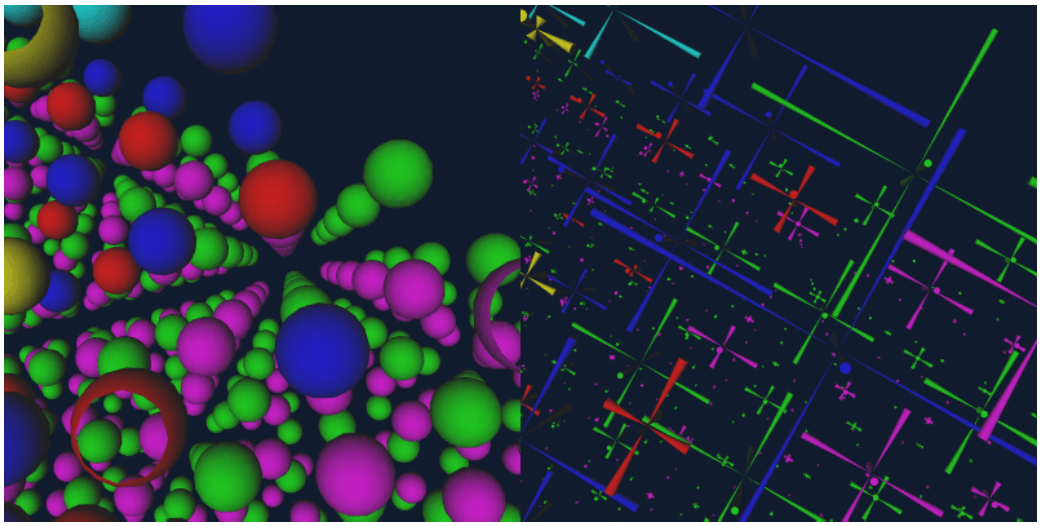
Mathematical and Computational Sciences Division

Summary of Activities for Fiscal Year 2004



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

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INFORMATION TECHNOLOGY LABORATORY

NIST National Institute of Standards and Technology

Abstract

This report summarizes the technical work of the Mathematical and Computational Sciences Division of NIST's Information Technology Laboratory for the period of October 2003 through December 2004. Part I provides a high-level overview of the Division's activities, including highlights of technical accomplishments during the previous year. Part II provides additional details covering many of the research activities of the Division. Part III provides listings of publications, technical talks, and other professional activities in which Division staff members have participated

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

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Part I

Overview

Introduction

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

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

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

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

The first area and second areas are accomplished primarily via collaborations with other technical units of NIST, supported by mathematical research in key areas. Projects in the third area are typically motivated by internal NIST needs, but have products, such as software, which are widely distributed. This work is also often done in conjunction with external forums whose goals are to promulgate standards and best practices in the computational sciences and engineering. In addition to these broad areas, we have identified two special focus areas.

4. Digital Library of Mathematical Functions
5. Quantum Information

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

Division customers span all of the NIST Laboratories, as well as the computational science community at large. We have developed a variety of strategies to increase our effectiveness in dealing with such a wide customer base. We take advantage of leverage provided via close collaborations with other NIST units, other government agencies, and external organizations. We develop tools with the highest potential impact, and make resources easily available online. We provide consulting, as well as educational and training opportunities for NIST staff. We maintain a state-of-the-art scientific visualization laboratory. Finally, we select areas for direct external participation that are fundamental and broadly based, especially those where measurement and standards can play an essential role in the development of new products.

Division staff maintain expertise in a wide variety of mathematical domains, including linear algebra, special functions, partial differential equations, computational geometry, Monte Carlo methods, optimization, inverse problems, nonlinear dynamics, and mathematical physics. We also provide expertise in parallel computing and scientific visualization and analysis. Application areas in which we have been actively involved this year include atomic physics, materials science, electromagnetics, manufacturing engineering, construction engineering, bioinformatics, and image analysis.

In addition to our direct collaborations and consulting, output of Division work includes publications in refereed journals and conference proceedings, technical reports, lectures, software packages, and Web services. MCSD staff members also participate in a variety of professional activities, such as refereeing manuscripts and proposals, service on editorial boards, conference committees, and offices in professional societies. Staff members are also active in educational and outreach programs for mathematics and computer science students at all levels.

Technical Approach

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

Information Science Research

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

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

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

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

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

Information Technology Research

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

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

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

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

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

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

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

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

Technology Transition

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

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

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

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

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

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

Technology Insertion

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

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

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

Example Projects.

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

Highlights

In this section we provide examples of some of the major accomplishments of the Division over the past year. Details can be found in subsequent sections.

Technical Accomplishments

MCSD has made significant technical progress in a wide variety of areas during the past year. Here we highlight a few examples.

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

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

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

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

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

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

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

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

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

Staff News

MCSD welcomed a variety of new staff members this year. In November 2003 Florian Potra of the University of Maryland Baltimore County joined MCSD as a faculty appointee to strengthen the Division's research program in applications of mathematical optimization methods. Scott Glancy joined the MCSD Boulder staff in September 2004 as an NRC Postdoctoral Fellow. A recent Ph.D. in Physics from the University of Notre Dame, Glancy will work with Manny Knill on the study of linear optics quantum computing.

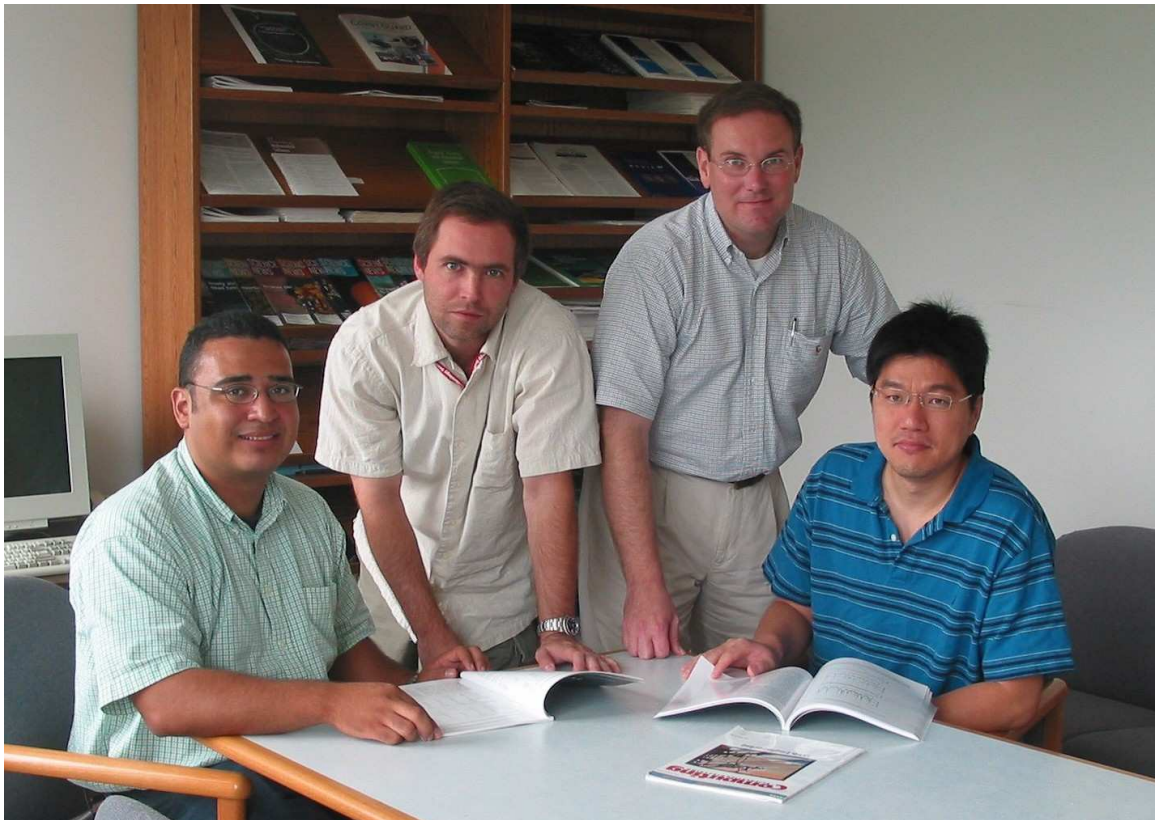
Several new guest researchers also became associated with MCSD in 2004. Anoka Yimsiriwattana, a computer scientist from the University of Maryland Baltimore County is collaborating with MCSD's quantum computing project. Eduardo Martinez-Vecino of the University of Salamanca, Spain, spent two months visiting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

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

Cristoph Witzgall of MCSD and Josef Stoer of Universitaet Wuerzburg

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

[1] http://math.nist.gov/workshops/wg25-2004/



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

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

MCSD provided support for 10 student staff members on summer appointments during FY 2004. Such appointments provide valuable experiences for students interested in careers in mathematics and the sciences. In the process, the students can make very valuable contributions to MCSD program. This year's students were as follows.

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

SURF: Summer Undergraduate Research Fellowship

Awards

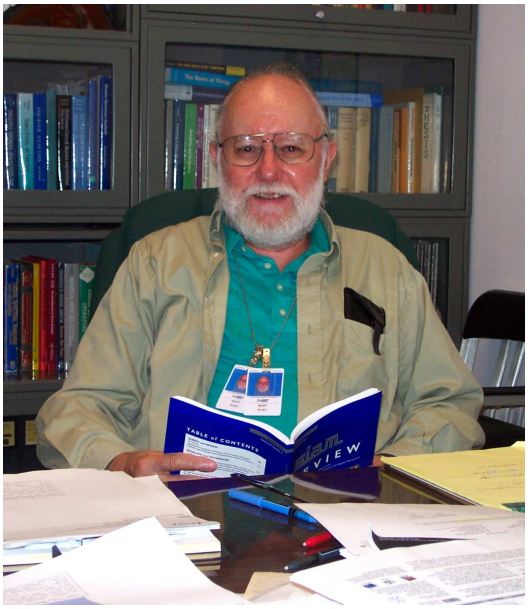
Left: Timothy Burns (center) with Debasis Basak and Richard Rhorer (MEL) in the NIST Kolsky Bar Lab. Burns and Rhorer were co-winners of the 2004 Allen V. Astin Measurement Science Award. *Right:* NIST Fellow Geoffrey McFadden.

Geoffrey McFadden of MCSD has been elevated to the position of ***NIST Fellow***. He was recognized for his prolific and high impact collaborative research in the mathematics of materials science, especially for his contributions to the theory of phase transitions. NIST Fellow status is conferred on less than 1% of NIST staff; McFadden is currently the only NIST Fellow from ITL.

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

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

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



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

Technology Transfer

MCSD staff members continue to be active in publishing the results of their research. This year 53 publications authored by Division staff appeared, 43 in refereed journals. Thirteen additional papers have been accepted and are awaiting publication. Another 35 are under review. MCSD staff members were invited to give 53 lectures in a variety of venues and contributed another 31 talks in conferences and workshops. The Division lecture series remained very active, with 25 talks presented (six by MCSD staff members); all were open to NIST staff.

MCSD staff members also organize workshops, minisymposia, and conferences to provide forums to interact with external customers. This year, staff members were involved in organizing 12 such events. Among these were minisymposia at the SIAM Annual Meeting, the SIAM Image Science Conference, and the Joint Mathematics Meetings. MCSD hosted three local symposia in 2004, a Symposium on Topics in Operations Research (May 2004), a Workshop on the Changing Face of Mathematical Software (June 2004), and a Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems, each with approximately 40 attendees.

Software continues to be a by-product of Division work, and the reuse of such software within NIST and externally provides a means to make staff expertise widely available. Several existing MCSD software packages saw new releases this year, including OOMMF (a problem-solving environment for micromagnetic modeling), TNT (Template Numerical Toolkit for numerical linear algebra in C), and OOF (a problem-solving environment for modeling of materials with complex microstructure). Many of our software packages experience substantial downloads. During the past 12 months, for example, OOMMF was downloaded 2,400 times. JAMA, the Java linear algebra package that we developed with the MathWorks registered 9,000 downloads, while TNT saw more than 10,500 downloads.

Web resources developed by MCSD continue to be among the most popular at NIST. The MCSD Web server at math.nist.gov has serviced more than 80 million Web hits since its inception in 1994 as NIST's first Web server. More than 25 million of these hits occurred in the past year. The

Division server regularly handles more than 16,000 requests for pages each day, serving more than 55,000 distinct hosts on a monthly basis. Altavista has identified more than 8,500 external Web links to the Division. Seven MCSD sites are listed among ITL's top 10:

1. NIST Math Portal, http://math.nist.gov/
2. Matrix Market, http://math.nist.gov/MatrixMarket/
3. Guide to Available Mathematical Software: http://gams.nist.gov/
4. Division home page: http://math.nist.gov/mcsd/
5. ACM Transactions on Mathematical Software: http://math.nist.gov/toms/
6. Digital Library of Mathematical Functions: http://dlmf.nist.gov/
7. Template Numerical Toolkit: http://math.nist.gov/tnt/

Professional Activities

Division staff members continue to make significant contributions to their disciplines through a variety of professional activities. R. Boisvert serves as Chair of the International Federation for Information Processing (IFIP) Working Group 2.5 (Numerical Software). He was recently named Co-Chair of the ACM Publications Board. D. Porter serves on the Tcl Core Team, which manages the development of the Tcl scripting language. D. Lozier serves as chair of the SIAM Special Interest Group on Orthogonal Polynomials and Special Functions. Fern Hunt serves on the Executive Committee of the Association for Women in Mathematics.

Division staff members serve on journal editorial boards of nine journals: *ACM Transactions on Mathematical Software* (R. Boisvert and R. Pozo), *Computing in Science & Engineering* (I. Beichl), *IEEE Transactions on Information Science* (E. Knill), *Interfaces and Free Boundaries* (G. McFadden), *Journal of Computational Methods in Science and Engineering* (M. Donahue), *Journal of Crystal Growth* (G. McFadden), *Journal of Numerical Analysis and Computational Mathematics* (I. Beichl and W. Mitchell), *Mathematics of Computation* (D. Lozier), *SIAM Journal of Applied Mathematics* (G. McFadden), *SIAM Journal of Scientific Computing* (B. Alpert).

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

Part II

Project Summaries

Applied Mathematics

Time-Domain Algorithms for Computational Electromagnetics

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

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.

Local Nonreflecting Boundary Conditions. A problem that has been revisited this year is that of nonreflecting boundary conditions for the wave equation (and Maxwell's equations). Although earlier work of these researchers was successful in producing a procedure that is both spectrally accurate and highly efficient, its lack of flexibility in the shape of the boundary limits the variety of settings in which it has been adopted. Alpert and his collaborators have since attempted to generalize the nonreflecting boundary procedures to rectangular domains. This year they became convinced that the highly nonlocal dependencies inherent in nonreflecting boundary conditions can be circumvented (or localized) by looking somewhat inside the domain. This hypothesis, arising in part by analytical work by Warchall, has prompted a renewed attempt to formulate an exact local nonreflecting boundary treatment. This work continues.

Impact. A paper presenting recent NIST collaborative research appeared: "Near-Field, Spherical-Scanning Antenna Measurements with Nonideal Probe Locations," R. C. Wittmann, B. K. Alpert, and M. H. Francis, *IEEE Transactions on Antennas and Propagation* **52** (8) (2004), pp. 2184-2186. A paper on an inner product for scattering problems, "Half Space Representation of Acoustic Waves from Compact Sources," B. Alpert and Y. Chen, has been accepted for publication in *Communications in Pure and Applied Mathematics*. The work has been recognized by researchers developing methods for computational electromagnetics (CEM) and has influenced work on these problems at Boeing and HRL (formerly Hughes Research Laboratories). It has also influenced researchers at Yale University and University of Illinois. In each of these cases, new research in time-domain CEM is exploiting discoveries of the project.

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

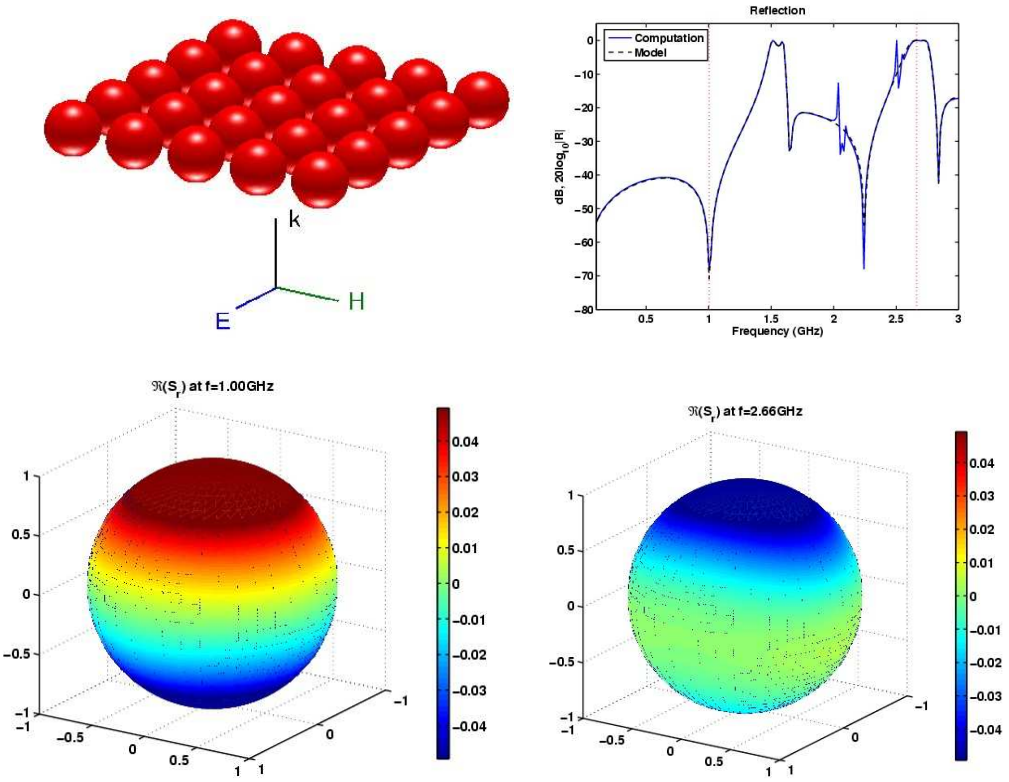
Resonant Optical Scattering by Nanoscale Periodic Structures

Andrew Dienstfrey

The emerging ability of scientists to fabricate materials at nanometer length scales has created new possibilities for the engineering of materials with novel optical scattering properties. These devices will have tremendous impact in a variety of commercial, defense-related, and scientific applications: magneto-optic storage, micro-antenna arrays, integrated optical circuits, quantum computing hardware, to name a few. Essential for the successful development of these devices, are specialized computational tools which can accurately guide researchers in fabrication and modeling efforts.

Broadly speaking, these materials are composite, nanoscale dielectric and metallic scatterers arranged in a periodic manner so as to harness resonant phenomena in their interaction with electromagnetic fields. Instances go by various names depending on the scientific community and/or the desired objective of the research. Research into *photonic crystals* is yielding new techniques for the use of patterned dielectric structures as nanoscale optical waveguides. In the emerging field of *plasmonics*, electromagnetic fields are coupled to surface electron fields in metals. The resulting interactions allow, for example, for highly-collimated optical beam formation. Control of this process could have significant impact in the development of future magneto-optic storage devices. Finally, research in *meta-materials* includes new ways of modeling frequency-selective services. These surfaces reflect or transmit light at variable yet controlled frequencies with high-efficiency and selectivity. They are currently the subject of intense study by multiple groups within NIST's Electromagnetics Division (EEEL) as well as in the physics community at large. In addition to having applications as tunable optical pass-band filters, these structures present theoretical modeling challenges as several homogenization theories that are currently in use entail paradoxical effects concerning the refraction and propagation speeds of electromagnetic fields.

As an entry point into this field, MCSD research over the past year has focused on developing a suite of programs for precise simulation of scattering of electromagnetic waves by meta-material structures. The computational task is challenging in that the problem requires full vector solutions to Maxwell's Equations capable of simultaneously capturing both near and far-fields so as to bridge, respectively, the coupling of resonances dictated by nanometer scale structures to the macroscopic scales at which fields become accessible to homogenization theories. In brief, the program represents near-fields as truncated expansions of spherical multipole vector fields. Although these vector functions appear in the classical solution to *single* sphere scattering initiated by Mie in 1903, algorithms for translating expansions, which are required in the case of scattering by *multiple* spheres, are still under development today. Given the complicated nature of these functions, efficient representations are essential and the program leverages several years of research efforts undertaken by Ron Wittmann and other NIST scientists working in near-field antenna measurements. With these choices made, there is an additional mathematical complication in that the model postulates an *infinite* array of scatterers. Therefore, it is necessary to develop algorithms for computing certain doubly-infinite formal sums. The convergence properties of these sums are extremely subtle and constitute a mathematical hurdle that must be overcome. Finally, the interplay between length scales associated with individual small scatterers on the one hand, and on the other hand an effective large scatterer consisting of infinitely many individuals, requires computations to go deep into what are referred to as evanescent modes so as to achieve numerical convergence. The instabilities associated with these modes are legion. The program overcomes these problems through careful scalings of internal representations. All of these problems have been addressed and initial results are promising. It is anticipated that, in parallel to fabrication and measurement experiments also underway within NIST, the computational tools developed by MCSD will aid in testing these theories.



Results of computation of electromagnetic scattering by a proposed meta-film. The upper left shows the geometry of the scatterers. The spheres are composed of yttrium iron garnet (YIG) and exhibit high dielectric and magnetic susceptibilities relative to free space ε=15, μ=45). The sphere radii and lattice constant are r=5 mm, d=12.79 mm respectively. In the computation the array extends to infinity. The upper right shows the magnitude of the reflection coefficients predicted by a NIST model and determined by the computation. Note the deep minimum in reflected energy predicted by both model and computation at $f \cong 1$ GHz and again at $f \cong 2.25$ GHz. The lower plots show the radial component of the electromagnetic energy flux at the surface of each scatterer. The plot on the left is consistent with the energy flow induced by the incident planewave radiation. Of theoretical interest is the inverted energy flow through the sphere at the frequency of maximum reflection shown in the lower right.

The plots above show results of a computation a meta-film consisting of an infinite array of dielectric/paramagnetic spherical scatterers situated in the XY-plane, illuminated from below by a linearly-polarized planewave traveling upward in the z-direction. This structure is being fabricated at microwave scales and measured in a waveguide by members of Magnetics and Radio-Frequency Electronics Groups (EEEL). In addition, a model has been developed by members of the Radio-Frequency Fields Group. The subplot in the upper left shows the geometry of the scatterers. In the upper right the magnitudes of the reflection coefficients predicted by the model and the computation are plotted as functions of frequency. One observes good agreement between the model and computation. In particular, both predict the deep minimum in reflection at 1GHz which implies a particularly high transmission of electromagnetic energy at this frequency. However, the computation predicts other resonances (for example, the structure near 2GHz) that the model can not account for at present. The nature of these resonances is currently under investigation.

Finally, the computation allows for the resolution of energy flow at unprecedented scales. The two lower plots show the magnitudes of the radial component of electromagnetic energy flux at the surface the spherical scatterers at two different frequencies. The plot on the left shows the flux at

the frequency of maximum transmission (approximately 1GHz). The negative values at the bottom and positive values at the top of the sphere (blue and red, respectively) are consistent with the incident planewave penetrating into the sphere at the bottom and emerging through the top with little impedance. The subplot on the lower right is in stark contrast. At this frequency (approximately 2.7GHz) the spheres exhibit maximum reflection, minimum transmission. Here one observes a reversal of energy flow from the previous picture in that, at least on the surface of the sphere, the energy is entering the sphere from the top and exiting from the bottom. This reversed flow of energy lies at the heart of the paradoxes and disputes circulating in the physics community studying meta-material structures. It is hoped that in the coming year continued investigation with the set of computational tools developed by MCSD will aid in resolution of some of these problems.

Phase-Field Modeling of Solidification under Stress

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Melting and solidification into either a crystalline or amorphous state in nano-volumes are basic mechanisms of modern phase change recording. This process exploits an amorphous-to-crystalline phase change to record information onto electronic media such as DVDs. Due to the density difference between phases, transformations in confined volumes are accompanied by internal stresses. Thus, it is necessary to take into account the effect of internal stress during phase change recording. In this project we have modeled this "writing" process by considering melting and solidification in a confined volume.

To simulate melting/solidification we employ a phase field model. Phase-field modeling is an effective approach for the analysis and prediction of the evolution of complex microstructures during phase transformations. This approach has been particularly successful when it has been applied to solidification problems. For single-component system the standard phase-field method requires solving two equations: the time dependent Ginsburg-Landau phase-field equation and the equation of heat transfer. The phase field model that we develop includes stress field during non-isothermal solidification of a one-component system. These stresses can be external or internal, i.e. they can arise as a result of boundary conditions at the external surface or they can be a result of elastic interactions between the phases. Thus, the phase field model takes into account the simultaneous evolution of three fields: a phase field, a temperature field and a stress/strain field.

To demonstrate this approach we consider the solidification and melting of a confined sphere. For this simple system the complete numerical solutions taking into account the time-space evolution of temperature, order parameter and strain-stress field is obtained. The simulation shows that at some boundary and initial conditions the evolution of a spherical symmetry system results in steady states corresponding time-independent distribution of order-parameter and uniform temperature. Comparison results of phase field modeling and thermodynamic analysis of a sharp-interface model shows that these steady states are equilibria which exist in systems with fixed volume. The analysis of these equilibrium states allows us to estimate the value of interface energy that are then verified by a phase field calculation of the energy of plane liquid/solid interface. The model can be used to simulate the process of "writing" to electronic media that exploit an amorphous-to-crystalline phase change for recording information.

Part of this work represents a collaboration with researchers at Northwestern University under an NSF Nanoscale Interdisciplinary Research Team (NIRT) grant. K. Thornton spent four weeks visiting MCSD under this program, and G. McFadden visited Northwestern and presented results at a nanotechnology workshop at Northwestern that was funded through the grant.

A conference proceedings paper on this work has been published: J. Slutsker, A. L. Roytburd, G. B. McFadden, and J. A. Warren, "Phase Field Modeling of Solidification and Melting of a Confined Nano-particle," International Workshop on Nanomechanics, July 14-17, 2004, Pacific Grove, CA, Tze-jer Chuang and Peter Anderson, eds.

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

Lateral Deformation of Diffusion Couples

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R. F. Sekerka (Carnegie Mellon U.)

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.

In this project G. McFadden collaborated with W.J. Boettinger, S.R. Coriell, and J.A. Warren of the Metallurgy Division, MSEL, and R.F. Sekerka, of Carnegie Mellon University on the modeling of stress effects during interdiffusion of solute in a diffusion couple. The work involves a continuum model that describes the creation and annihilation of lattice vacancies at defects in the crystal, which can produce swelling or shrinkage of the sample locally.

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. 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 measurments of the deformation observed in gold-silver alloys. This work has been submitted for publication in *Acta Materialia*.

An extension of the work is being used to model the bending of a thin plate, for which experimental data is also available. This work is intended to address problems in which stress is produced in nano-scale samples due to the effects of multicomponent diffusion.

The Effect of Contact Lines on the Rayleigh Instability of a Crystalline Interface

G. McFadden
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M. Miksis (Northwestern U.)

In continuum models of nanoscale structures, the importance of surface energy effects often become a critical factor as the ratio of surface to volume increases. In previous work the effects of surface tension anisotropy on interfacial instabilities in crystalline rods or wires was considered. These instabilities can lead to break-up of the structures, with associated mechanical or electrical failure of the system. These instabilities are generalizations of the classical modes studied by Lord Rayleigh in liquid jets, and are capillary effects that reflect the lower surface energy associated with the decrease in surface area near a necking region.

We are currently generalizing our previous work for isolated crystalline bodies by including the effects of a substrate that supports the crystalline rod or wire. The junction of the rod and substrate at a contact line can significantly stabilize the system, since the contact line restricts the form of perturbations that can lower the overall energy of the system. We have performed an energy analysis of the system that leads to a coupled eigenvaue problem, with associated boundary conditions arising from the balance of energies at the contact line. The results are relevant for studies of quantum wires on circuit boards or other types of substrates.

This work represents a collaboration with researchers at Northwestern University under an NSF Nanoscale Interdisciplinary Research Team (NIRT) grant.

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

Configurational Forces at a Liquid-Liquid Interface

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

In this work we address the problem of formulating directly nonequilibrium interfacial conditions for an interface between two fluids. The approach we adopt here is based on the formalism of configurational forces as developed by Gurtin. We specifically apply these ideas to fluid-fluid systems in which phase transitions may occur. Of particular interest are interfacial conditions such as the nonequilibrium version of the Gibbs-Thomson equation. Our discussion of configurational forces leads naturally to the inclusion of effects such as interfacial viscosity and interface kinetics. This work is being submitted to the *Journal of Fluid Mechanics*.

Phase-Field Model of Line Energies at a Corner or Tri-Junction

G. McFadden
A. Wheeler (U. of Southampton)

Phase-field models of multiphase systems represent interfaces between different thermodynamic phases as regions of finite width, rather than mathematically-sharp surfaces. These models can incorporate physical effects such as interface kinetics and surface tension anisotropy in a natural manner, since the underlying formalism is based on a consistent thermodynamic description of the system. If the level of surface tension anisotropy is large enough, the interface can develop corners where the system prefers to omit certain high-energy orientations all together. Surprisingly, phase-field models can describe such missing orientations even though the interface has finite width; to do so, the solutions develop singularities through the whole interfacial region, where each contour of the phase-field variable describing the interface has a corner with limiting angles that are determined by the surface tension anisotropy. It is natural to associate a line energy with such a corner, and to consider further generalizations of the phase-field formalism that selectively smooth the corners at an even smaller length scale. To do this, we have developed a model in which the free energy of the system consists of both convectional gradient energy terms that account for the surface energy, and a new term that involves the square of the Laplacian to account for line energies. We performed an asymptotic analysis that recovers the conventional sharp corner conditions in the limit of small smoothing. Professor Wheeler visited for two one-week periods this year during this collaboration.

Linear Stability of Cylindrical Couette Flow in the Convection Regime

G. McFadden
M. Ali (King Saud U., Riyadh, Saudi Arabia)

The viscous fluid flow created between differentially rotating coaxial cylinders has provided a fertile testing ground for both linear and nonlinear stability theory. Beginning with the work of G.I. Taylor in 1923, numerous experimental and theoretical studies on flow transitions and morphologies of supercritical circular Couette flow have appeared. Initial studies on thermally-driven circular Couette flow were motivated by technological problems in the cooling of rotating electrical machinery. Early theoretical attacks neglected gravity and usually considered only axisymmetric disturbances in the limit of infinite aspect ratio. There has been a renewed interest in the problem of radially heated rotating flows, partially from a continued effort to enhance the cooling of rotating machinery, but also with the aim of understanding and controlling instabilities in nematic liquid crystal systems, in chemical vapor deposition processes, and in the solidification of pure metal.

The stability of viscous isothermal circular-Couette flow generated by rotation of the inner cylinder is controlled by the radius ratio, the aspect ratio, and the Taylor number. Stationary counter-rotating toroidal cells of uniform width stacked one above the other appears at a critical Taylor number. In the absence of rotation, natural convection between vertical differentially heated concentric cylinders depends crucially on the magnitude of the imposed thermal heating and the system aspect ratio. Early experimental studies fostered the identification of three distinct flow regimes in both planar and cylindrical gaps: conduction, transition, and convection. Here we consider the convection regime, where axial boundary layers form along each cylinder walls, and a vertical temperature gradient develops in the interior of the sample. We have developed an analytical solution for the base flow in the convection regime in a vertical annulus with a rotating inner cylinder and a stationary outer cylinder. The stability of this base flow is then computed numerically with respect to both axisymmetric and asymmetric disturbances. A paper has been submitted to *Physics of Fluids*.

Linear Stability of Spiral Poiseuille Flow with a Radial Temperature Gradient

D. L. Cotrell
G. B. McFadden

For fluid flow in an annulus driven by the combination of an axial pressure gradient, rotation of the inner and outer cylinders, and a radial temperature gradient (spiral Poiseuille flow with a radial temperature gradient), we are investigating the transition from the simplest flow possible (steady flow with two nonzero velocity components and a radial temperature gradient that vary only with radius) to the next simplest flow possible (steady flow with three nonzero velocity components and a temperature profile that vary in the radial and axial directions). This work is motivated by electrochemical processes in rotating cylinder electrodes, heat transfer in rotating machinery, flow-amplified electrophoretic separations, and vortex flow reactors for shear-sensitive biological systems. This work extends the case of isothermal spiral Poiseuille flow for which D. Cotrell and A. Pearlstein (University of Illinois at Urbana-Champaign) recently computed complete linear stability boundaries for several values of the radius ratio and rotation rate ratio, and shows how the centrifugally-driven instability (beginning with steady or azimuthally-traveling-wave bifurcation of circular Couette flow) connects to a non-axisymmetric Tollmien-Schlichting-like instability of nonrotating annular Poiseuille flow (flow driven solely by an axial pressure gradient). Results for the non-isothermal case show that the stability boundary shifts either up or down depending on the sign of the temperature difference. For the isothermal case, it is also known that in many instances there is no instability for small enough axial flow rates. For the non-isothermal case, however, we have shown that for any nonzero temperature difference between the inner and outer radii, a new non-isothermal mode of instability causes the base state to be destabilized under these conditions. This work has been submitted to *Physics of Fluids* for publication.

Axial Flow Effects on the Linear Stability of Circular Couette Flow with Viscous Heating

D. L. Cotrell
G. B. McFadden

For fluid flow in an annulus driven by the combination of an axial pressure gradient and rotation of the inner and outer cylinders, G. McFadden and D. Cotrell are investigating the effect axial flow has on the linear stability of circular Couette flow with viscous heating. We note that it is extremely important to consider viscous heating in hydrodynamic stability calculations and experiments, because unlike externally imposed temperature gradients, viscous heating is a strong function of the fluid properties and cannot be easily controlled or eliminated. The analysis extends previous results with no axial flow (and computes the correct asymptotic behavior at large temperatures, a case for which we believe incorrect results are in the literature), and accounts for non-axisymmetric disturbances of infinitesimal amplitude. D. Cotrell has implemented the linear stability analysis for this case using spectral methods, but because the number of collocation points needed to fully resolve the strong internal thermal layer is large, He has also solved the linear stability problem by solving a two point boundary value problem (using the program Support) whose results will be used to check solutions in parts of parameter space for which the spectral method approach requires significant spatial resolution. Comparison between the two methods is good, but limited due to the fact that the boundary value problem approach uses Newton iteration to find critical eigenvalues and the domain of convergence is very small. Because of this, Cotrell has implemented spectral domain

decomposition in the spectral collocation code. Because this generates a global matrix eigenvalue system that is sparse, Cotrell is in the process of implementing the sparse eigenvalue solver ARPACK which finds only a specified number of eigenvalues clustered around a point you pick (i.e., the real part of the temporal growth rate is zero).

Linear Stability of Modified Couette Flow

D. L. Cotrell
G. B. McFadden

The stability of flow in the annular region between two concentric cylinders driven by rotation of either one or both cylinder walls has been investigated since the work of Taylor (1923). One of the simplest geometric perturbations of the "standard" flow is when one of the axisymmetric boundaries is allowed to have an axially-periodic radius. This problem is important is wavelength selection, cases where one might want to prescribe the wavelength of the resulting vortices, and in trying to stabilize axisymmetric Taylor vortices beyond the range seen for the smooth walled case. D. Cotrell has used the finite element method to implement the axisymmetric linear stability for this steady 2-D base state, and is currently in the process of using previous computational and experimental results to validate the code. Cotrell is in the process of implementing the nonaxisymmetric case as well.

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

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The usefulness of computer simulations of rapid deformation processes using commercial finite-element software packages is often limited by the lack of material response data in the regimes of interest. For example, high-speed machining processes involve the plastic deformation of materials at very high rates of deformation, and this leads to rapid heating of the material in the cutting zone. The relationship of stress (force per unit area) to strain (a dimensionless tensor quantity that measures how much a material deforms in compression and shear), often referred to as the material constitutive response (or the stress-strain curve in simple cases), can be much different at high strain rates and high temperatures than typical "handbook" data. Therefore, a vital step in the development and implementation of effective machining models is to provide appropriate stress-strain relationships for materials of interest to industry. In 2001, a project was started at NIST, *Materials Data and Metrology for Machining Simulation*, which included building a unique testing apparatus that couples a traditional Kolsky (split-Hopkinson) high-strain-rate material response testing bar, with an existing NIST fast pulse-heating facility. The Kolsky compression test involves sandwiching a sample of the test material between two long, hardened steel rods. One of the steel rods is impacted by a shorter rod of the same material, sending a stress pulse into the sample. While the steel rods remain elastic in their response to the impact loading, the sample 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. The goal of the new facility has been to develop the capability to preheat a material sample rapidly using an electrical pulse, and then almost immediately perform a Kolsky bar

compression test, thereby providing high-strain-rate, pulse-heated material response data that would be useful for high-speed machining studies. While the pulse-heating and temperature control capabilities were being developed for the Kolsky bar, and experiments were being performed on materials of interest in the automobile and aircraft industries, the twin towers at the World Trade Center in New York City were destroyed, and several NIST laboratories were tasked by Congress with analyzing the specific sequence of events that led to the collapse of the buildings. Constitutive response data were required for the many types of steel that had been used in constructing the towers, and the NIST Kolsky Bar Facility was employed for this purpose. When ATP funding for the original project ended in FY2004, all of the major goals had been met, and a unique materials testing laboratory had been built with the help of personnel from several NIST laboratories, along with the help of interested personnel from universities and other government laboratories with expertise in the many different areas required to get the facility up and running.

During the past fiscal year, while studies have continued on the modeling of high-speed machining of materials of interest in manufacturing, funding has been obtained from the National Institute of Justice (NIJ) through the NIST Office of Law Enforcement Standards (OLES) to use the NIST Kolsky Bar to study the constitutive response of frangible bullets (i.e., ammunition made from materials other than lead that breaks up on impact), and to develop a related tension-testing bar to study the mechanical behavior of soft body armor woven from fibers of the advanced polymeric materials PBO (Zylon) and Aramid (Kevlar). The test data will be used by the US Department of Justice to determine what actions are required to ensure that soft body armor provides adequate protection to police officers in the field. Experimentally validated finite element models of bullet-vest interactions will be developed as part of this new program, which is expected to be funded for another two fiscal years.

This work has been supported in part by the NIST Advanced Technology Program (ATP) and the National Institute of Justice (NIJ).

Micromagnetic Modeling

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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 2004 alone, the software was downloaded more than 2,400 times, and use of OOMMF was acknowledged in more than 40 peer-reviewed journal articles.

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

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

The MCSD micromagnetic project produced six journal papers and three conference presentations in the fiscal year 2004. Project staff also contributed to the National Nanotechnology Initiative Interagency Workshop on Instrumentation and Metrology for Nanotechnology.

This work is supported in part by the NIST Competence Program.

Optimization Problems in Smart Machining Systems

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The goals of Smart Machining Systems (SMS) are to produce the first and every product correct, improve the response of the production system to changes in demands (just in time), realize rapid manufacturing, and provide data on an as needed basis. These systems are envisioned to have the capability of: self recognition and communication of their capabilities to other parts of the manufacturing enterprise; self monitoring and optimizing their operations; self assessing the quality of their own work; and self learning and performance improvement over time. To accomplish this, the SMS must cope with uncertainties associated with models and data. Robust optimization is an approach for coping with such uncertainties.

Optimization plays a crucial role in SMS. A general optimization problem consists in determining some decision variables $x_1, x_2, \ldots, x_n$, such as feed, depth of cut, spindle speed, in such a way that a set of given constraints are satisfied and a desired objective function is optimized. The constraints are determined by both empirical, heuristics and theoretical considerations, and they can usually be expressed as a system of inequalities. If we denote by x the vector of decision variables and by $f_0(x)$ the objective function, then the optimization problem can be written as

$$\text{minimize} \quad f_0(x) \tag{1}$$

$$\text{subject to} \quad f_i(x) \le 0, \qquad i = 1, 2, \ldots, m. \tag{2}$$

An example of an objective function that we would like to minimize in machining is the surface location error. The above general form of an optimization problem can handle also objective functions that we would like to maximize, like the material removal rate. This is accomplished by

replacing $f_0(x)$ with $-f_0(x)$ in (1). If the objective function $f_0(x)$, as well as the functions $f_1(x), f_2(x), \ldots, f_m(x)$ defining the constraints, such as cutting force, machine tool power and torque, tool life, surface roughness and spindle speed, are linear in the decision variables, then the optimization problem (1)-(2) becomes a linear programming problem (LP) that has been extensively studied, and for which efficient algorithms are known. However, in most application both the objective function and the functions defining the constraints are nonlinear. By introducing an additional variable x_0, we can always consider that the objective function is linear. Indeed it is easily seen that that the optimization problem (1)-(2) is equivalent to

$$\text{minimize} \quad x_0 \tag{3}$$

$$\text{subject to} \quad f_0(x) - x_0 \le 0, \tag{4}$$

$$f_i(x) \le 0, \quad i = 1, 2, \ldots, m. \tag{5}$$

While in a traditional deterministic setting, where $f_0(x), f_1(x), \ldots, f_m(x)$ are considered precisely determined, the form (3)-(5) can be conveniently extended to deal with uncertainty in the data defining the optimization problem. Indeed, in real applications the functions $f_0(x), f_1(x), \ldots, f_m(x)$ depend on some parameters $\varsigma_1, \varsigma_2, \ldots, \varsigma_p$ that are only approximately known. In some cases we can define an "uncertainty set", or set of possible parameter values, $U \subset R^p$ that contain all possible values of the parameter vector ς. If U contains a single vector then we are in the traditional deterministic setting. Otherwise, we consider the robust optimization problem

$$\text{minimize} \quad x_0 \tag{6}$$

$$\text{subject to} \quad f_0(x, \varsigma) - x_0 \le 0, \quad \forall \varsigma \in U \tag{7}$$

$$f_i(x, \varsigma) \le 0, \ i = 1, 2, \ldots, m, \ \forall \varsigma \in U \tag{8}$$

The robust optimization problem above aims at determining the vector of decision variables x such that the objective function is minimized and the constraints are satisfied *for all* possible values of the parameter vector ς. Although this seems hopeless, recent progress in optimization theory and practice shows that for many engineering problems we can formulate robust optimization problems that can be efficiently solved by modern optimization algorithms.

Currently a model for maximizing the material removal rate for a turning center by estimating the appropriate tool feed rate and turning speed has been proposed by MEL. It currently requires only an LP solver, but a script has been written in Matlab to examine the effect of varying parameters over a wide range of values. Graphs of feasible regions have been developed that can aid a machine operator in selecting the optimal or near-optimal parameter settings. The current script has been interfaced to GUI by MEL so that an operator can test the consequences of selecting parameters within the allowed ranges. A full robust optimization code requires the development of a more extensive script, but the current version allows MEL Engineers to begin studying the affects of parameter adjustment on material removal rate and comparing results against machining experiments.

Hierarchical Control of Systems Governed by Differential Equations

Anthony Kearsley
Paul Boggs (Sandia National Laboratories)
Jon Tolle (University of North Carolina)

The study of optimal control problems arising in the control of fluids in non-standard geometries has become an extremely active area of research. Motivated by a desire to detect, simulate and even control contaminant transport (perhaps from security applications) numerical algorithms are actively being investigated by numerous research groups. Our small group has developed a theory and approach to these problems based on multiple but ranked (or hierarchical) objectives. Typically, one wants to control a state equation, an approach involving well-ordered multiple objectives. These problems belong to the class of problems called multicriteria optimization. There is no unique mathematical formulation of these types of problems. In practice these problems are often solved by minimizing a weighted sum of the deviations from the targets with the weights corresponding to the preferences. Another formulation, sometimes referred to as goal programming, insists that the preferred targets must be satisfied to within certain tolerances and the others are reduced as much as possible within these constraints. Both of these approaches involve the choice of a set of weights or tolerances for which there can be little theoretical guidance. Yet another approach, called bilevel optimization nests optimization problems, optimizing with respect to one target and using the solutions as parameters in a larger problem.

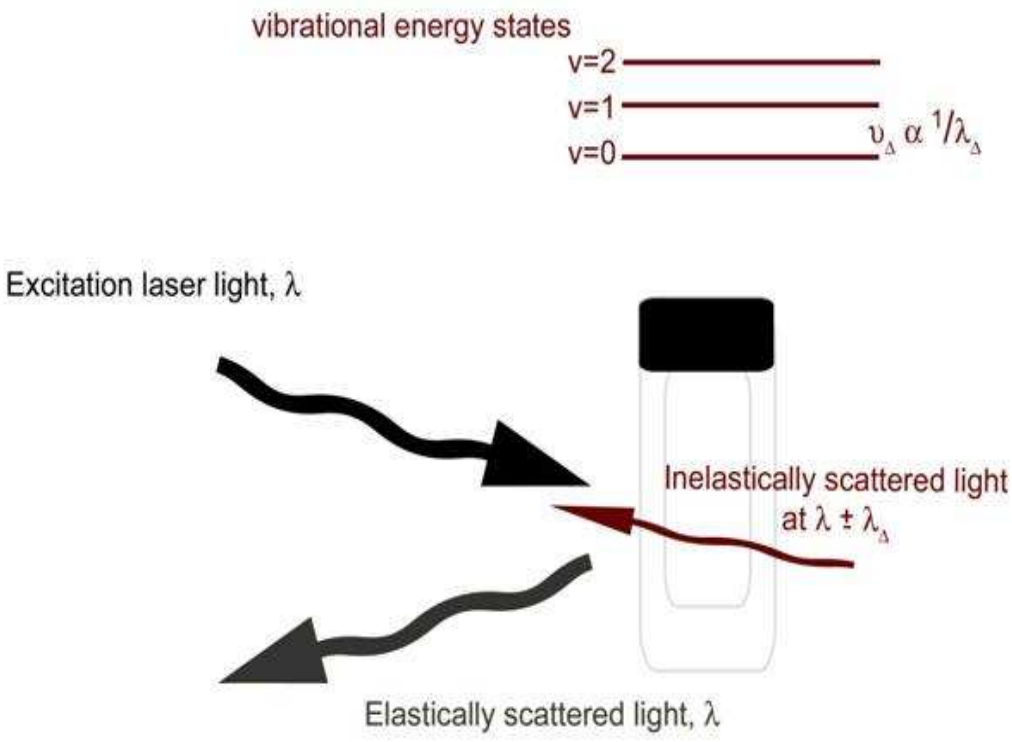
We have successfully developed a nonlinear programming approach to these hierarchical optimization problems. Given a fairly arbitrary (general) geometry, a constitutive flow equation and a collection of well-ordered objectives, we have derived an optimality system whose solution yields optimal controls and state variables that seek to achieve objectives in the order that they have been placed.

Analysis of Extrema Arising in Laser Sampling Techniques

Anthony Kearsley
Peter Ketcham
Geoffrey McFadden

Raman spectroscopy is a technique that measures molecular vibrational energies of chemical compounds. It is a form of vibrational spectroscopy complementary to infrared absorption. Raman spectra are generated by a monochromatic light source (e.g., a laser) to a sample and detecting the light that is inelastically back-scattered. The majority of the scattered light has the same energy as the laser; this is elastic scattering or Rayleigh scattered radiation. A very small portion of the incident laser light (~10-6%) is scattered inelastically by a discrete amount of energy that is related to the molecular vibrational energy of the molecular bond. This is known as Raman scattering (see Figure), which can be used to help elucidate the structural characteristics of the sample.

Raman spectroscopy instruments offer the capability to rapidly screen an unknown sample without requiring the operator to physically handle or prepare the sample. Additionally, Raman can be performed through a variety of container types, including glass, paper, and some plastics. These characteristics make Raman a suitable candidate for field analyses of a forensic nature. An evaluation of several portable Raman instruments was undertaken to help identify requirements for an improved fieldable Raman instrument that could be used by first responders. Key characteristics of these systems include portability, energy control, and ease of use by field agents who may not have extensive training in spectroscopy.



An illustration of the Raman scattering process.

To determine specifications for the next-generation field-portable Raman systems each of the instruments is in the process of being evaluated for use by first responders in the field. During the course of these evaluations, the need for an improved, fully automated, sample identification and peak-matching algorithm became clear. The algorithm currently under development consists of multi-stage computer processing that

1. selects peaks and troughs in spectroscopic data in a fully automated fashion,
2. identifies a sub-selection of statistically relevant peaks,
3. compares the statistically relevant peaks to a previously compiled database of spectral files, and
4. calculates a score that indicates the strength of the correlation between the collected spectrum and a database entry.

We have started developing an algorithm that we believe may be appropriate for this application. The real strength of this algorithm is that it functions independent of the number of data points, data-point spacing, spectral range, and the instrument's resolving power. This is intended to forestall the need for additional database development each time instrument specifications or optical designs are changed.

This work is partially supported by the Federal Bureau of Investigation (FBI).

Automated Numerical Algorithms for Advanced Mass Spectrometry and Standard Reference Materials

Javier Bernal
Anthony Kearsley
Peter Ketcham
Charles Guttman (NIST MSEL)
William Wallace (NIST MSEL

Modern mass spectrometry (MSpec) has been producing important material science information in a wide variety of scientific applications. Most recently, this work has become very important in the analysis and identification of chemicals for pharmaceutical industries, homeland security applications and manufacturing optimization. Loosely speaking a mass spectrometer (see Figure 1) detects the presence of chemicals inside a sample by bombarding the sample, suspended in a matrix, with ions (in the form of a laser) and then counting the ions "bounce" off the matrix prepared sample (see Figure 2). Each chemical causes ions to bounce off in a different way thus leaving a signature. Very often, one is interested in testing for the presence of a particular chemical inside a sample material, a MSpec experiment can be designed to result in large peaks being produced when the chemical in question is detected by ions (for example one must identify, separate and sum the matrix peaks present in the Bradykinin MSpec output in Figure 3). This accurate method for determining the presence of chemicals has been employed with more and more frequency by scientists.

While very detailed chemical procedures have been developed for MSpec sample preparation, very little work has been done on the development of automated numerical methods for the analysis of MSpec output. Today, analysis of such data requires a huge investment of time by highly trained professionals, limiting its usefulness in law enforcement and homeland security applications.

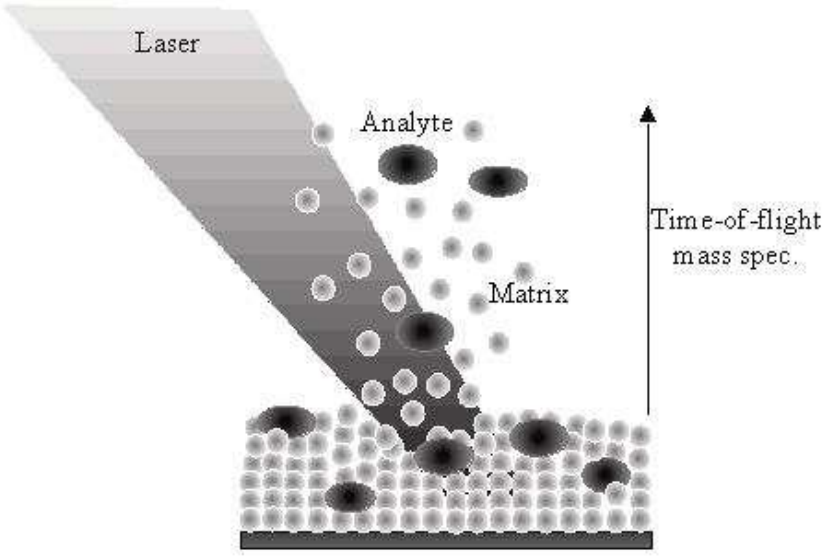


Figure 1: Illustration of MALDI Time-of-Flight Mass Spectrometer

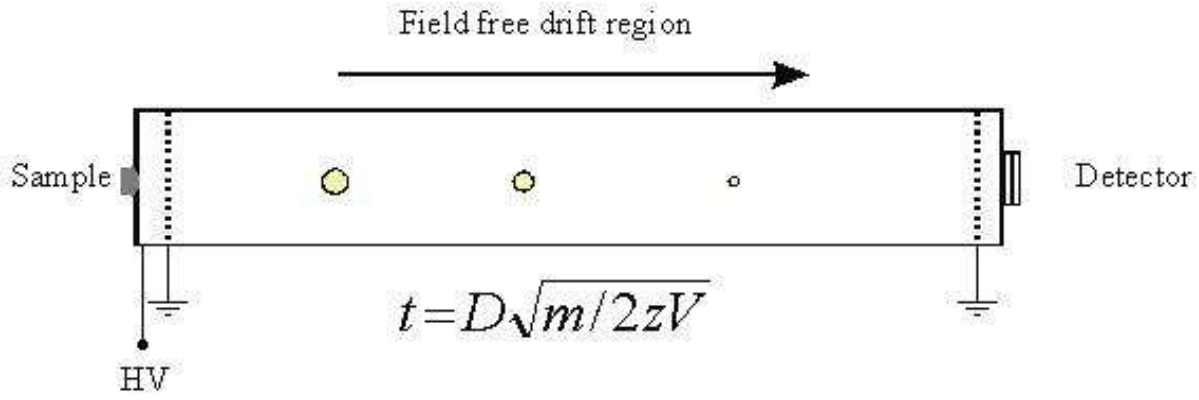


Figure 2: Detection mechanism in MALDI Time-of-Flight Mass Spectrometer

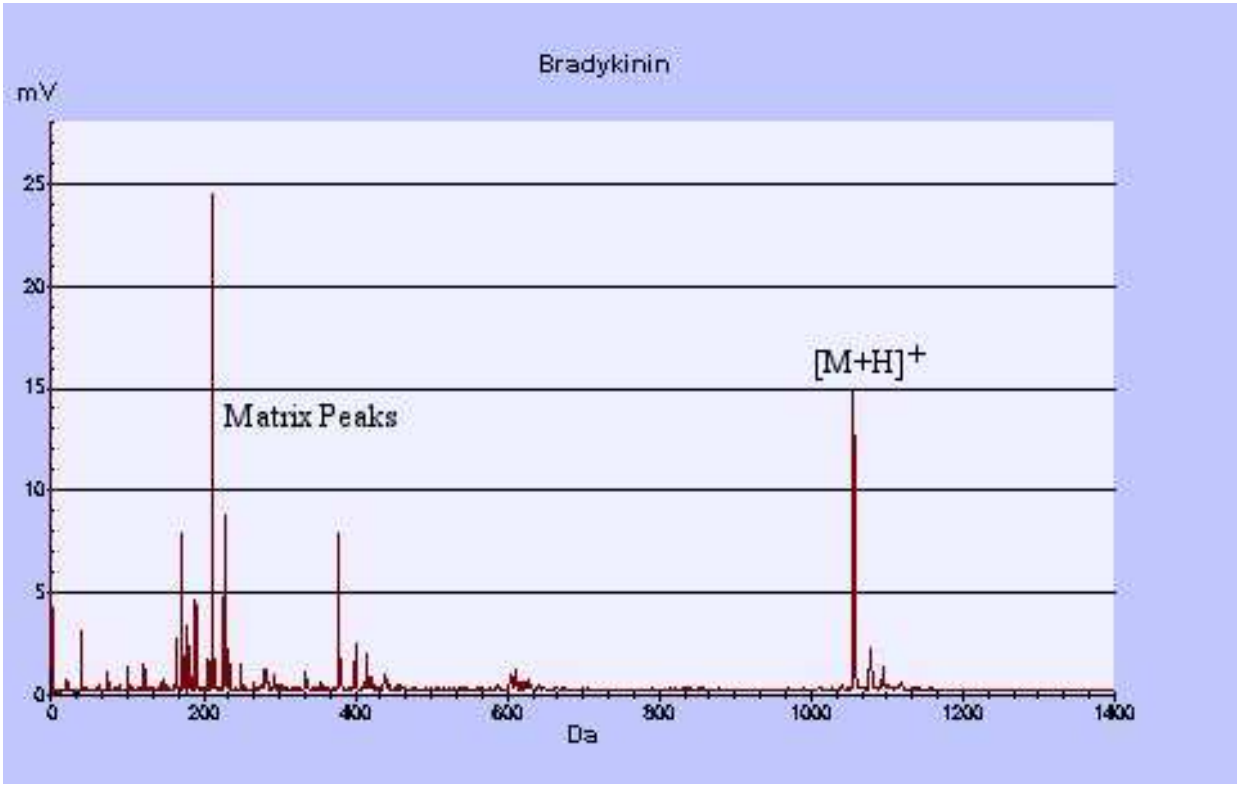


Figure 3: Bradykinin Mspec Output

The objective of this project is to develop a reliable, and robust algorithm for *automatically* analyzing raw output from mass spectrometers and to demonstrate the algorithm by building a from-everywhere accessible public-domain web-based tool making a high quality implementation of the algorithm available. An elementary version of the algorithm has been made available on the web and has been very popular (the algorithm was accessed by over 5,000 different sites in its first month of availability). This trial web tool was constructed in such a way that one can directly analyze noisy mass spectrometer output and generate unbiased machine-independent analysis of the noisy data in a timely fashion, greatly reducing (or eliminating) the need for laborious and painstaking manual analysis.

Modern mass spectrometers produce astonishingly high-quality data. Scientists are regularly faced with the difficult and time consuming task of sorting through many enormous noisy data sets in search of data structures (for example one must assume a “peak” shape or a “trough” shape) corresponding to the presence of chemical in question. Likewise, to determine the similarity or origin of fibers requires the analysis of chemical compositions usually acquired with a mass spectrometer. Because of unavoidable measurement errors committed when using a mass spectrometer outputs from different laboratories, machines or test runs can vary even when analyzing identical samples. When this data is then analyzed to determine the presence of a chemical substance that professionals must carefully examine the data by hand to identify the structure indicative of the chemical presence in question. This expensive and time consuming task is usually done with the aid of packaged computational algorithms many of which are `black-box' codes sold by software vendors or by companies manufacturing mass spectrometer hardware. In practice, these codes are often massaged into performing correctly by changing large numbers of algorithmic input parameters and/or testing subsets of the output data independently before analyzing the entire mass spectrometer output. Numerical behavior of currently available software can vary drastically as a function of numerous extraneous factors including parameter selection, choice of peak shape for example, machine precision, and even the computer platform on which the software is being run. Simply put, this is a very difficult problem.

We have succeeded in developing, implementing and testing an algorithm that, given raw MSpec data, can efficiently identify peak and trough structure without assuming any a priori size or shape structure. This algorithm is unique in that it requires no arbitrary parameter selection but instead allows the user to input a readily available estimate of machine noise produced by all time of flight mass spectrometers. Preliminary results are promising as the algorithm is now being used to analyze MSpec data (by members of the Polymer division at NIST, staff members at the Bureau of Alcohol Tabbacco and Firearms, the Federal Bureau of Investigation, the National Institutes of Health and a number of private companies).The webtool has been mentioned in general science journals like *Science*, *Nature* and *Radiochemistry News*.

The following papers related to this project have recently appeared.

- Bernal, C. Guttman, A. Kearsley and W. Wallace ``Automated Peak Picking and Integration Algorithm for Mass Spectral Data'', in Proceedings of the 51st ASMS Conference on Mass Spectrometry and Allied Topics, June 2003, Montreal Canada.
- J. Bernal, C. Guttman, A. Kearsley and W. Wallace ``A Numerical Method for Mass Spectral Data Analysis'', Applied Mathematics Letters (in revision)
- W. Wallace, A. Kearsley C. Guttman ``An Operator-Independent Approach to Mass Spectral Peak Identification and Integration'', Analytical Chemistry, 76, 2446-2452 (2004).

Mathematical Problems in Construction Metrology

Javier Bernal
David Gilsinn
Christoph Witzgall
Geraldine Cheok (NIST, BFRL)
Alan Lytle (NIST, BFRL)
William Stone (NIST, BFRL)

During the past decade, laser-scanning technology has developed into a major vehicle for wide-ranging applications such as cartography, bathymetry, urban planning, object detection, and dredge volume determination, just to name a few. The NIST Building and Fire Research Laboratory is actively investigating the use of such technology for monitoring construction sites. Here laser scans taken from several vantage points are used to construct a surface model representing a particular scene. Another aspect of the project envisions that CAD-generated geometry sets will be transformed into a library of 3D construction site objects, which will serve multiple purposes during construction. The objects would be loaded into an augmented simulation system that tracks both equipment and resources based on real-time data from the construction site obtained from laser scans. With some additional enhancements, the end result will be a world model of the site, in which as-built conditions can be assessed, current construction processes can be viewed as they occur, planned sequences of processes can be tested, and object information can be retrieved on demand. A project could be viewed and managed remotely using this tool. Pick-and-place control of construction site objects is another application of the 3D construction site object library. With automation and robotics entering on construction site scene, vision systems, such as LADAR (laser direction and ranging), will be incorporated for real time object identification, using the 3D library templates. Once objects, such as I-beams, are located and their pose determined, robotic crane grippers can be manipulated to acquire the I-beam.

LADAR technology is currently being tested by the NIST Building and Fire Research Laboratory for locating equipment on construction sites. LADAR scans of I-beams of multiple lengths and angular poses relative to the scanning LADAR have been generated (See Figure 1). A database of design specifications for potential I-beam candidates has been created. The LADAR scans generate a large number of points, ranging in the millions, in a typical scan that can be acquired in a matter of seconds. These scans usually contain a large number of noisy data values arising from ground hits to phantom pixels caused by beam splitting at sharp edges.

Figure 2 shows the scan obtained by the LADAR. Although each of the points in the figure are associated with an (x, y, z) coordinate relative to the LADAR, the identification of the nature of the objects scanned is not as clear as a photograph provides. Whereas the photograph provides a clear image it does not provide coordinate information. The challenge then is to use the database of design specifications, in this case of I-beams, to locate an object in the scanned image that essentially matches the length, width and height of an I-beam from the database and to report its center-of-mass location and angular pose relative to the LADAR. The scanned image consist of nothing more than coordinate points. In order to compare efficiency as well as speed, two algorithms have been developed to process the coordinate points obtained from a scan. One algorithm depends on binning of the scanned points to reduce the number of points processed. The bins are then examined to identify those that are likely to be phantom points or floor hits. These bins are eliminated from further analysis. Bins are then grouped into potential objects and bounding boxes place around them. These boxes are compared with bounding boxes defining the I-beams in the database and the best fit one is reported as the likely I-beam in the scan. At the same time to center and pose of the object bounding box is reported. The second algorithm relies on using Triangulated Irregular Networks (TINs) to mesh the scanned data. The density of the triangulated points is then examined to identify those triangle groups most likely to form solid objects in the scanned field-of-view. The bounding box procedure is then applied to these groups and the bounding boxes are compared with the bounding boxes of I-beams specified in the database. Again, location and pose relative to the LADAR is also determined.

Joining cent-of-mass estimates with principle components analysis has been shown to be a reliable method of determining location and pose of the I-beams.

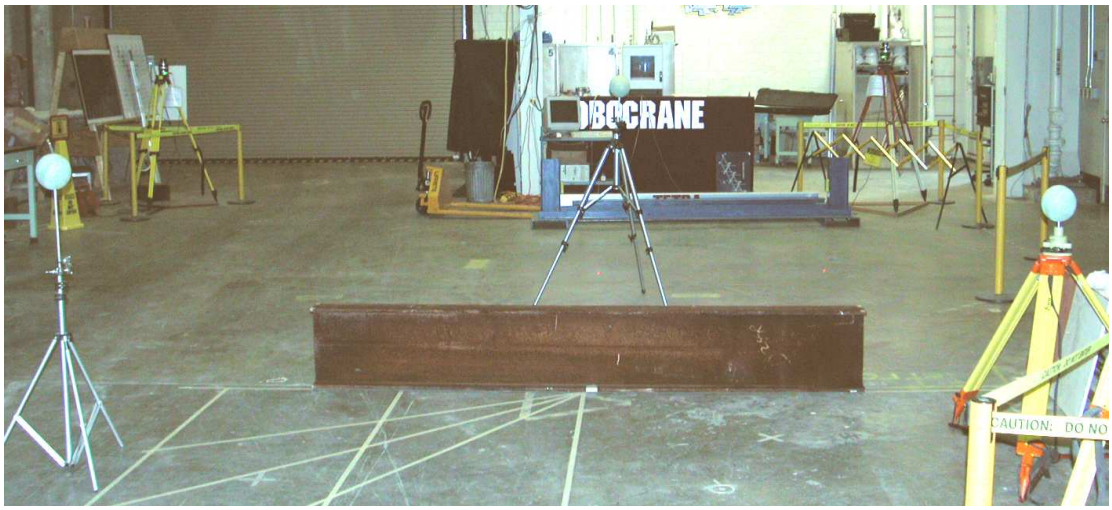


Figure 1: This figure shows the experimental configuration used for scanning an I-beam by a LADAR placed approximately at the camera location. The white lines on the floor are alignment marks for setting the I-beam at different angles relative to the LADAR. The spheres on tripods are located for coordinate registration with a world coordinate system.

Figure 3 shows a comparison being made between a bounding box of an I-beam from the database and a potential object in the field-of-view of the scanner. The red outlined box is the bounding box constructed from the database and the blue outlined box is the bounding box of the scanned object. Note that the algorithms have isolated the potential objects from the noise, floor hits and phantom pixels. Figure 4 shows a close fit between an I-beam bounding box constructed from the database and an isolated object scanned by the LADAR.

Other approaches to modeling objects in 3D construction sites have also been investigated including multivariate splines and finite elements. Traditional least squares fitting can lead to ringing at sharp edges of objects or buildings. A new minimum energy principle has been developed that fits Clough-Tocher finite elements to objects with sharp edges in such a way that ringing is suppressed. The minimization algorithm joins a Gauss-Seidel relaxation algorithm with a reweighting and regularization algorithm. It has shown promise on various test problems but requires further analysis to understand the nature of the algorithms convergence.

Urban environments provide challenges for first responders. Situation management for them now finds it desirable for the command and control center to have instant access to the location of both threats and assets. That is, they need to know the 3D whereabouts of their personnel during an incident. To date, no such system exists that will reliably and accurately track the movement of emergency and law enforcement personnel inside a building. Previous substantial research by NIST BFRL has proven that ultra-wideband tracking is viable through several meters of non-metallic construction material. Crucial to the accuracy of the use of ultra-wideband tracking is knowledge of the quantitative behavior of electromagnetic (EM) wave propagation through construction materials, since EM propagation speed varies dramatically depending on the type of material involved (e.g. concrete, brick, masonry block, plywood, etc.). Lack of accurate material properties could yield location estimates that are in error by a factor of 10 or more from their true location.

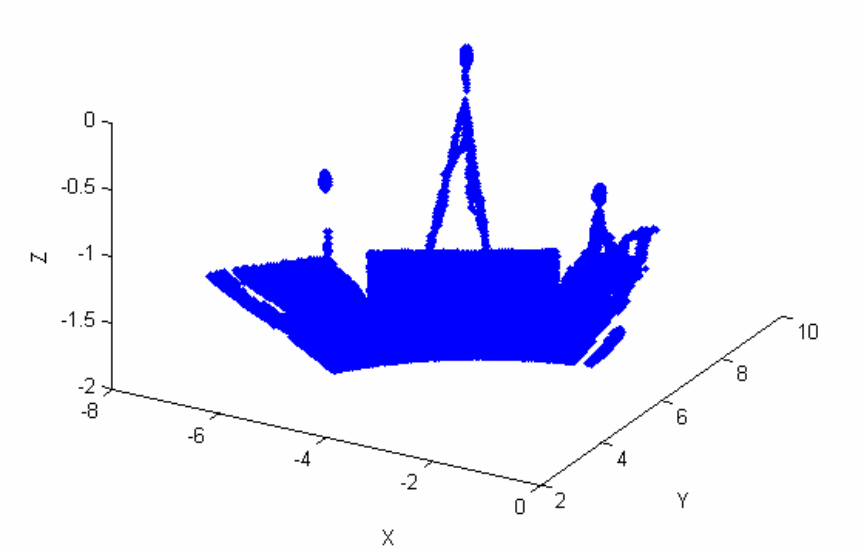


Figure 2: This figure shows the results of a LADAR scan of the I-beam in Figure 1. The flat areas on either side of what appears to be the I-beam are floor hits. Notice the results of hits on the three tripods.

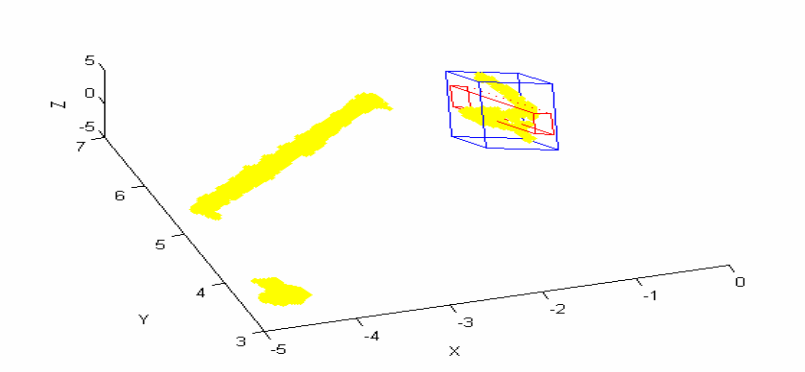


Figure 3: This figure shows the lack of fit between a bounding box defining an ideal I-beam (red) from the database and a bounding box defining an object in the LADAR field-of-view (blue).

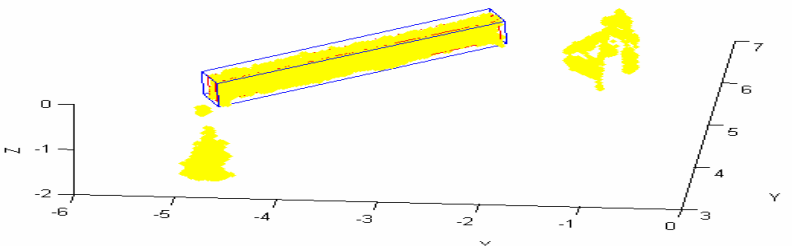


Figure 4: This figure shows the close fit of a bounding box defining an ideal I-beam (red) and a bounding box defining the isolated scanned object (blue).

The key characteristic needed to predict 3D location is the frequency-dependent dielectric constant for a broad class of construction materials. NIST BFRL began investigating ultra-wideband methods for tracking the movement of objects inside buildings as early as 1994. That program initially investigated time-of-flight through-wall tracking in the 0.5 to 2 GHz regime (which includes that of most cell phones) and then later extended the research to include all frequencies between 0.5 to 8 GHz.

BFRL obtained FY04 funds from the NIST Office of Law Enforcement Standards to investigate the possibility of computing the dielectric constants of construction materials. D. Gilsinn of MCSD was approached by BFRL to determine the feasibility of using this data and a known model from the EM literature that related dielectric constants to the transmission coefficients available in the experimental data, as a way to estimate the dielectric constants of the materials. A script was written in Matlab to perform a nonlinear least squares estimate of the dielectric constants. For low frequency values in the 0.5 GHz range unique minima were obtained. However, as frequencies increase multiple minima showed up in the form of lobes. After consultation with colleagues in the EM field it became clear that the multiple minima were due to the fact that at higher frequencies it took multiple wavelengths to penetrate the material. For wavelengths approximately the width of the test material a single minimum was produced. Another thing that was found out was that the dielectric constants had to be treated as complex quantities. Thus it was necessary to search for minima in the complex plane. BFRL has proposed to OLES to continue the investigation of computing the dielectric constants in FY05.

This work was supported in part by the NIST Building and Fire Research Laboratory.

Modeling and Computational Techniques for Bioinformatics Based Data Mining

Fern Y. Hunt
Agnes O'Gallagher

The purpose of this project is to develop generic bioinformatics algorithms that can utilize large-scale and fast computational methods to perform the comparison and alignment of a large number of long biological sequences. Almost all methods currently in use are based on an optimization problem that is solved using the methods of dynamic programming. Starting from a Markov decision theory approach, we solve a linear programming problem. Our goal is to avoid the exponential increase in computation as the number of sequences increases and to avail ourselves of the high performance algorithms available for solving this type of problem. Potential applications for this work are in drug discovery where large numbers of sequence sites must be evaluated for use as drug targets and the development of of pharmacogenomic therapies, i.e. therapies that are tailored to genetic-makeup of the patient. Multiple sequence alignment also plays an important role in the characterization of biological threats.

The software package growing out of our algorithm development requires training data, i.e. a set of aligned sequences that are used to determine the underlying model parameters. Much of our time in 2004 was spent in looking for ways to obviate the need for this. For example rather than relying on data from sequences aligned by other methods we sought to construct data sequences by simulating (in a controlled way) the evolution of protein or DNA sequences.

We used the program ROSE to simulate the evolution of an entire bacterial genome. This produced a set of evolutionary related sequences that were used as a training set. Thus we were able to align the genomes of the original and several other sequences using our method. In addition to enhanced computational efficiency, the robustness to changes in the alignment due to changes in the input parameters can be measured. This is a feature that is to our knowledge, unique to our approach.

Last year we examined the sensitivity of the solutions of the linear programming problem to small changes in the costs. The latter could occur because of changes in the scoring matrix used to score the alignments. This year we examined the sensitivity of the alignments and found them to be quite robust. Theoretical calculations of the degree of sensitivity bear out our observations.

Three invited presentations including one hour talk at the American Mathematical Society were given. Two papers describing our work were submitted to refereed journals and both were accepted for publication.

Virtual Measurements from Computational Quantum Chemistry Models

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

http://srdata.nist.gov/cccbdb

A virtual measurement is a prediction determined from a computational model together with its associated uncertainty for the value of a measurand. We are developing practical methods to quantify the uncertainty associated with the predictions from computational quantum chemistry models and also trying to address other important issues in quantum chemistry. Interest in virtual measurements is increasing for reasons of economics and safety. They are becoming critical in research and development of chemical processes, new materials, and drug discovery. Predictions from quantum chemistry models are usually reported without uncertainties making them incomplete and less useful. The uncertainties in computed values arise largely from systematic biases rather than random errors; therefore, a new approach is needed.

We have developed an approach to quantify the uncertainty associated with enthalpies of formation based upon the *Guide to the Expression of Uncertainty in Measurement*, published by the International Organization for Standardization (ISO) and the NIST Computational Chemistry Comparison and Benchmark Database (CCCBDB), which contains data for over 600 molecules, over 100 calculations for each molecule, and over 4000 vibrational frequencies (Irikura, K. K.; Johnson, R. D., III; Kacker, R. N. *Metrologia* **41** (2004), pp. 369-375). The challenging issue here is identifying a suitable class of molecules in the CCCBDB for which the biases are similar to the bias for the target molecule. Predictions from ab initio calculations of vibrational frequencies are scaled to compensate for their estimated differences from the experimental values. The scaling factors carry uncertainty, yet it is not quantified. We are in the process of quantifying these uncertainties. For the vibrational frequencies we found the uncertainties to be orders of magnitude larger than previously believed. We plan to continue extracting such information from the CCCBDB to determine the uncertainties for other calculated properties as well. By convention, uncertainties in quantum chemistry are expressed as intervals with a stated coverage probability such as 95 %. Often, the available information and the method of propagating uncertainties do not provide a definitive coverage probability. We are investigating the corresponding probability distributions. There is great interest in using quantum chemistry models to help identify unknown molecules by vibrational spectroscopy and to quantify the probability that the molecule is correctly identified.

Lipschitz Space Characterization of Images

Alfred S. Carasso

Previous MCSD work on characterizing the lack of smoothness of natural images, is gaining wide acceptance, and is influencing the direction of research in image analysis.

Most commonly occurring images *f(x,y)* display edges, localized sharp features, and other fine-scale details or *texture*. In particular, *f(x,y)* is very seldom a differentiable function at every point (x, y). Correct characterization of the lack of smoothness of images is a fundamental problem in image processing.

It turns out that so-called *Lipschitz spaces* are the appropriate framework for accomodating non-smooth images. The L^p Lipschitz exponent α for the given image, where $0 < \alpha < 1$, measures the fine-scale content of that image, provided the image is relatively noise free. Heavily textured imagery has low values for α, while large values of α indicate that the image is relatively smooth.

During the past year, four presentations of this general circle of ideas were made. The venues were the MCSD Colloquium, the University of Maryland Wavelet and Harmonic Analysis Seminar, the SIAM Image Science Conference in Salt Lake City, and the George Washington University Summer Program for Women in Mathematics. In addition, a MiniSymposium on *Loss and Recovery of Image Texture* was organized at the Salt Lake City SIAM Conference, featuring eight speakers and drawing a sizeable audience. A paper entitled "Singular Integrals, Image Smoothness, and the Recovery of Texture in Image Deblurring" was published in the *SIAM Journal on Applied Mathematics*, Volume **64**, Issue 5 (2004), pp. 1749-1774. That particular SIAP issue is notable for including four major papers on image analysis among its fourteen published articles, indicating strong current interest in this research topic.

Considerable effort was also expended in seeking U.S. Patent protection for MCSD's technique for measuring image Lipschitz exponents, and the accompanying new MCSD deblurring methodology. Intensive interaction with patent attorney Dr. Noreen Welch, of the Washington, DC law firm of Stevens, Davis, Miller and Mosher, over a three month period, resulted in the filing of an application entitled *Singular Integral Image Deblurring Method* on August 31 2004.

Improving Image Resolution in Nanotechnology

Alfred S. Carasso,
András E. Vladár (NIST MEL)

A recurring theme at the January 2004 *NIST Grand Challenge National Nanotechnology Workshop*, was the relatively low quality of current nanoscale electron microscopy micrographs, and the urgent need for improved imagery to support future research. Of major interest to the Nanoscale Metrology Group at NIST is the continuing development of improved mathematical tools for image analysis, and the use of such tools to effect measurable increases in resolution in state-of-the-art scanning electron microscopy. One very major difficulty lies in the large image sizes, often on the order of 1024x1024 pixels, or larger. This presents formidable computational challenges. Many new techniques are based on nonlinear partial differential equations, and typically require thousands of iterations, and several hours of CPU time, to achieve useful results. *Real-time* image processing algorithms are exceedingly rare and very highly sought after.

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

Nevertheless, in recent years, considerable progress was achieved by MCSD in developing mathematical technologies that lead to real-time image processing algorithms. In addition, a unique new capability was created, the so-called *APEX method*, that can achieve useful blind deconvolution of 1024x1024 SEM imagery in about 60 seconds on current workstations. Because of its manifold applications, this technology is the subject of intense and continuing research and development.

Very recently, a new Hitachi Scanning Electron Microscope was acquired by the Nanoscale Metrology Group, capable of producing higher quality imagery than had previously been possible. A major challenge for MCSD's deconvolution algorithms was to demonstrate measurable increases in sharpening of such state of the art imagery. Two sharpness measures were used, the image Lipschitz exponent α, and the image discrete *total variation* or TV norm. Image sharpening increases the TV norm, due to the steepening of gradients, while it decreases the Lipschitz exponent as finer scale features become resolved. Examples of such sharpening are shown in Figures 1 and 2. In Figure 1A, the original 1024x1024 Tin sample micrograph has TV norm of 13000 and Lipschitz exponent $\alpha = 0.40$. The APEX-sharpened Figure 1B has TV norm = 34000 with $\alpha = 0.29$. In Figure 2A, the original 1024x1024 Magnetic Tape sample has TV norm = 14000 with $\alpha = 0.35$. The APEX-processed Figure 2B has TV norm = 39000 with α = 0.26. These very substantial sharpness increases are typical of those obtained in numerous other test images.

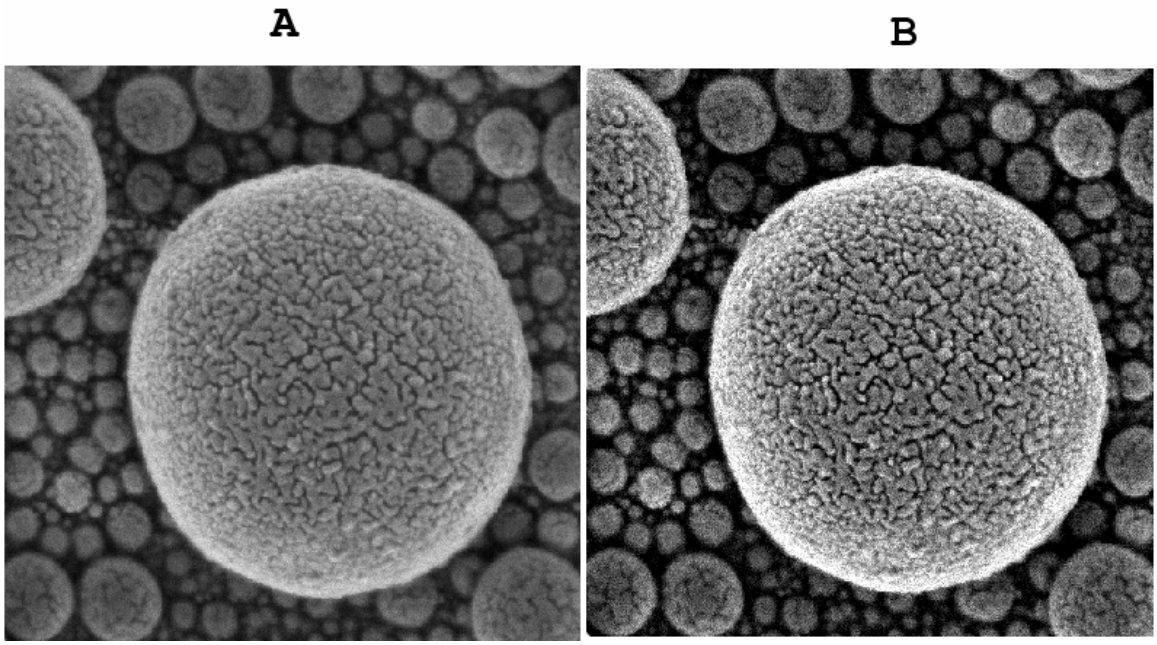


Figure 1. APEX blind deconvolution of state of the art Scanning Electron Microscope imagery produces measurable increases in sharpness. (A) Original 1024x1024 Tin sample micrograph has Lipschitz exponent $\alpha = 0.40$ and TV norm = 13000. (B) Sharpened image has $\alpha = 0.29$ and TV norm = 34000.

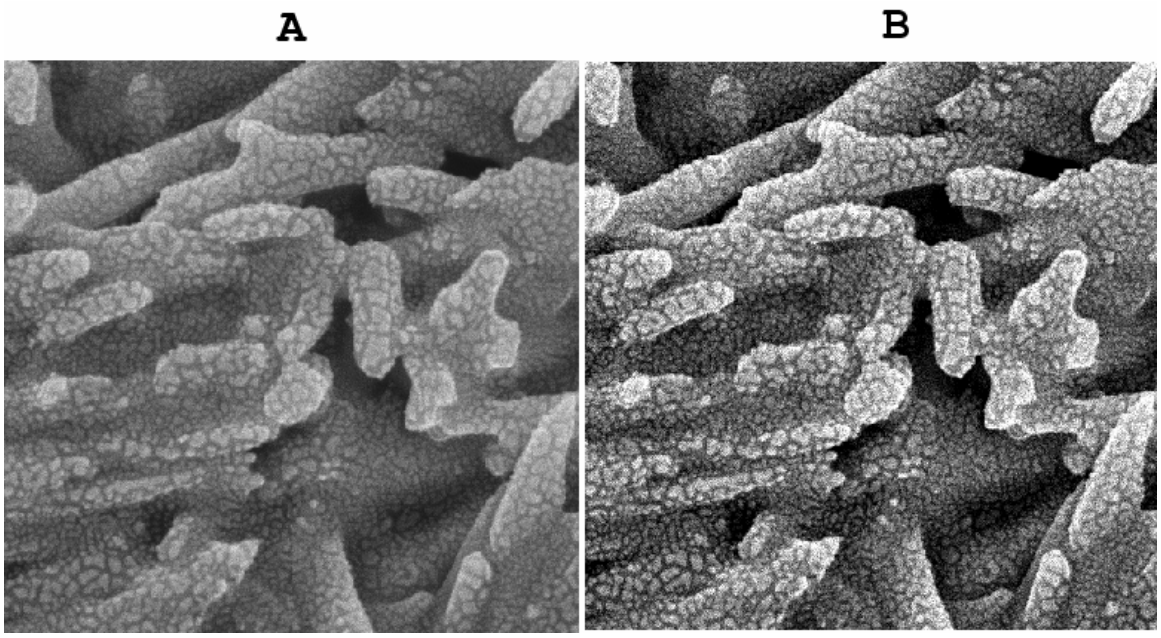


Figure 2. APEX sharpening of SEM imagery. (A) Original 1024x1024 Magnetic Tape sample has $\alpha = 0.35$ and TV norm = 14000. (B) Sharpened image has $\alpha = 0.26$ and TV norm = 39000.

Color Blind Deconvolution

Alfred S. Carasso

As previously observed, blind deconvolution of images is a difficult mathematical problem that is not fully understood, and one for which little reliable theoretical or computational expertise actually exists. MCSD's *APEX method*, as originally published in *SIAM Journal on Applied Mathematics* **63**, 2 (2002), pp. 593-618}, deals with gray-scale imagery. The method is based on identifying a blurring kernel in the form of a Lévy stable density function, by appropriate one dimensional Fourier analysis of the blurred image. Using that kernel, an ill-posed parabolic backwards in time continuation problem must then be solved to obtain the deblurred image.

Typically, the detected point spread function turns out to be too wide, *erroneously*. However, this can be compensated for by early termination of the continuation algorithm. This requires visual monitoring of the unfolding deconvolution process, by a user familiar with the physical or medical context underlying the image. Very striking results have been obtained with the APEX method, in quite diverse gray-scale imaging applications.

Blind deconvolution of color imagery appears to be a much harder problem. A color image can be decomposed into its RGB components, and the APEX method may be applied to each component in turn. However, the crucial APEX element that involves visual monitoring of the continuation algorithm is no longer feasible. An experienced user may be unable to decide whether or not the blue image, say, has been properly deblurred. Conceivably, in reconstituting the individual deblurred components into a single color image, one of the components may turn out to have been too aggressively sharpened, resulting in such false coloring as yellow eyes or green lips in Figure 3B. Clearly, considerable useful research remains be done, exploring various mathematical constraints that might be imposed to ensure proper balancing of the individual components. Most important, such constraints should avoid nonlinear formulations that require large numbers of iterations, as this would destroy the real-time advantage of the APEX method.

One real-time approach that has been found surprisingly successful is based on enforcing quasi conservation of radiant flux in each RGB component. In the above-mentioned backwards in time continuation problem, both the discrete L^1 and TV image norms can be calculated at each time step. Typically, the TV norm increases by a factor of 2 or 3, while the L^1 norm increases very slowly. It is found that useful color sharpening is obtained by terminating backwards continuation in each RGB component when the L^1 norm exceeds the original L^1 norm by more than 5%.

One intriguing potential application for color APEX processing lies in Hubble Telescope imagery. As shown in Figure 4, significant sharpening of some images appears to be possible.

Figure 3. Blind deconvolution of color imagery must result in correct balancing of RGB components and preserve natural coloring appropriate to subject matter. *Left:* Original Lizabeth Scott image. *Right:* Real time APEX sharpening with L^1 norm conservation preserves natural colors.

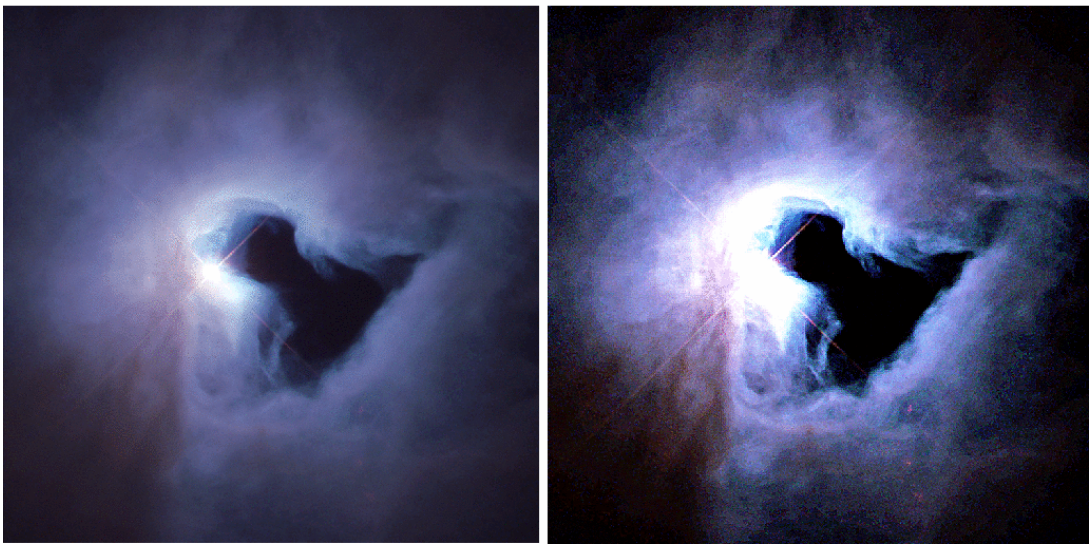


Figure 4. Hubble Telescope imagery presents interesting candidates for APEX processing. *Left:* Original Hubble image of Orion reflection nebula NGC 1999. *Right:* Real time APEX enhanced image.

Monte Carlo Methods for Combinatorial Counting Problems

Isabel Beichl
Francis Sullivan (IDA Center for Computing Sciences)

In the previous year we had developed a new method to estimate the number of independent sets in a graph. An independent set is a subset of the set of nodes of a graph where none of the subset has any connections with any other elements of the subset. This problem is important because of applications in thermodynamics and data communications. It is dual to the problem of counting the number of cliques in a graph and thus gives graph connectivity information. In this year, we applied the method to a first principles calculation of the hard sphere entropy constant in three dimensions. Calkin and Wilf had made an estimate in 2-dimensions. On the way to our 3-dimensional result, we reproduced their two-dimensional result. Calkin and Wilf also computed tight analytic upper and lower bounds on the constant. We have also been able to compute these bounds in three dimensions. This was done using the transfer matrix of the lattice, a technique originally developed in statistical mechanics. The trace of the transfer matrix for aperiodic lattices is just the largest eigenvalue of the transfer matrix for the periodic case. Calkin and Wilf didn't know this. Computing the largest eigenvalue can be done for these 0-1 matrices in very large cases by doing bit operations instead of using the floating point representation. Without this trick, we would not have been able to compute a large case and hence not obtain tight bounds.

Surface Reconstruction with the Power Crust

Javier Bernal

The problem of surface reconstruction is that of approximating the surface of an object from a set of sample points on the surface. Sample points are usually obtained from real objects with the aid of laser scanners.

The power crust is a piecewise-linear approximation of the surface of an object that is computed from an approximation of the medial axis of the object. The medial axis is a skeletal shape associated with the object with the property that each point in the medial axis is the center of a maximal empty ball that meets the surface of the object only tangentially at two or more points.

Currently a program is being implemented for computing the power crust. The main tools being used are the Voronoi diagram and the weighted Voronoi diagram or power diagram. The medial axis is first approximated by a subset of the Voronoi vertices of the set of sample points called poles. When the set of sample points is good the poles lie near the medial axis and the union of the Delaunay balls centered at poles inside the object approximates the object. The squared radii of the Delaunay balls centered at poles define weights on the poles and a power diagram of the set of weighted poles is computed. By taking advantage of the natural graph that the power diagram defines on the set of poles, poles are labeled as either inner or outer with respect to the object. The union of the power cells of inner poles is then a polyhedral solid that approximates the object and whose surface is the Power crust. Even when the set of sample points is not totally good because of noise or because it is too sparse, a good Power crust can usually be obtained by carefully selecting the poles.

Modeling the Behavior of Cryocoolers

Abbie O'Gallagher
John Gary

The REGEN3.2 package developed by John Gary and Abbie O'Gallagher over the last several years has become a dependable tool for researchers in cryocooler technology. It models the behavior of these devices and accepts a large number of parameters to describe the design, including the material properties of the device, the device geometry (screens, plates, spheres or some other configuration), its porosity, hydraulic diameter, cross sectional area, etc. It also has the capability of allowing a design that includes layers made up of different materials. Until now, Regen3.2 has not been capable of allowing those layers to have different configurations (for example screens in one layer and spheres in another) or different factors by which the thermal conductivity could be adjusted. This year A. O'Gallagher added these two capabilities.

Elastic Wave Model

Abbie O'Gallagher

Abbie O'Gallagher has been exercising a special version of a 3-D finite element wave code for Marv Hamstad of the Materials Reliability division. This work supports the database of waveforms that is being produced producing using this code. As part of this work, O'Gallagher revised a Matlab script for filtering output from the wave code. This work is reported in three papers appearing in the *Journal of Acoustic Emission.*:

- K. S. Downs, M. A. Hamstad and A. O'Gallagher, "Wavelet Transform Signal Processing to Distinguish Different Acoustic Emission Sources," *Journal of Acoustic Emission* **21** (2003), pp.52-69.
- M. A. Hamstad, K. S. Downs and A. O'Gallagher, "Practical Aspects of Acoustic Emission Source Location by a Wavelet Transform," *Journal of Acoustic Emission* **21** (2003), pp.70-94.
- M. A. Hamstad and A. O'Gallagher, "Modal-Based Identification of Acoustic Emission Sources in the Presence of Electronic Noise," to appear in *ournal. of Acoustic Emission*.

Measures of Approximation in Delay Differential Equations

David Gilsinn

Delay differential equations have arisen in the modeling of machine tool dynamics and, in particular, the problem of chatter. Machine tool chatter is a self-excited oscillation of a cutting tool against a machined workpiece. Acoustically it can be detected as a high frequency squeal in a machine shop. The suppression of chatter is significant to producing a high quality surface finish on the workpiece. Modeling chatter and other machining instabilities has been a problem of long-term interest to the NIST Manufacturing Engineering Laboratory. Mathematically, chatter is characterized as a limit cycle for a nonlinear delay differential equation.

D. Gilsinn of MCSD has implemented algorithms that compute various parameters needed in order to employ a precise measure of how near an approximate periodic solution is to the "real" limit cycle. The measure is more precise than a standard order-of-magnitude error estimate. Whereas in ordinary differential equations there are well-developed Green's function methods of determining the

initial conditions for periodic solutions as well as constructing fundamental solutions, in delay differential equations there are no such easily constructed relations. The stability of limit cycles is determined by the characteristic multipliers. For exact periodic solutions to delay equations there is always a characteristic multiplier of one with the location of the other characteristic multipliers identifying the nature of the stability of the solution. In ordinary differential equations the computation of characteristic multipliers becomes an algebraic problem. However, in delay differential equations the determination of characteristic multipliers can be performed by solving an eigenvalue problem for a Fredholm-type integral equation. Another parameter needed to implement the precise measure involves solving the adjoint delay differential equation associated with the variational equation of the nonlinear delay differential equation about the approximate solution. Solving the adjoint requires a reverse direction integration of the adjoint equation. However, delay differential equations usually solve in forward time steps. It is necessary then to formulate a variation of constants formula for the adjoint in such a way that only forward integration of the fundamental solution if required. Finally, a precise bound must be obtained relating the magnitude of a nonhomogeneous term to a solution in the case of a linear nonhomogeneous delay differential equation. Matlab programs have been written to compute these parameters and a precise location of the solution to a Van der Pol equation with delay has been demonstrated. Further study of more efficient algorithms for computing the necessary parameters is currently under way along with an analysis of the convergence of the parameter identification algorithms.

Modeling a Radioactive Decay Chain

Bert W. Rust
Dianne P. O'Leary

A conceptually simple physical problem which produces a numerically difficult fitting problem involves modeling a radioactive decay chain, with unknown decay rates, to explain a single times series of radiation measurements. Solving the system of ODEs to derive an expression for the observed radiation time series yields a linear combination of real exponentials whose rate constants and amplitudes (linear coefficients) must be estimated by nonlinear least squares. Many years ago, Lanczos called this the "separation of exponentials" problem and vividly demonstrated its ill conditioning [C. Lanczos, "Applied Analysis," Prentice Hall (Englewood Cliffs, 1956) pp. 272-280]. A more recent review of the numerical difficulties has been given by Dianne O'Leary [D.P. O'Leary, *Computing in Science and Engineering* **6** (May-June 2004), pp. 66-69]. The presence of measurement errors in the observed data makes the estimation problem practically impossible if there are more than three species (two decays) in the chain. But recent developments in extragalactic astronomy have renewed interest in chains with three decays. Type Ia supernovae have been the object of much government sponsored research because of their promise as "standard candles" for measuring distances to other galaxies. The light curve of such a supernova is given in Figure 1. It is generally believed that the decaying luminosity, beginning a few days after peak brightness, is powered by the radioactive decays

$$\text{Ni-56} \rightarrow \text{Co-56} \rightarrow \text{Fe-56}\,,$$

even though the observed luminosity decay rates do not exactly match the known terrestrial half lives of the nickel and cobalt isotopes. In 1976 evidence was presented by Rust, et. al. [B.W. Rust, M. Leventhal and S.L. McCall, *Nature* **262** (1976), pp. 118-120] which suggested that this mismatch in rates was caused by an acceleration of the nuclear reactions which arises because they occur in the high density interior of a white dwarf star. The evidence, gleaned from 15 light curves, indicated that for any given supernova, both decay rates were increased by the same factor. This means that for each supernova, the ratio of the two observed rates would be the same as the ratio of the terrestrial half

lives, but the acceleration rate would vary from one supernova to another. Thus only 3 (rather than 4) free parameters were required for the sum of two exponentials used to model the decaying part of the light curve. This reduction is almost inconsequential for modeling only the decaying part of the light curve, but it becomes crucial when the model is extended to also accommodate the rise to maximum luminosity.

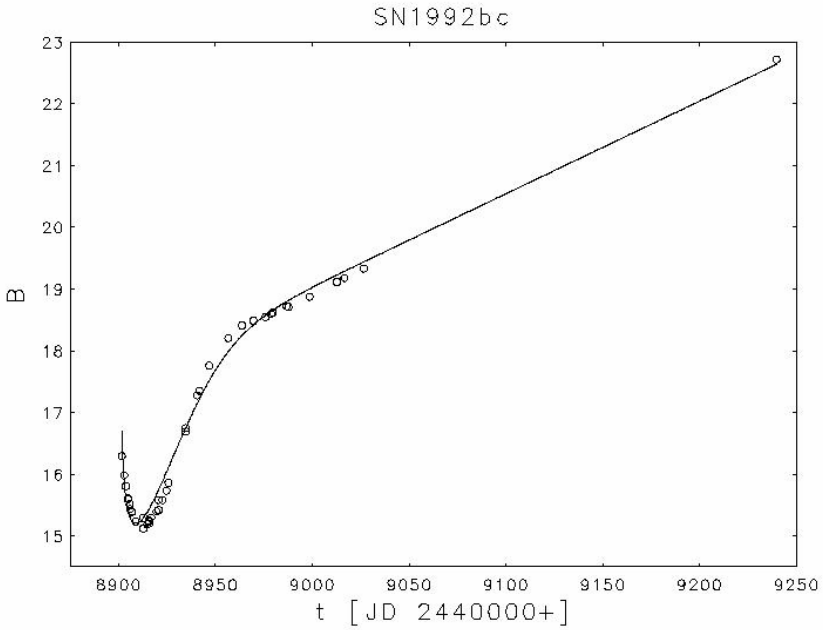


Figure 1. The B-magnitude (blue band) light curve of the Type Ia supernova SN1992bc. The abcissa is time measured in units of Julian Days, and the ordinate is apparent luminosity measured in magnitudes. Because smaller magnitudes indicate greater luminosities, the minimum at approximately 24400008910 days actually corresponds to the peak brightness of the supernova. The circles represent the measured values and the curve is the nonlinear least square fit of the model described in the text below.

A simple model for the entire light curve can be gotten by considering a three stage chain of nuclear reactions of the form

$$\text{(lighter isotopes)} \rightarrow \text{Ni-56} \rightarrow \text{Co-56} \rightarrow \text{Fe-56},$$

with the last two stages being the decays described above. The first stage combines a number of rapidly occurring fusion reactions which build the nickel from lighter nuclei. The model does not consider the details of these reactions, but assumes only that, taken all together, they occur on an exponential time scale with a well defined rate constant to be determined by fitting the measured light curve data. Assuming that all three stages contribute to the total luminosity yields a linear combination of three exponentials with three linear and three nonlinear adjustable parameters. The above-described reduction of the number of effective rate constants from three to two was offset by the inclusion of the time of the initial explosion as an additional free parameter. The six parameter model is completely intractable because of the ill conditioning noted above. But it can be transformed into a model in which, for physical reasons, all six parameters must be nonnegative. This does not alleviate the ill-conditioning, but it suggests the possibility of stabilizing the fits by using a nonnegatively constrained optimization algorithm. The reformulation also isolates the contribution to the luminosity of the first stage of the above reactions, and if that term is dropped from the model, the result is a five parameter model which is not intractable. The curve in Figure 1 is a fit of that reduced

model. Even without the luminosity contribution from the fusion reactions, the fit tracks the data well enough to justify further efforts to stabilize the six parameter fit. The reward for success in such an effort would be considerable because it is well known that the rate of decline in luminosity is correlated with the peak luminosity. Thus, a good fit to the light curve of a distant supernova would yield estimates of both its apparent luminosity, from the light curve itself, and its intrinsic luminosity, from the estimate of the acceleration of the decay rate. The two could then be combined to give an estimate of the distance to the supernova.

Systems Identification and Parameter Estimation

Bert W. Rust

An important scientific modeling problem is to find a system of ordinary differential equations (ODEs) which describe the dynamical relationships between a set of measured time series variables. The ODEs will usually depend on several unknown constants and/or initial values which must be estimated by simultaneously fitting each separate ODE to its corresponding time series of observations. The fitting procedure (e.g., nonlinear least squares) will usually seek to minimize some measure of the mismatch between the solutions to the ODEs and the observations. Designing a measure of the mismatch which properly weights the contribution of each time series may be difficult because the measurements and/or their uncertainties may be numerically incommensurate, and the time series may not all have the same length.

A current example of great interest involves modeling the relationships between global fossil fuel carbon dioxide emissions $P(t)$, atmospheric concentrations of carbon dioxide c(t), and global average tropospheric temperatures $T(t)$. Good measured time series of annual values of these quantities are readily available on the Web. Previous work [B.W. Rust, ICCS 2004, *Lecture Notes in Computer Science* **3039** (2004), pp. 1226-1233] has suggested the following system of ODEs for modeling these three time series,

$$\frac{dP}{dt} = \alpha P - \beta\left\{\eta P + A\cos\left[\frac{2\pi}{\tau}(t+\phi)\right]\right\}P\,, \qquad P(t_0) = P_0$$

$$\frac{dc}{dt} = \gamma P\,, \qquad c(t_0) = c_0$$

$$\frac{dT}{dt} = \eta P + A\cos\left[\frac{2\pi}{\tau}(t+\phi)\right], \qquad T(t_0) = T_0$$

with free parameters α, β, η, A, τ, ϕ, P_0, γ, c_0, and T_0. Evidence for the indicated feedback between $T(t)$ and $P(t)$ was first noted in 1982 [B.W. Rust and B.L. Kirk, *Environment International* **7** (1982), pp. 419-422] and updated in 2003 [B.W. Rust, *Computing in Science and Engineering*, **5** (2003), pp. 74-79]. Evidence for the very simple relation between $c(t)$ and $P(t)$ was given in the ICCS 2004 paper noted above. The connection between $c(t)$ and $T(t)$ is the most uncertain link in the system. The above equations assume a linear relation between the two. Although this is a very simple assumption, it seems to be a good first approximation. It also allows the second equation to be dropped and the first and third to be simultaneously fit to their respective time series with only eight free parameters.

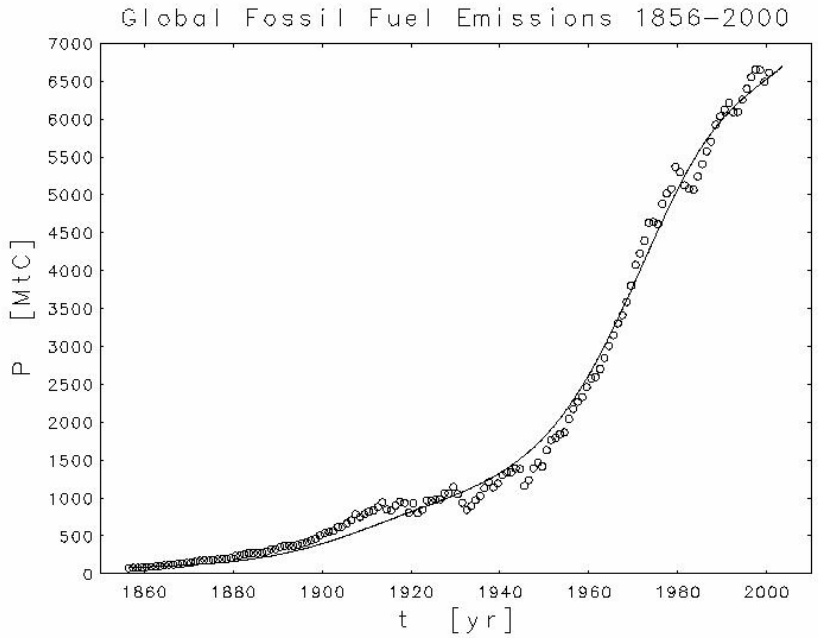


Figure 1. Annual global total fossil fuel carbon dioxide emissions measured in megatons of carbon. The circle are the observed values, and the curve is the *P(t)* fit obtained by simultaneously fitting the first and third ODEs in the above system to their respective data sets.

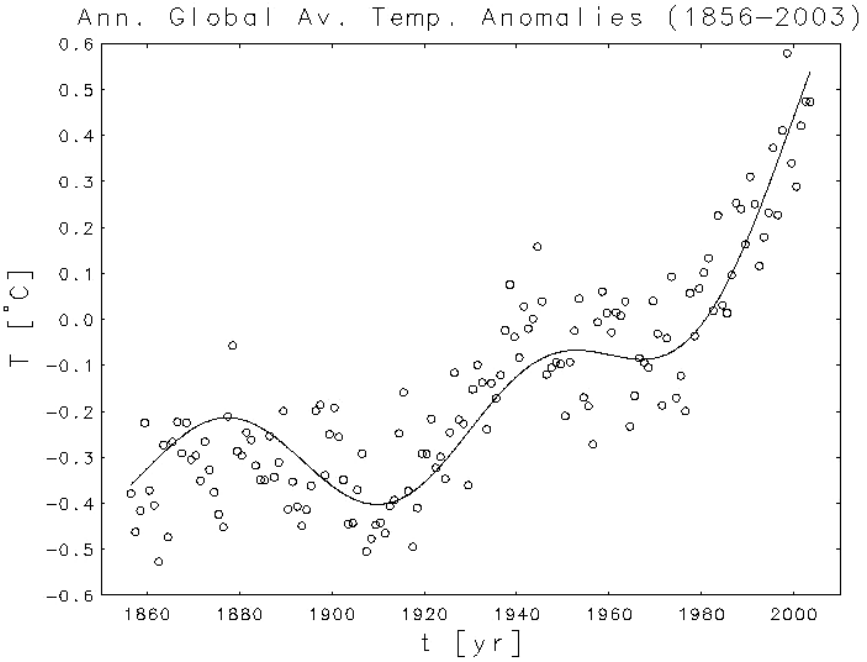


Figure 2. Annual global average tropospheric temperature anomalies (departures from the average temperature for the period 1961-1990) measured in degrees Centigrade. The circles are the observed values, and the curve is the *T(t)* fit obtained by simultaneously fitting the first and third ODEs in the above system to their respective data sets.

Plots of the *P(t)* and *T(t)* time series are given in Figures 1 and 2. The fits were obtained by combining a nonlinear least squares code with an adaptive multi-value ODE integrator. The quantity minimized was a linear combination of the sums of squared residuals for the two separate fits. Inspecting the two plots reveals that the magnitudes of the *P(t)* measurements are roughy 10,000 time larger than those for the temperature measurements, so in the first attempt, the observations in each time series were weighted inversely with the largest magnitude measurement in that series. This produced a good fit for the temperatures but a not so good fit for the emissions. Adding additional weighting for the emissions improved that fit but the temperatures fit was not as good as before. It was easy to improve one fit at the expense of the other by varying the relative weighting. The fits shown here were obtained by weighting the emissions data with an additional factor of 20. That value was a compromise chosen subjectively by inspecting the two fits for several different additional weighting factors. Thus far, no attempt has been made to optimize the choice because other considerations seem more important.

The most important of these considerations is a more realistic relation between *c(t)* and *T(t).* Studies of proxy records obtained from Antarctic ice cores, spanning more than 400,000 years, indicate slight, but not drastic, departures from a linear relation. The small relative uncertainties in the 8 parameter estimates obtained here, and the absence of any large correlations between them, suggest that the data may support at least one more adjustable parameter. The next step will be to replace the linear relation between *c(t)* and *T(t)* with a power law in which the exponent is also a free parameter.

Using a more complex relation between *T(t)* and *c(t)* will require that the *c(t)* time series also be included in the simultaneous fits. This will complicate the choice of weights for the sums of squared residuals because the *c(t)* data go back only to 1959. But the *c(t)* measurements are more precise than those for the other two time series, so the weighting must be adjusted to assure a good fit to them. If such a fit is also accompanied by good fits to the other two data sets, then confidence in the model will be enhanced.

A successful completion of the program outlined above would provide a predictive tool for informing policy decisions on future fossil fuel use. For example, by altering the differential equation for *P(t)* to conform to the provisions of the Kyoto treaty, and comparing the extrapolation of the altered model into the future with the one gotten by continuing on with the current model would allow one to predict whether or not the adoption of the Kyoto treaty would actually produce a significant reduction in the rate of global warming. Replacing the *P(t)* equation with one which provides for a gradual replacement of fossil fuels with alternative energy sources would allow a prediction of the final equilibrium temperature and the time scale on which it would be attained.

Mathematical Software

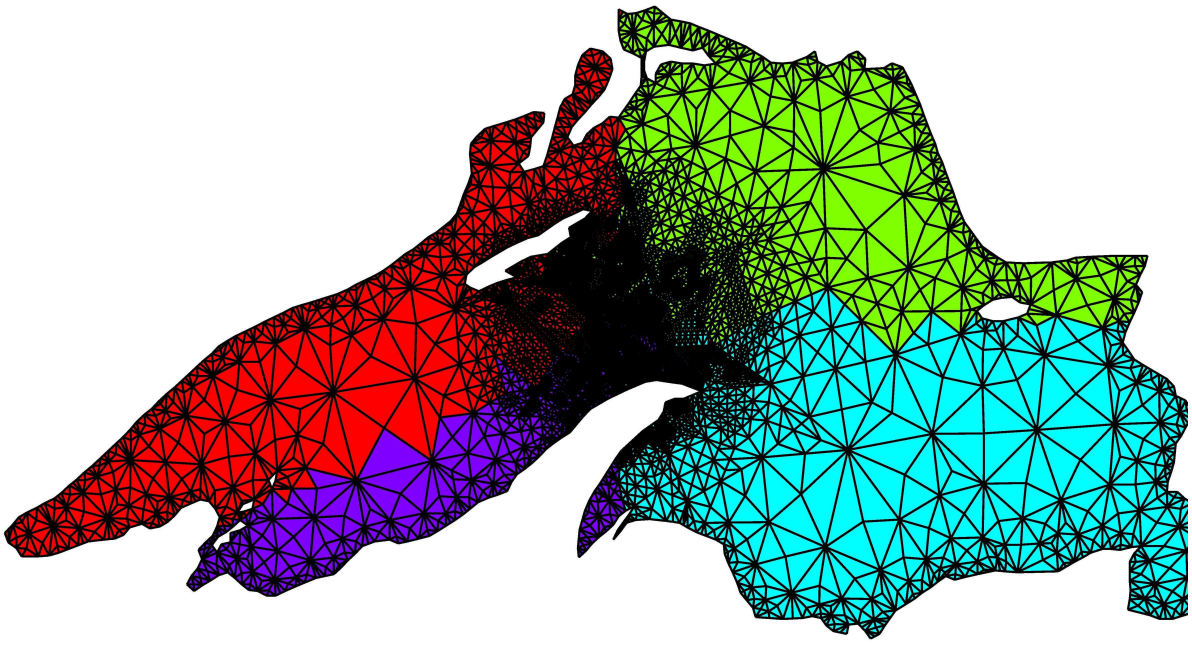
Parallel Adaptive Refinement and Multigrid Finite Element Methods

William F. Mitchell
Eite Tiesinga (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: improvement and extension of the PHAML software, 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 2004 are the following:



An adaptive grid generated by PHAML on 4 processors for a solution with a sharp peak over a Lake Superior shaped domain. Color indicates the assignment to processors.

- Performed an experiment to study the performance of preconditioners applied to GMRES for the solution of the linear systems that arise when using ARPACK to solve the discretized Schroedinger equation. Results of this experiment were presented at Preconditioning '03.
- Determined that the most trivial trajectory through the space of pseudopotential functions is likely the most effective path to use to initialize the solution of the relevant Schrödinger equation.
- Made improvements to the PHAML code that sped up the solution of Schrödinger's equation by a factor of 50, allowing the solution of a more realistic model of Cesium atoms.
- Extended PHAML to solve coupled systems of equations (i.e. multcomponent solutions), and applied the new code to solve 2-channel Schrödinger equations.
- Extended PHAML to solve partial differential equations on arbitrary polygonal domains, with the help of the freely available grid generation package Triangle. This involved developing a new method to create an initial grid suitable for PHAML from an arbitrary triangulation.
- Extended PHAML to use high order finite elements to obtain more accurate solutions with fewer grid points.
- Extended PHAML to handle periodic boundary conditions.
- Several other minor improvements to PHAML were made, and eight minor releases of the code occured as the code evolved.

In addition, three talks were given at conferences on this topic, two of which were invited lectures, and two papers were accepted for publication in refereed journals.

Future work will continue to enhance PHAML with additional capabilities and robustness, extend PHAML to an hp-adaptive method with adaptivity in the polynomial degree as well as spacial resolution, study multigrid methods for high order finite elements, study error estimators for eigenvalue problems and high order finite elements, improve the robustness of the Schrödinger application code, and extend the application to a multi-channel model with time-dependent systems of equations.

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. SciMark includes computational kernels for FFTs, SOR, Monte Carlo integration, sparse matrix multiply, and dense LU factorization, comprising a representative set of computational styles commonly found in numerical applications. SciMark can be run interactively from Web browsers, or can be downloaded and compiled for stand-alone Java platforms. Full source code is provided, in Java and C programming languages for comparison under different compilers and execution environments. The SciMark result is recorded as megaflop rates for the numerical kernels, as well as an aggregate score for the complete benchmark. The current results database lists over 2,400 submissions form computational platforms ranging from hand-held devices to high-end servers and supercomputers. The reports contains data representing nearly every operating system and Java Virtual Machine (JVM) environment currently in use, including Solaris, FreeBSD, MacOS, Sun OS, IRIX, OSF1, Linux, OS/2, and Windows 95, 98, 2K, ME, NT, XP platforms.

SciMark and its kernel components have become a pseudo-standard in industry and academia. They were adopted by the Java Grande Benchmark Forum, and Sun Microsystems used

SciMark 2.0 to demonstrate the floating-point improvements to their JVM 1.4.2[2]. As of December 2004, the record for SciMark is over 570 Mflops, with some of its kernels, such as LU factorization, running at over 1.2 Gflops. One major area of improvement for JVM implementations was the Monte Carlo kernel, which makes extensive use of synchronized methods. This helped identify synchronization overheads in common JVMs, and as a result the latest implementations show an improvement from single-digit Mflops to over 100 Mflops.

Sparse BLAS Standardization

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

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

MCSD has played a leading role in the standardization effort for the Basic Linear Algebra Subprograms (BLAS) and continues to be a major contributor for the design and development of reference software and documentation. The BLAS are kernels for computational linear algebra subroutines comprising of fundamental matrix/vector operations common to most scientific computing applications. By standardizing such interfaces, computer manufacturers and software vendors can provide high-performance implementations especially suited to a specific hardware platform. By developing their applications in terms of BLAS, computational scientists can achieve high levels of performance and portability. 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. To this, 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) has formed an updated BLAS standard which addresses 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, and NIST was first to develop and release a public domain reference implementation in ANSI C for early versions of the standard, which helped shape the final specification. After the standard was formally approved and accepted, the complete technical specification was published, and a special issue of the ACM Transactions of the Mathematical Software (TOMS) was devoted to the new BLAS standard, including a paper co-authored by R. Pozo and other subcommittee members providing an overview of the sparse matrix interface.

This year saw the public release of an ANSI C reference implementation of the Sparse BLAS (http://math.nist.gov/spblas/SparseBLAS.html) and the development of a new compact C++ implementation that adheres to the reference interface. This new version is quite small, and uses advanced features of ANSI/ISO C++ and key ingredients of object oriented design to provide similar functionality in a small fraction of the lines of code, and a framework that is much easier to extend with user-defined sparse matrix formats. This new design was motivated by integration of the Sparse BLAS with the NIST Template Numerical Toolkit (see below). The TNT interface provides an object oriented framework to support fundamental sparse matrix operations and memory management in application codes, while the reference implementation provides stand-alone code that serves as a testing and validation module for platform-dependent versions of the Sparse BLAS library.

[2] 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

MCSD maintains an active research program in the design of object oriented mathematical software libraries. This work has led to some of the most highly used object oriented linear algebra packages, including Lapack++, Iterative Methods Library (IML++), Sparse Matrix Library (SparseLib++), Matrix/Vector Library (MV++), and the Template Numerical Toolkit (TNT). Together, these packages receive more than 60,000 downloads a year from the NIST web site, not counting numerous mirror sites which also host these codes. This software is currently in use in a variety of industrial and commercial applications.

TNT incorporates many of the ideas explored by R. Pozo and colleagues with previous software designs and advanced features of the ANSI/ISO C++ programming language. The package includes support for both C and Fortran multidimensional array layouts, arrays sections, and application modules, such as linear algebra, which includes fundamental algorithms for matrix decompositions (LU, Cholesky, SVD, QR), eigenvalue problems, and sparse matrix support such as vector scatter/gather operations, and matrix multiplication.

This year, the TNT project saw several public software releases and critical design updates. The latest TNT implementation has a separate interface specification which allows library developers to create specialized modules that take advantage of particular hardware platforms, utilize vendor-specific libraries, or implement different C++ strategies. An important new extension is the support for iterative methods used in the solution of large scale linear systems, including commonly used nonstationary methods such as Conjugate Gradient (CG), Generalized Minimal Residual (GMRES), Quasi-Minimal Residual (QMR), and related variants. 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.

OOF: Finite Element Analysis of Material Microstructures

Stephen Langer
Andrew Reid (Drexel University)
Seung-Ill Haan (UMBC)
Edwin Garcia (Penn State University)
Eric Ma (Montgomery Blair High School)
Edwin Fuller (NIST MSEL)
Craig Carter (MIT)

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

The OOF Project, a collaboration between MCSD, MSEL's Ceramics Division and the Center for Theoretical and Computational Materials Science, and MIT, is developing software tools for analyzing real material microstructure. The microstructure of a material is the (usually) complex ensemble of polycrystalline grains, second phases, cracks, pores, and other features occurring on length scales large compared to atomic sizes. The goal of OOF is to use data from a micrograph of a real material to compute the macroscopic behavior of the material via finite element analysis. OOF is intended to be a general tool, applicable to a wide variety of microstructures in a wide variety of physical situations.

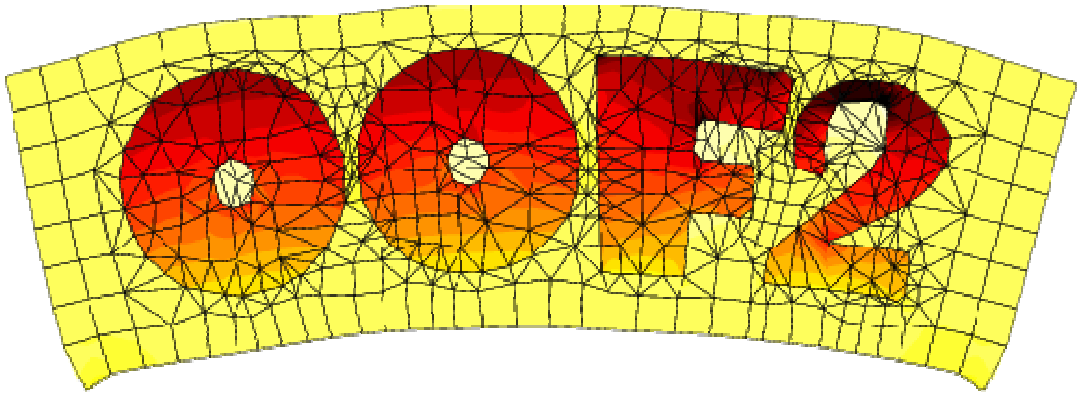
This year saw the first beta release of OOF2. OOF2 is a completely new version of the program, designed to be much more powerful and flexible than the original. The first release of OOF2 solved linear elasticity and thermal conductivity problems, like OOF1, but can easily be

extended to a wide variety of other physical problems, such as chemical diffusion and reactions, and piezoelectricity.

Most of the effort this fiscal year centered on the large number of features, bug fixes, and optimizations required to get OOF2 ready for release. These included improvements to the contour plotting code, better methods for defining graphical outputs, better tools for examining solutions, more compact data file formats. The program is now threaded, so it can perform multiple simultaneous tasks with the user interface remaining sensitive during CPU-intensive computations.

OOF2 can automatically create documentation of its command set. The OOF2 developers are working with the MatCASE (Materials Computation and Simulation Environment) project at Penn State University to create a suite of tools to simulate materials on all length scales, from microscopic quantum mechanical to macroscopic effective property calculations. OOF2 will perform the macroscopic calculations. Automatic generation of the API documentation facilitates the integration of OOF2 into the MatCASE environment. The documentation is written in XML so that it can also be converted into both on-line and printed manuals.

Eric Ma, a student in the Math and Science Magnet Program at Montgomery Blair High School, spent his second summer developing OOF code at NIST. He is working on techniques to detect grain boundaries in images of polycrystalline materials. These grain boundaries can be easy for humans to see but very difficult for a program to detect. If OOF2 can automatically detect grain boundaries, then it will be much easier for a user to assign material properties to individual grains. Eric has adapted and merged several edge detection algorithms from the image processing literature to form a promising new technique for finding boundaries in micrographs.



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

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

Jeffrey Fong
Barry Bernstein
Ronald Boisvert
Dan Lozier
Geoffrey McFadden.
James Filliben (ITL SED)
Hung-kung Liu (ITL SED)
Nell Sedransk.(ITL SED)
Terri McAllister (NIST BFRL)
Emil Simiu (NIST BFRL)
Howard Baum (NIST BFRL)
Kuldeep Prasad (NIST BFRL)
Ronald Rehm (NIST BFRL)
Roland deWit (NIST MSEL)
Richard Fields (NIST MSEL)

Beginning in Feb. 2004, researchers from MCSD (Fong and McFadden), ITL Statistical Engineering Division (James Filliben), and BFRL (Howard Baum, Terri McAllister, Kuldeep Prasad, and Emil Simiu) have been working together on a five-year Competence Project entitled *Complex System Failure Analysis: A Computational Science Based Approach.* The objective of the project is to create the scientific basis for building failure investigation procedures that (1) will allow NIST to accomplish its mission under the National Construction Safety Team Act (P.L. 107-231, Oct. 1, 2002), and (2) is likely, over time, to be applicable for failure analysis and uncertainty determination of a broad range of complex physical, chemical, biological, and engineered systems of interest throughout NIST.

Since the physics of structural failure due to fire and other extreme loadings involves complex models and multi-physics simulations based on an incomplete knowledge of the governing equations and a strong variability in material properties, geometric dimensions, joint characteristics, and loading spectra, one of the first questions to address is to find a rational basis for the verification and validation of computational models of complex engineering systems. On Nov. 8-9, 2004, a workshop co-sponsored by NIST and DOD was held to address this important question. Two MCSD working documents containing preprints of 41 papers and 25 discussions were distributed to 50 attendees of the workshop. The attendees represented such organizations as Applied Research Associates (Littleton, CO), Auburn University, DOD Defense Modeling & Simulation Office, Lawrence Livermore National Laboratory, MIT, NSF, Oak Ridge National Laboratory, Sandia National Laboratory, Southwest Research Institute, SRI International Inc., Stanford University, Texas A&M University, University of Cincinnati, University of Houston, University of Iowa, and XYZ Scientific Applications (Livermore, CA). The workshop provided MCSD with valuable input regarding its potential role in the growing Verification and Validation community.

Fortran 90 Version of ODRPACK Used in Package StatistiCAL

Abbie O'Gallagher
D. Williams (NIST EEEL)

Abbie O'Gallagher and D. Williams of EEEL have developed a special version of an unreleased, Fortran 90 version of ODRPACK, a package for orthogonal distance regression originally developed by MCSD staff in the 1990s. The work was in response to a problem that arose when Williams interfaced a DLL containing the Fortran 90 version of ODRPACK with StatistiCAL, a network analysis package that he has developed. A version suitable for a desired Visual Basic code is currently under development.

High Performance Computing and Visualization

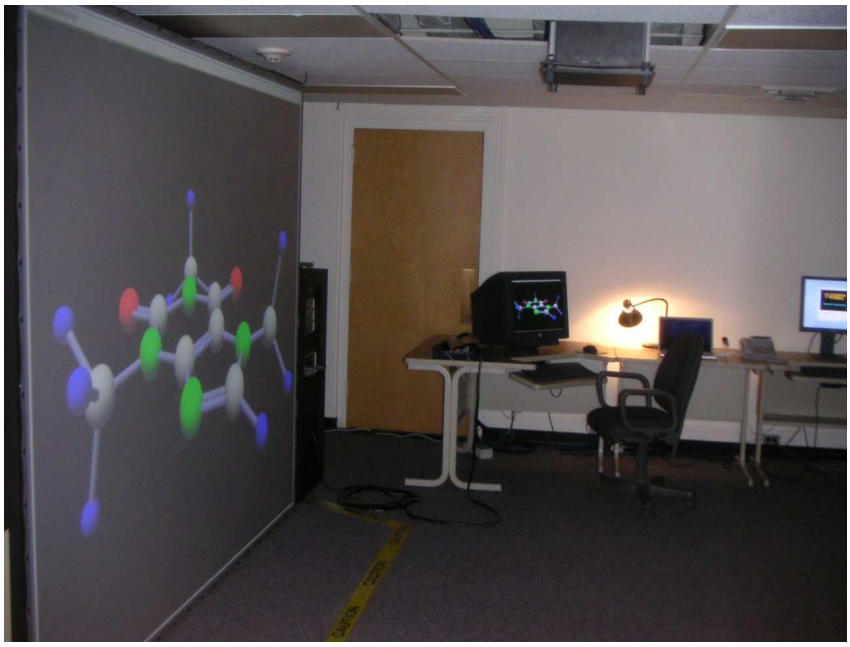
Research and Development in Visual Analysis

Judith Devaney
Terrence Griffin
John Hagedorn
Howard Hung
John Kelso
Adele Peskin
Steve Satterfield

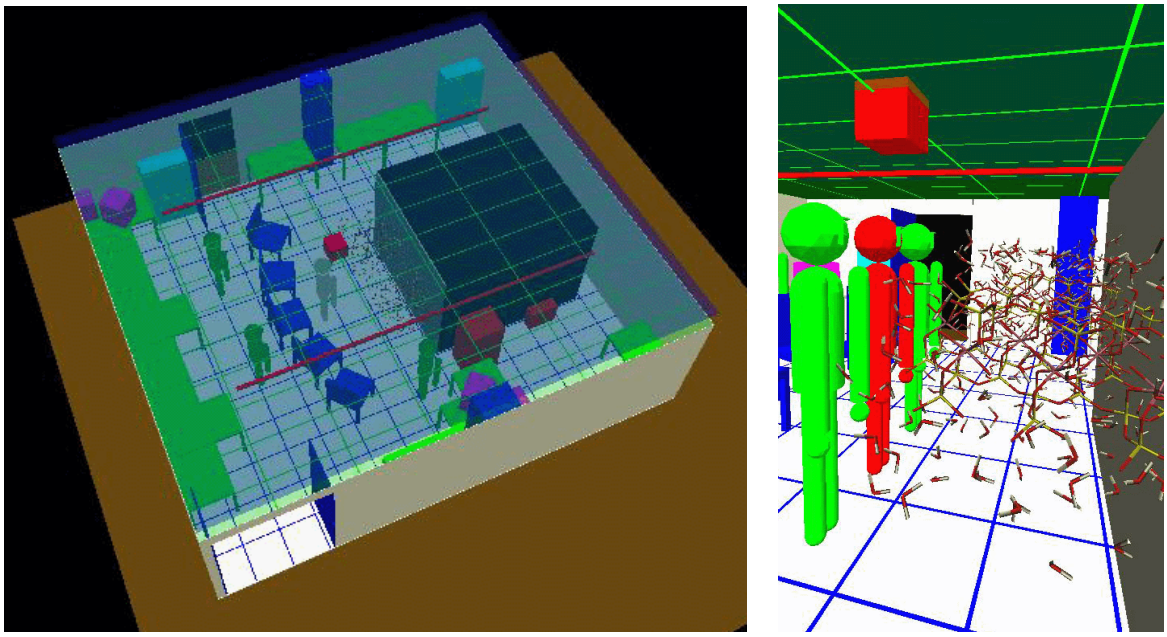
Computational and laboratory experiments are generating increasing amounts of scientific data. Often, the complexity of the data makes it difficult to devise *a priori* methods for its analysis, or the data is from new landscapes, such as the nano-world, where we have little experience. Moreover, there may be ancillary data, from databases for example, that would be helpful to have available. We are developing visual analysis capabilities in an immersive environment that allow NIST scientists to interact with data objects in a three-dimensional landscape rather than simply viewing pictures of them. With 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.

Immersive Visualization Environment

The center of our visual analysis system is an immersive visualization environment. This environment is distributed and has software components and hardware components. A major goal of the project is to keep up with advances in hardware while insulating the scientists from these changes. The hardware for visualization is moving towards commodity cards and processors. We track these changes and update our environment at a pace that does not interfere with our ability to perform visual analysis on scientific data. A major accomplishment this year was the installation of an immersive environment at NIST Boulder, driven by an SGI with commodity graphics cards.



Boulder Immersive Environment



Top view (left) and side view (right) of mock up of Boulder immersive visualization facility.

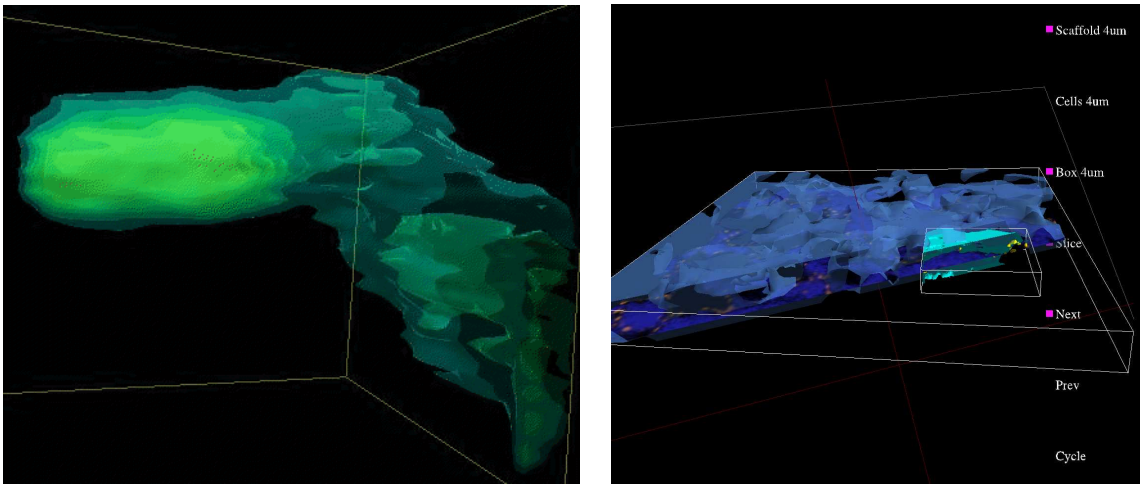
Another goal is to allow scientists to preview their data on their desktop with a Linux machine. These machines would be kept in sync with our primary environment. This year we have placed one machine on the desk of Nick Martys (BFRL) in support of the VCCTL project.

Visual Analysis Software (http://math.nist.gov/mcsd/savg/software)

Our software includes methods to get data into the immersive environment, methods to represent the data, and methods to interact with the data and the underlying computational environment. We analyze both the output of computational experiments as well as laboratory experiments. Following are some highlights of our accomplishments this year.

SAVG FileFormat. We have defined a file format and written an immersive visualization loader to input results of specific analyses we create directly, as well as to facilitate displaying of results we create with specialized packages. This file format is ASCII based. It describes geometric primitives including tri-strips, polygons, line segments, points, color, transparency, surface normals, and other rendering properties. The input file format is extensible and application independent, and will allow many applications to easily generate efficiently displayable data. We have written an OpenDX to SAVG converter and Kitware has written a program to output this format from VTK, their visualization toolkit. Kitware will include this in their next release. We have also written a toolbox that creates objects in this format and that contains tools for coloring, scaling, translating these objects. We have released the format and loader.

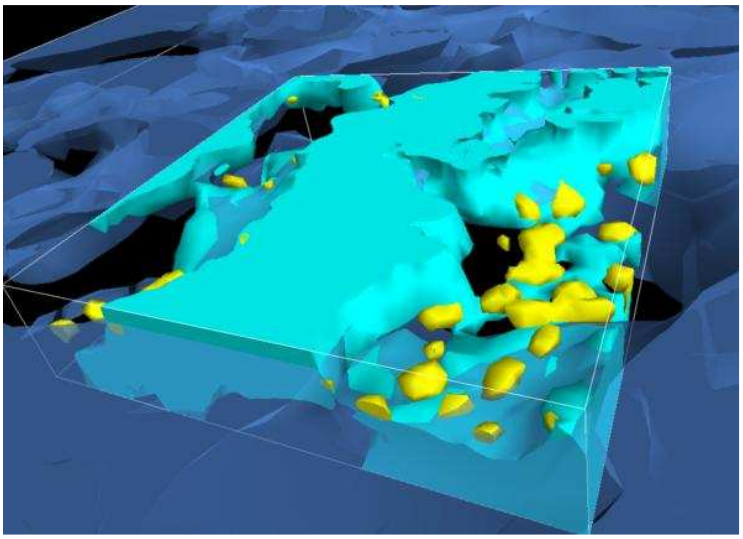
Transparency. We have created a nested transparent surface viewer for viewing of dense volumetric data in the RAVE. This viewer layers the colors for maximum view depth. The SAVG loader was written to display transparency with arbitrary nestings. The visualization of transparency is complex because what one sees depends on the sequence of transparent objects that intersect with the viewer's line of site. This sequence must be combined correctly to show the correct color to the viewer. There are efficiency issues as well. See figure below for an application.



Left: Bayesian reconstructions of a circuit with an electromigration void showing nested transparent isosurfaces. *Right:* A portion of the immersive display showing several features of the system (interactive menus, 2D cross-sections, interactive clipping plane, and transparency).

Clipping Planes. Many datasets are three dimensional dense datasets. Being able to see into them easily is a priority. We have created a set of interactive clipping planes that enable the user to prune away any data between them and the plane. This can also be a clipping box where all but the data in the box is made invisible. At the extreme of a very narrow box, the result is a three dimensional contour plane. The figure above (right) is an example with the tissue engineering data set.

Segmentation and Registration. We have incorporated the capability to perform segmentation and registration on data to derive additional representations. For example, we used level set segmentation to derive surfaces for the tissue engineering project. See the figure below.



Polymer and cell surfaces derived from segmentation of the tissue engineering project data using level sets. The blue is the polymer scaffold with the darker blue scanned at a higher resolution than the light blue. The yellow depicts the cells. The primary laboratory data is noisy, but the level set segmentation method produces a scientifically meaningful segmentation.

Navigation Through Differing Scales. In an immersive environment, the size of the objects in the virtual space relative to the scientist interacting with the objects becomes significant. For example, in the tissue engineering and cement fibers datasets, when data from both scales of the data are displayed simultaneously, some of the data was either too small to see properly or some was too large to see properly. The most important issue was the navigation through the differing scales of the data. We solved this by implementing a method for interactively changing the size of the data in the immersive environment in a continuous fashion. This enables the user to make small features large for detailed inspection or to make large volumes smaller to enable overviews of the data.

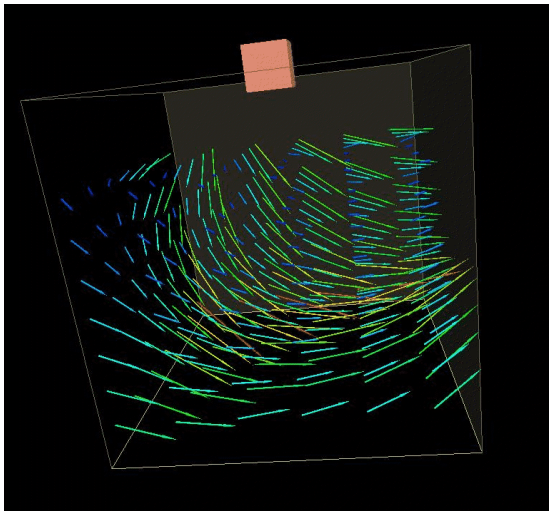
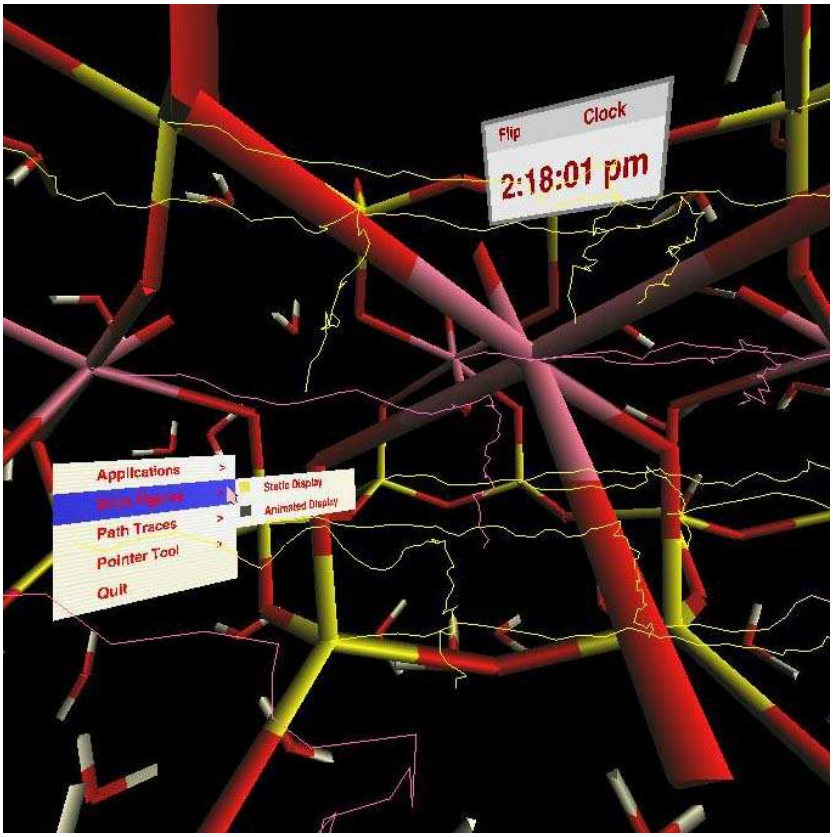


Image from tracker calibration project. Arrows show magnitude and direction of errors.

Tracker Calibration. Virtual reality environments need a method of referencing where a user is positioned, so that the images projected are centered on the viewer's perspective. This is accomplished by using a tracking system. The electromagnetic tracking system is the most widely used today, but it is not without flaws. The idea behind tracking is very simple. Through the use of sensors, the position and orientation of a user is sent to the tracking mechanism. The problem is that when the coordinates are transmitted to the receiver, they are not precisely accurate, resulting in a distorted image projected to the user. This distortion is due to the sensitivity of the electromagnetic tracking system to metal objects. By calibrating the tracking system, the distortion is compensated by assigning a known value to offset the abnormality in transmission. The quadratic Shepard method for trivariate interpolation of scattered data was used on points sampled from the space. This algorithm enables the interpolation of a single-valued function on points in three dimensional spaces. Three separate interpolations were needed to derive corrected values for the X, Y, and Z coordinates.

Technology Insertion. In order to spur commercial development of immersive visualization tools, we developed a solicitation entitled *Device Independent Interaction Framework for Immersive Scientific Visualization* for the FY 2004 NIST Small Business Innovative Research (SBIR) program. A company named Open Tech of Blacksburg, VA submitted a winning proposal. They will be developing tools that enable scientists to select computer hardware devices and interaction techniques that are most appropriate to their investigation, without necessitating modifications to their software to manage the particular devices, platform, and configuration selected. We have received a first delivery of menuing software for the immersive environment from Open Tech. Their interface works on the desktop as well as in the immersive environment. The windows are centered on the user's head and provide a natural method of interaction that includes response to gestures. The figure below provides an example.



This figure demonstrates the OpenTech VEWL menuing system based on the OpenGL Polygon Based menu for the smart gel data.

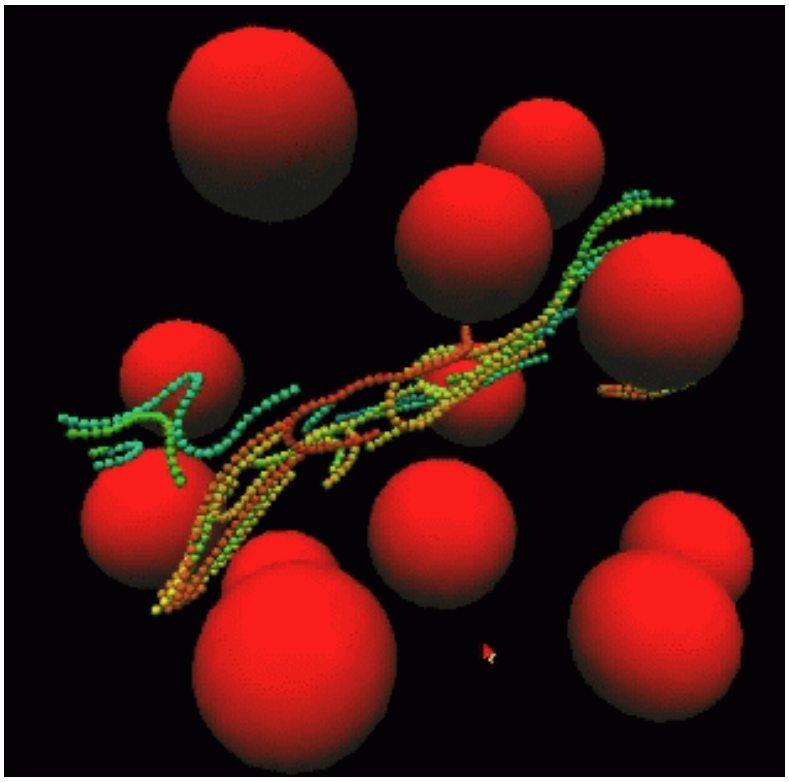
Virtual Cement and Concrete Testing Laboratory (VCCTL)

Judith Devaney
William George
Terence Griffin
John Hagedorn
Howard Hung
Steve Satterfield
James Sims
Clarissa Ferraris (NIST BFRL)
Edward Garboczi (NIST BFRL)
Nicos Martys (NIST BFRL)

The NIST Building and Fire Research Laboratory (BFRL) does experimental and computational research in cement and concrete. Recently, MCSD has been collaborating with BFRL in the parallelization of their codes and in creating visualizations of their data. In January 2001 the Virtual Cement and Concrete Testing Laboratory (VCCTL) Consortium was formed. MCSD assisted in this effort through presentations of our work with BFRL and demonstrations of visualizations in our immersive environment. The consortium consists of NIST (BFRL and ITL) and nine industrial members: Cemex Trademarks Worldwide, Ltd., Holcim (US) Inc., Master Builders Technologies, National Ready Mixed Concrete Association, Association Technique l'Industrie des Liant Hydrauliques (ATILH), International Center for Aggregate Research (ICAR), W.R. Grace, Sika Technology AG, and Portland Cement Association. The overall goals of the consortium are to develop a virtual testing system to reduce the amount of physical concrete testing, and to expedite the

research and development process. This will result in substantial time and cost savings to the concrete construction industry as a whole. MCSD continues to contribute to the VCCTL through collaborative projects involving parallelizing and running codes, creating visualizations, as well as presentations to the VCCTL current and prospective members. For example, in November 2003, J. Devaney made a presentation to the VCCTL entitled *Cement and Concrete: Parallel Computing, Scientific and Information Visualization*, and in November 2004 a presentation entitled *Automatic Labeling with Machine Learning*. The following projects are included in this effort.

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



S. Satterfield worked with N. Martys (NIST BFRL) to create an immersive visualization showing the results of a dynamic simulation of concrete flow with fibers.

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

Omelayan (hence the Q in QDPD). 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 W. George, in collaboration with N. Martys of BFRL, completed a major modification to the QDPD application, consisting of re-write of the inner-most computational core to add a second level of parallelization on top of the higher-level MPI based message-passing parallelism. A simplification to the MPI level of parallelism is also being considered as a result of this modification. This effort is intended to expand the capabilities of this application in order to scale it from the current 10s of processors up to an application that will run on 1000s of processors. This will allow for the simulation of much larger systems as well as the inclusion of additional physics to the computation. This second level of parallelism has added multi-threading to the main computation in the inner-most loops of the algorithm. This change has been made to take better advantage of the hybrid architecture of current parallel machines, such as the IBM-SP, that consist of 10s to 100s of SMP nodes each of which consists of 2-16 CPUs.

For initial development and testing, J. Devaney and W. George have obtained user accounts at NERSC (National Energy Research Scientific Computing Center, Lawrence Berkeley National Laboratory), and have obtained a small allocation of 2000 CPU hours on the NERSC parallel machine Seaborg, a 6080 CPU IBM SP RS/6000 (380 16-CPU nodes). This account has been used to further develop this QDPD application and to compare the performance of the new multi-level parallel version with the pure MPI version.

In addition to the work on the IBM SP, we have performed a series of benchmark tests of the new multi-level parallel QDPD application on an 8-CPU SGI. The results so for, after some code tuning, show no performance improvement of the multi-level version of QDPD over the pure MPI version given the same number of CPUs. This is true regardless of the ratio of MPI processes to threads used. In all cases the pure MPI version of QDPD outperforms the multi-level parallel version. If similar results are obtained on the distributed memory IBM SP this direction of algorithm development will be changed.

Immersive Visualization of Concrete Aggregate Flow. In support of the VCCTL, X-ray tomography has been used to create a database of aggregates spanning about four decades in size. Examples include cement particles, sand and, even, rocks. These realistic aggregate shapes can be incorporated into codes used to model the rheological properties of cement based materials. The purpose of this project is to develop techniques to display flows of multiple types of aggregate in an immersive visualization environment.

T. Griffin is developing a visualization of aggregate directly from the database to insure that the visualization and the codes reference the same aggregate particles. This will run directly on a Linux laptop or in the immersive environment. While the visualization references the same aggregate, it can be shown with differing levels of realism.

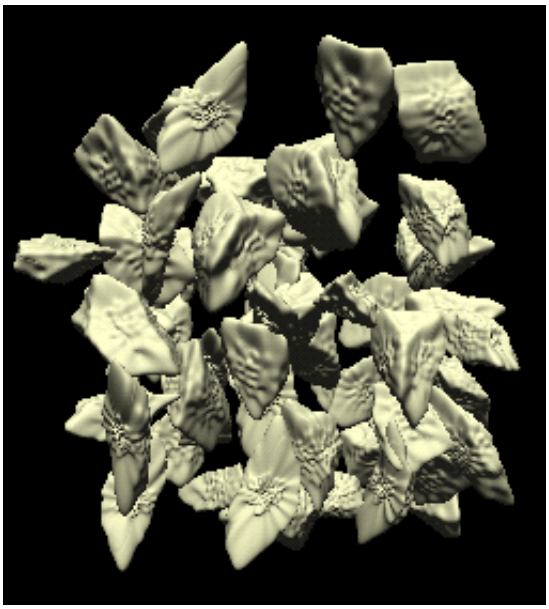


Image of modeled actual aggregate in a shear flow.

Parallelization of Fluid Flow in Complex Geometries. The flow of fluids in complex geometries plays an important role in many environmental and technological processes. Examples include oil recovery, the spread of hazardous wastes in soils, the processing of polymer blends, droplet breakup, phase separation and chemical analysis in confined geometries, and the service life of building materials. The latter two applications are of particular concern for our NIST collaborators in BFRL. The detailed simulation of such transport phenomena in varying geometries and subject to varying environmental conditions or saturation, is a great challenge because of the difficulty of modeling fluid flow in random pore geometries and the proper accounting of the interfacial boundary conditions. In order to model realistic systems, BFRL has developed a lattice Boltzmann (LB) algorithm that simulates multiple fluids, various forces, and wetting characteristics within arbitrary geometries. We have parallelized this algorithm using MPI to enable the study of large systems.

This year the code was extensively exercised in a study leading to the following paper: J. Hagedorn, N. Martys, and J. Douglas, "Breakup of a Fluid Thread in a Confined Geometry: Droplet-Plug Transition, Perturbation Sensitivity, and Kinetic Stabilization with Confinement," *Physical Review E* **69** (5) (2004). J. Hagedorn is currently collaborating with N. Martys on modeling the permeability of two 3D images of paper provided by the Avery Dennison Corporation.

Visualization of Smart Gels

Steve Satterfield
Carlos Gonzalez (NIST CSTL)

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

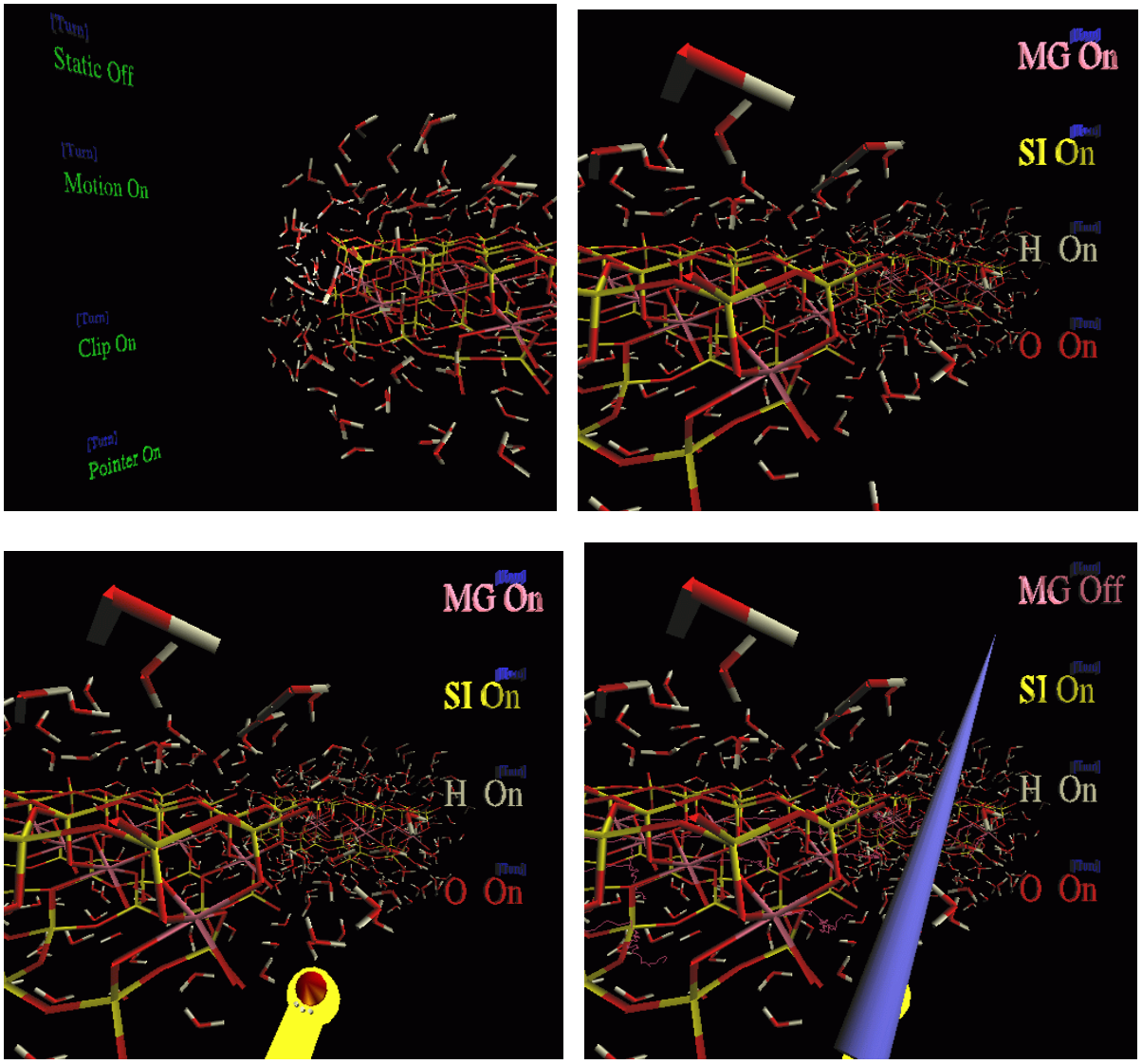
A smart gel is a material that gels in response to a specific physical property. For example, it may gel at a specific temperature or pressure. The mechanisms that create a gel in response to given stimula are not well understood. Developing this understanding is the key to being able to create materials that gel under precise control. The potential for applications of smart gels is enormous. For example, they could be useful in applications such as an artificial pancreas that releases insulin inside the body in response to high sugar level. Smart gels might someday be used to make exotic foods, cosmetics, medicines, and sensors.

The NIST team is studying a subclass of these materials called shake gels. Through some complex and as yet unknown process, these watery mixtures of clays and polymers firm up into gels when shaken, and then relax again to the liquid phase after some time has passed. A shake gel might be used, for example, in shock absorbers for cars. The material would generally be a liquid but would form a gel when the car drove over a pothole; the gel thickness would adjust automatically to the weight of the car and the size of the pothole. A more esoteric application might be the formation of gelled areas within a liquid where holograms could be created using a laser.

Working with our collaborators in CSTL, we have created a dynamic immersive visualization of the results of a molecular level computational simulation of shake gel formation. This visualization provided NIST scientists with unprecedented insight into the processes controlling the formation of shake gels. This work received wide notoriety during the last year, including the following, each of which described Smart Gel work of Carlos Gonzalez and immersive visualization of S. Satterfield. Film reports were done in the MCSD RAVE immersive visualization lab.

- Segment in opening video of the SC 2003 Conference, November, 2003, Phoenix, AZ.
- News report on local Fox Network affiliate (Channel 5) on October 30, 2003
- *Design News* article in their October 20, 2003 issue.

- A segment of the science series NEXT@CNN that aired on CNN on Saturday January 3. J. Devaney and S. Satterfield were both interviewed. An associated article was posted on the CNN site[3].
- *HPCWIRE* article (106741) in their January 9, 2004 issue.



Four images of the shake gel visualization illustrating menu controls and pointing devices which have been developed by MCSD to enable interactive exploration of the data.

[3] http://www.cnn.com/2004/TECH/science/01/02/coolsc.visualization/index.html

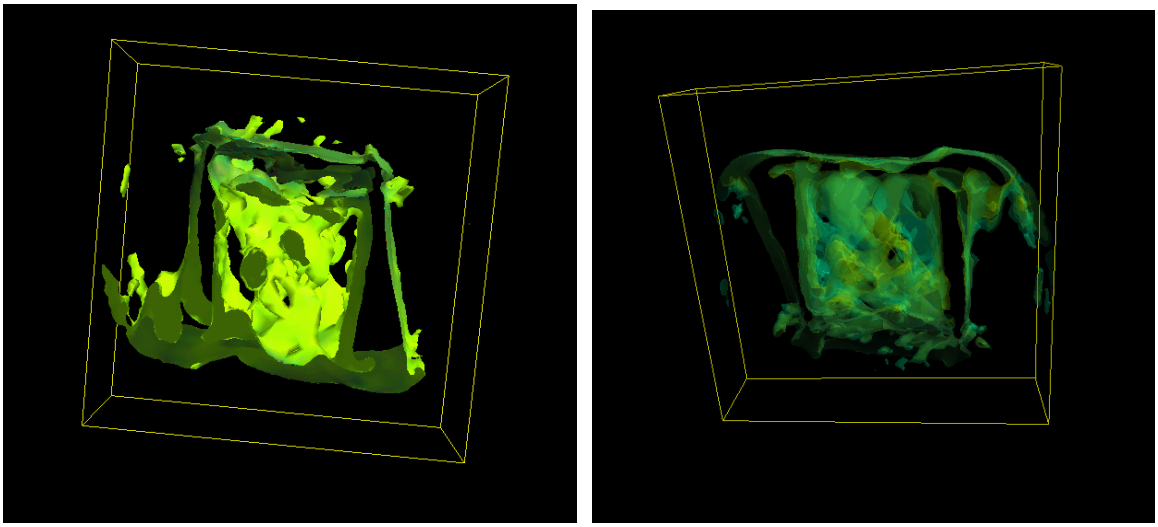
3D Chemical Imaging at the Nanoscale

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

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

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

- Techniques for the interactive visualization of 3D isosurfaces in an immersive environment
- Segmentation techniques for 3D datasets
- Standardization of file formats



Visualizations of reconstructed tomographic data of a photonic crystal sample. This is a photonic band gap material, approximately 3 micrometers across. An artificially periodic crystal was created by exposing photoresist to four laser beams. The sample was sectioned with a focused ion beam, than a tilt series of 76 views was obtained using a transmission electron microscope. The views were aligned to five fiducial markers, than reconstructed using a Bayesian algorithm. The reconstruction was Fourier filtered. *Left:* the structure is represented as an opaque surface approximating the surface of the structure. *Right:* the structure is represented with two transparent surfaces in order to reveal additional internal detail in the data.

In addition, W. George has designed an architecture and API for a 3D Chemical Imaging service. This architecture is client/server based using Jini (a Java based distributed computing infrastructure) to link a client application on the user's workstation to a compute server on a parallel machine. A parallel Monte Carlo Simulator, probably in Fortran/MPI, will be the main computation. Other applications will be needed to prepare the input and post-process the output from this simulator. The computation will run on an MCSD multiprocessor SGI system using semi-dedicated CPUs.

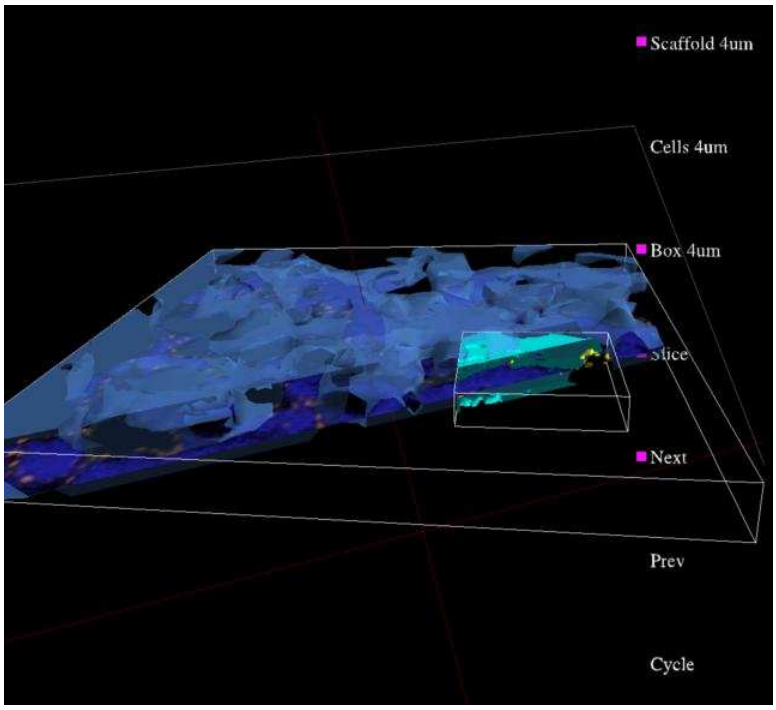
This project is sponsored by the NIST Competence Program.

Multi-Modal Imaging and Visualization for Integrating Functional and Structural Information

John Hagedorn
Steven Satterfield
John Kelso
Adele Peskin
Judith Devaney
Joy Dunkers (NIST MSEL)
Marcus Cicerone (NIST MSEL)
Lyle Levine (NIST MSEL)
Gabrielle Long (NIST MSEL)

We can no longer advance material science simply by studying model systems that are idealized in dimension and function. We must comprehend realistic, complex, three-dimensional systems in terms of their structure, function, and dynamics over a broad scale from nanometers to millimeters. In this collaboration with the NIST Materials Science and Engineering Lab, which is sponsored by the NIST ATP program, we are combining data from different measurement devices that reflect both functional and structural information. The multiple data sets taken from a single sample are then combined and visualized in our interactive, immersive, virtual reality environment in order to gain new insights into the physics and materials science of complex systems.

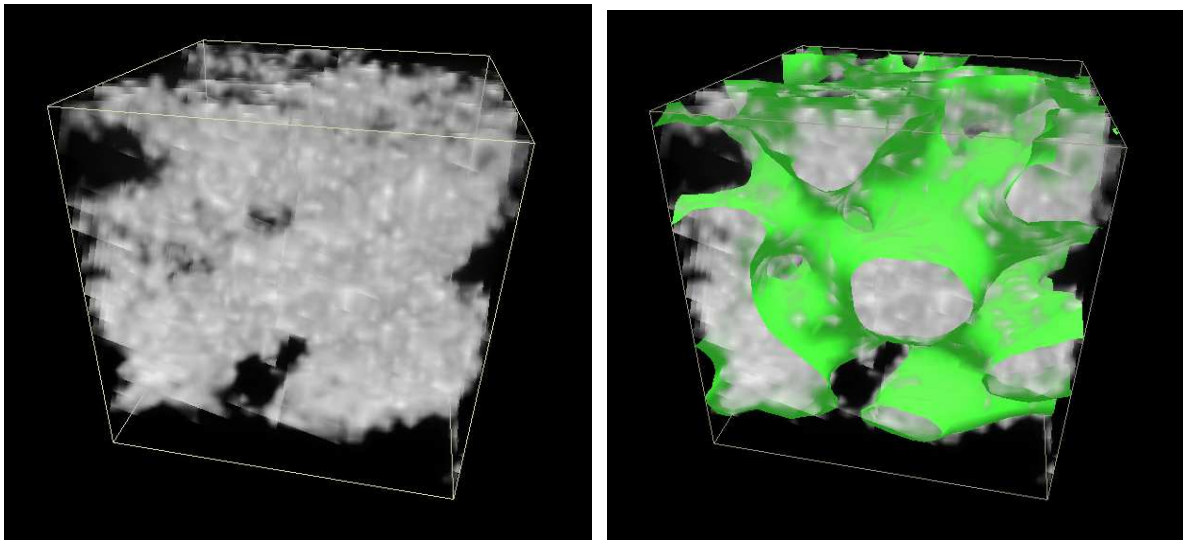
Our collaborators are gathering measured data using a variety of techniques, including optical coherence tomography (OCM) and confocal fluorescence (CFM) imaging. When data from these different devices is combined in a manner that is visually apparent, unprecedented insight towards the comprehension of complex relationships among large amounts of correlated data can be obtained. These methods have applications to the characterization of biomaterials, the failure analysis of polymer composites, and the reliability of semiconductor devices. In this project we are concentrating on an application in tissue engineering. The system being imaged is that of cells growing on polymer scaffoldings.



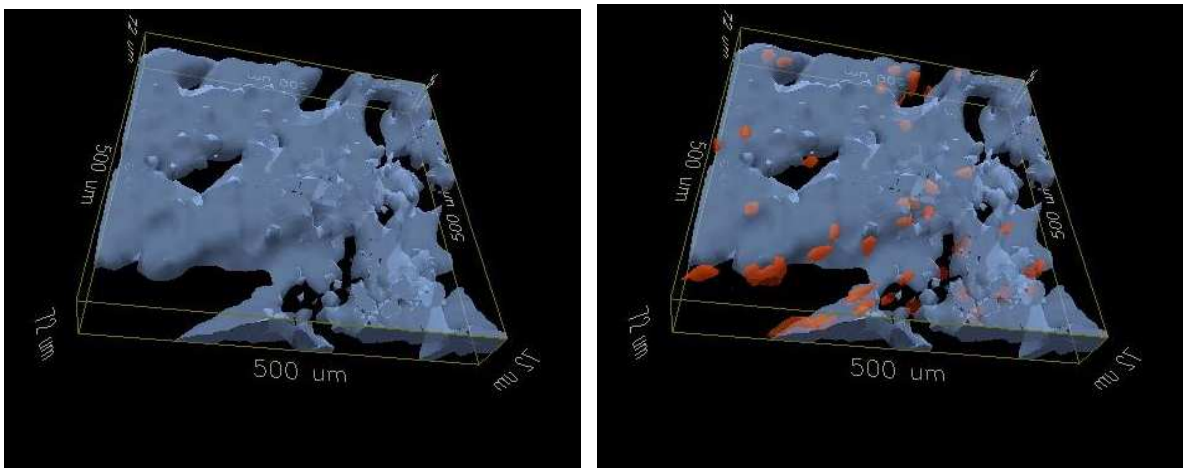
A portion of the immersive display showing several features of the system: interactive menus, 2D cross-sections, interactive clipping plane, and transparency.

Visual analysis of data of this type presents a variety of challenges. The data is three-dimensional. Separate noisy data sets from different instruments must be cleaned, combined, and registered. Data of different resolutions must be combined for use in a single visualization. Complex porous surfaces within the volume must be identified. Interactive volume-rendering techniques, surface-rendering techniques, and combined volume/surface-rendering techniques must be available. We have developed a flexible framework that supports such complex visual analysis of combined CFM and OCM data in our immersive environment. Our display makes use of transparency, lighting effects, simultaneous viewing of 2D and 3D data, annotation, clipping, and menus. The figures below illustrate a variety of these features.

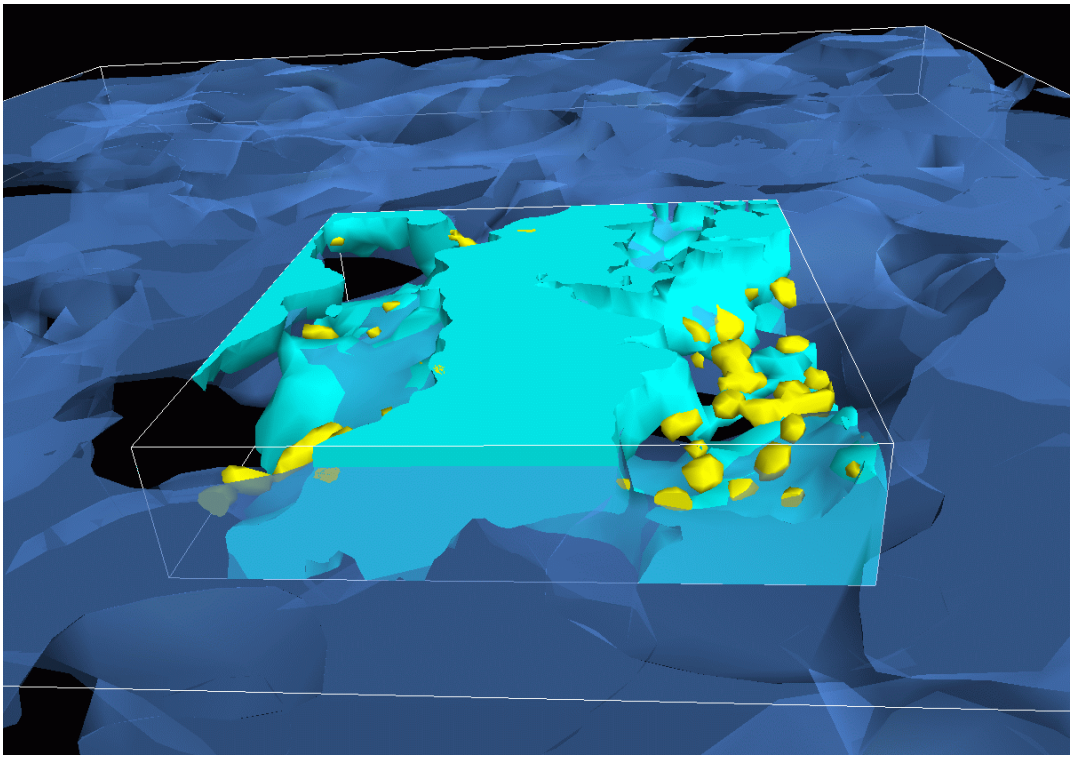
This project is sponsored by the NIST Advanced Technology Program.



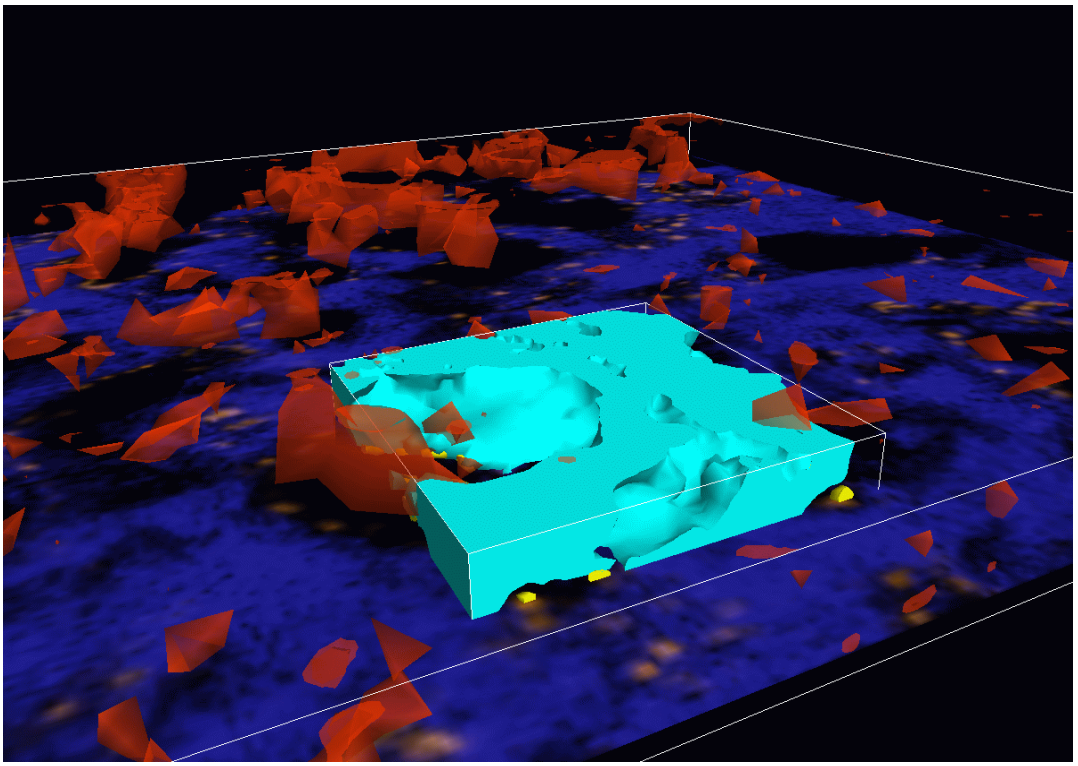
Left: Volume visualization of scaffolding. *Right:* A segmentation of the scaffolding from the pore space. Both are directly viewable in the RAVE.



Left: The surface of the scaffolding as a transparent surface. *Right:* Cells (in red) are shown growing on the scaffolding. This is a fusion of data from two separate instruments. It is directly viewable in the RAVE as scaffolding only, cells only, or scaffolding and cells.



High resolution (opaque blue) scan of polymer scaffolding with high resolution scan of cells (yellow) combined with lower resolution scan (transparent blue) of polymer scaffolding

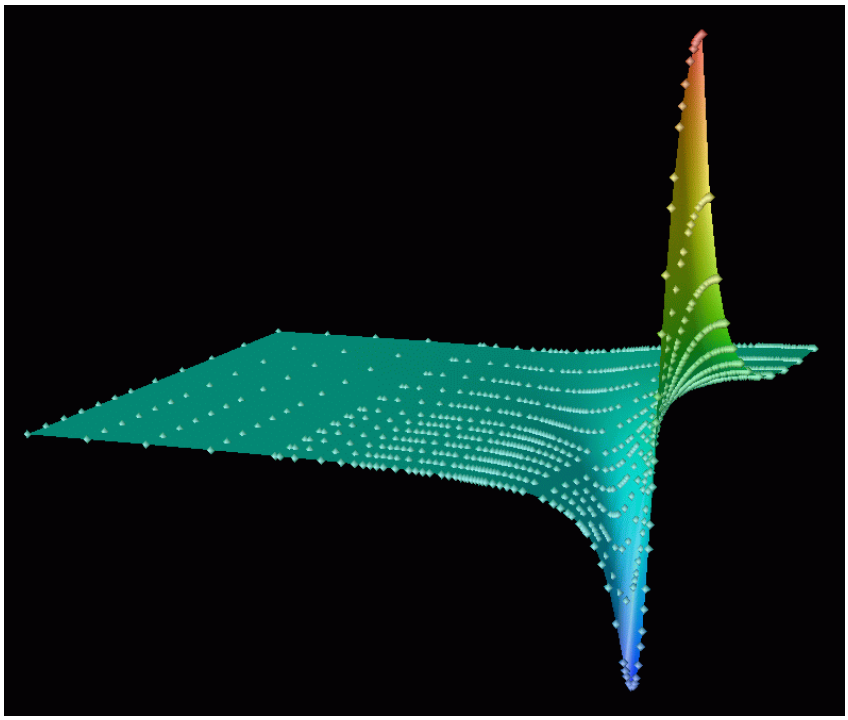


High resolution (opaque blue) polymer scaffolding with cells (yellow) scans combined with cross section of lower resolution scans of polymer scaffolding (dark blue) and cells (red)

Physics Models for Transport in Compound Semiconductors

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

Physics models for carrier transport in semiconductors are essential inputs of computer programs that simulate the behavior of micoelectronic and optoelectronic devices. Such simulations increase understanding, reduce times-to market, and assist in making selections from among competing or alternative technologies. As devices shrink in size to nanometers, performing experimental measurements becomes more costly and time-consuming. This means that computer simulations will become more essential for advances in future nanotechnologies. Unlike many physics models that are based on using variations in parameters to fit experimental data, the NIST physics models developed in this project are based on quantum mechanical calculations with no fitting parameters to account for dopant ion effects and many-body physics effects.



This figure summarizes the computed theoretical calculations of the real part of the complex electric susceptibility for n-type GaAs with a dopant density of 10^{18}cm^{-3} and at a temperature of 300K.

The calculations include many body quantum effects and bandgap narrowing due to dopant ion carrier interactions. The many body quantum effects treat both electron-electron and electron-hole interactions. The results are unique because all other reported treatments for the electric susceptibility 1) do not treat these effects self-consistently; 2) are Taylor series expansions in either (Q/A) or (A/Q), where Q is the magnitude of the normalized wave vector and A is the normalized frequency used in such measurement methods as Raman spectroscopy; and 3) do not give the structure shown in the figure below. These results will change the way researchers and process engineers interpret non-destructive measurements to extract the carrier concentrations of GaAs wafers. The wafer carrier concentration is a key figure of merit associated with a go-no-go decision for determining whether a wafer meets specifications and should undergo further processing.

We are collaborating with EEEL to develop efficient computational methods for this problem, and to develop evocative displays of the results in our immersive environment. In particular, H. Hung has worked with H. Bennett of EEEL to develop new Fortran subroutines to evaluate Lindhard electric susceptibility integrals with singular integrands. They calculated the electric susceptibility for GaAs as a function of frequency for given reciprocal wave vectors at 300K

in n-type GaAs with a dopant density of 10^{18} cm^{-3}. These results will be used by CSTL to develop an algorithm for non-destructively determining the carrier density of GaAs wafers from Raman measurements. Displays of the results were developed using Dataplot, IDL, and OpenDX T. Griffin created an OpenDX viewer for the 3D output which was then converted to a format readable by DIVERSE and the results viewed in the RAVE immersive environment.

Computation and Visualization of Nano-structures and Nano-optics

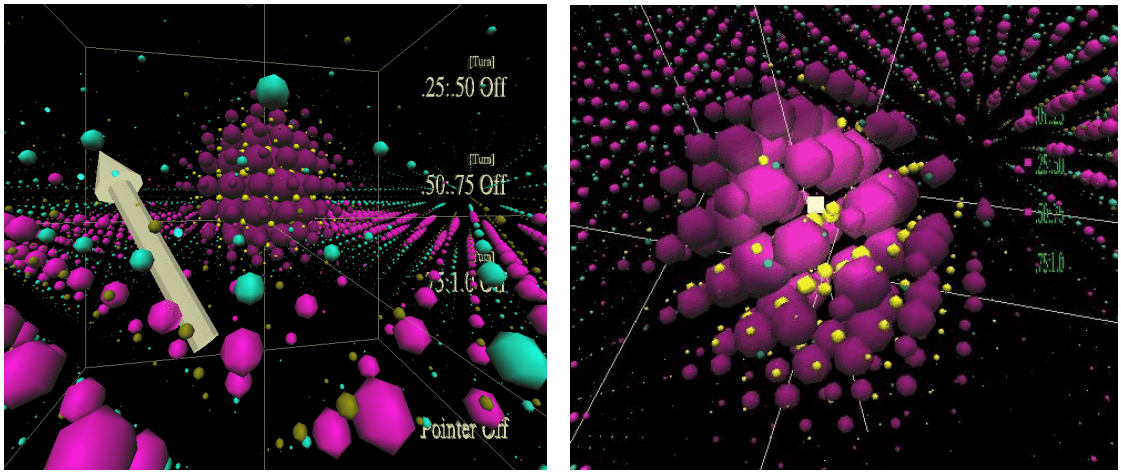
James Sims
John Hagedorn
Howard Hung
John Kelso
Steve Satterfield
Adele Peskin
Garnett Bryant (NIST PL)

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

Accurate atomic-scale quantum theory of nanostructures and nanosystems fabricated from nanostructures enables precision metrology of these nanosystems and provides the predictive precision modeling tools needed for engineering these systems for applications including advanced semiconductor lasers and detectors, single photon sources and detectors, biosensors, and nanoarchitectures for quantum coherent technologies such as quantum computing. Theory and modeling of nanoscale and near-field optics is essential for the realization and exploitation of nanoscale resolution in near-field optical microscopy and for the development of nanotechnologies that utilize optics on the size-scale of the system. Applications include quantum dot arrays and quantum computers. Atomic-scale theory and modeling of quantum nanostructures, including quantum dots, quantum wires, quantum-dot arrays, biomolecules, and molecular electronics, is necessary to understand the electronic and optical properties of quantum nanostructures and nanosystems fabricated from component nanostructures.

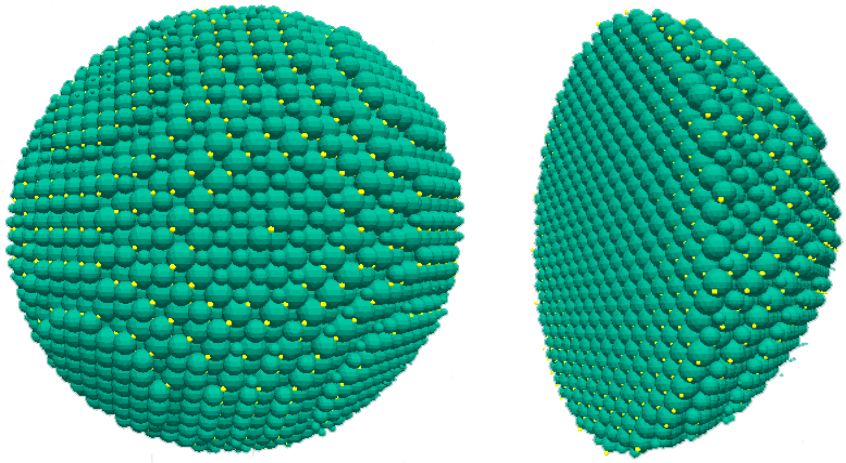
We are working with the NIST Physics Lab to develop computationally efficient large-scale simulations of such nanostructures. We are also working to develop immersive visualization techniques and tools to enable analysis of highly complex computational results. Among the accomplishments of the past year are the following.

- J. Sims completed and benchmarked a parallelization of the simulation code across one dimension. The code shows a speedup of 27 on 41 processors of our Linux cluster. On a 96 processor SGI it shows a speedup about twice as fast as a 32 processor run, so the code is scaling well up to the limit of the 1D treatment (around 60+ processors).
- J. Sims also completed a second parallelization effort that includes spin-orbit interaction, which introduces complex arithmetic and hence is even more in need of parallelization. The complex version of PARPACK is being used in this effort (some bugs in PARPACK were discovered in the process). J. Sims and H. Hung will be co-authors with G. Bryant on a talk on this to be given at the March American Physical Society meeting. This work required parallelization for size as well as speed, with matrices spread among processors. The latest runs are diagonalizations of 3.7 million by 3.7 million matrices.
- H. Hung, S. Satterfield, J. Hagedorn, J. Kelso, and A. Peskin and have developed visualizations of the atomic structure of lattices of electrons. The display of s-electron orbitals has been made. Data sets with of up to 377,777 atoms have been successfully processed and displayed in the RAVE.



Left: Visualization of s-orbitals of a pyramidal structure. *Right:* visualization of a quantum dot.

- J. Kelso investigated how to most efficiently display large numbers of these objects, including techniques such as billboarding, small-feature culling, level of detail and image based rendering.
- J. Sims has begun work on the next major step the computational part of the project, i.e., calculations on arrays of nanoparticles. The basic idea is to consider each nanoparticle as part of its own cluster, using the same input data as now, but as the computation proceeds information from neighboring atoms in each cluster has to be distributed to the appropriate processor in neighboring clusters, thereby "stiching" the calculations on the clusters in the array together. This involves using some of the communication facilities of the previous code, but also some new ones. For the new problems presented by stiching together structures, Sims is using a set of irregular communication routines that are available from Steve Plimpton (part of the Zoltan package).



These visualizations of HgS S-orbitals showed a state that had never been seen before: "I'm astonished that it is so constant throughout. I have never seen a state like this before." -- Garnett Bryant, PL

Computation of Atomic Properties with the Hy-CI Method

James Sims
Stanley Hagstrom (Indiana U.)

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

Impressive advances have been made in the study of atomic structure, at both the experimental and theoretical levels. For atomic hydrogen and other equivalent two-body systems, exact analytical solutions to the nonrelativistic Schrödinger equation are known. It is now possible to calculate essentially exact nonrelativistic energies for helium (He) and other three-body (two-electron) systems as well. Even for properties other than the nonrelativistic energy, the precision of the calculation has been referred to as "essentially exact for all practical purposes", i.e., the precision goes well beyond what can be achieved experimentally. These high-precision results for atomic two-electron systems have been produced using wave functions that include interelectronic coordinates, a trademark of the classic Hylleraas (Hy) calculations done in the 1920s. The challenge for computational scientists is to extend the phenomenal He accomplishments (the ability to compute, from first principles alone, any property of any two electron atom or its ion to arbitrary accuracy) to molecules and to atomic systems with three, four, and even more electrons. Where three electron atomic systems (i.e., lithium (Li) and other members of its isoelectronic series) have been treated essentially as accurately as He-like systems, demand on computer resources has increased by 6,000 fold. Because of these computational difficulties, already in the four-electron case (i.e., beryllium (Be) and other members of its isoelectronic series) there are no calculations of the ground or excited states with an error of less than 10 microhartrees (0.00001 a.u.). This is where a technique developed by Sims and Hagstrom in a series of papers from 1971 to 1976 becomes important. They developed the Hy-CI method, which includes interelectronic coordinates in the wave function to mimic the high precision of Hy methods, but also includes configurational terms that are the trademark of the conventional Configuration-Interaction (CI) methods employed in calculating energies for many-electron atomic (and molecular) systems. Because of this, the Hy-CI method has been called a hybrid method. This is the power of the method, because the use of configurations wherever possible leads to less difficult integrals than in a purely Hy method, and if one restricts the wave function to at most a single interelectronic coordinate to the first power, then the most difficult integrals are already dealt with at the four electron level and the calculation retains the precision of Hy techniques, but is greatly simplified.

Two papers on this work appeared this year.

- J. S. Sims and S. A. Hagstrom, Erratum: Comment on "Analytic Value of the Atomic Three-electron Correlation Integral with Slater Wave Functions," *Physics Review A* **68** (2003), p. 059903.
- J. S. Sims and S. A. Hagstrom, "Math and Computational Science Issues in High-Precision Hy-CI Calculations I. Three-electron Integrals," *Journal of Physics B: At. Mol. Opt. Phys.* **37** (7) (2004), pp. 1519-1540.

In the second paper, Sims and Hagstrom discuss changes they have made to their Hylleraas-Configuration Interaction (Hy-CI) methodology to most effectively use modern day computers to increase the size (number of terms) and accuracy of the calculations. The availability of cheap CPUs, which can be connected in parallel to significantly (orders of magnitude) enhance both the CPU power and the memory that can be brought to bear on the computational task, has made techniques that appeared hopeless only five years ago doable (assuming the linear dependence problem can be obviated with extended precision). The goal is to extend techniques which are known to give the most accurate upper bounds to energy states to four and more electrons. The first step in this process was to efficiently evaluate the only difficult integral arising when using the Hy-CI technique in the case of the number of electrons greater than or equal to three, the three-electron triangle integral. Sims and Hagstrom focus on recursive techniques at both the double precision and quadruple precision level of

accuracy while trying to minimize the use of higher precision arithmetic. Also, they investigate the use of series acceleration to overcome problems of slow convergence of certain integrals defined by infinite series. They find that a direct + tail Levin u-transformation convergence acceleration overcomes problems that arise when using other convergence acceleration techniques, and is the best method for overcoming the slow convergence of the triangle integral.

They are now at work on Papers II and III in this series, "Math and Computational Science Issues in High Precision Hy-CI Variational Calculations II. Four-electron integrals," and "Math and Computational Science Issues in High Precision Hy-CI Variational Calculations III. Nuclear attraction and kinetic energy integrals". The latter paper is coming out of a need effort to modify their codes to handle the more general case of non-spherically symmetric Slater-type orbitals (STOs). Once these papers are finished, they will be ready to tackle the difficult matrix assembly problem, and then to do a benchmark Be calculation. Progress to date has included finding a new Be radial limit (s-orbital CI, no r_{ij}) that is better than any published result. Also integrals are being calculated in blocks, each block independent of all others, so different blocks can be calculated on different processors in the final big runs.

In addition to atoms, work is underway to extend high precision electronic energy calculations to diatomic molecules. A calculation is underway on the hydrogen molecule, the two electron molecular analog of helium. Progress to date has been to calculate the ground state energy with an accuracy of nanohartrees (10^{-9}) which is better than all but one previous calculation, an explicitly correlated gaussian (ECG) calculation. The goal is to achieve accuracy on the order of 10^{-12}, worthy of publishing in the *Journal of Chemical Physics*. Sims has completed a parallelization of the code. Building the H and S matrix and the matrix diagonalization (solving) are both parallelized. We focus on diagonalizing the matrix since that dominates the calculation.

All results are for a 3485-term wave function with a total energy of -1.1744 7571 4018 7855 1344 4640 2249 9 a.u. We have achieved a speedup of 24.5 on 32 processors of our Linux cluster, a good scaling (76.4 % scalability), and a more favorable speedup of 30 on 32 processors (93.7 % scalability) on a 96 processor SGI. Furthermore that scaling holds well up through the 90 processor run, where we get a factor of 80 on 90 processors, an (89.1 % scalability). This parallelization is relevant not only to H_2 but atomic states (Be, etc.) as well.

Finally to verify that they can do a better H_2 calculation than ECG, they have done an H_2^+ calculation and get, with 63 terms,

No. terms	E (R=2.0)	
63	**-0.6026 3421 4494 9464 1673**	***Our result***
160	**" " " 911**	***ECG (Cencek and Kutzelnigg)***

So they have achieved energy with 18 digits accuracy, five more digits than ECG. So it looks like for H_2 as well as the other 2-electron diatomics that Hy-CI will beat ECGs in the long run.

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

Screen Saver Science (SSS)

William L. George
Samuel Small (Johns Hopkins U.)
Jacob Scott (U. of California, Berkeley)
Angel L. Villalain Garcia (U. of Puerto Rico)

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

The SSS project aims to develop a computing resource composed of a heterogeneous set of PCs, scientific workstations, and other available computers, that can be easily used by scientists to execute large highly distributed, compute intensive applications. Each individual computer in this system would make itself available for participating in a computation only when it would otherwise be idle, such as when its screen saver would be running. This project is based on Jini, open software architectures built in 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 and workstations 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 research on Grid computing has been accelerating and this SSS computing environment will allow us to develop and experiment with new highly parallel and distributed algorithms more suitable for grid type environments. Finally, the use of Java for scientific applications is of interest in general and so the development of applications for SSS will give us the opportunity to explore this topic on actual production quality applications.

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

The SSS project began in the summer of 2002. Substantial progress has been made in designing, implementing, and testing the basic SSS infrastructure. A generic compute server has been implemented and a new Jini service, a remote file server, has been developed to provide SSS applications with basic file I/O capabilities.

In this last year, W. George has restructured the server side of SSS to facilitate the addition of security features and to simplify the installation of SSS on user's PCs and workstations. In the summer of 2004, W. George, in collaboration with SURF student Angel Garcia, began adding much needed security features to SSS including login authentication, integrity verification of downloaded code, confidentiality (encryption) in all network communication within SSS, and trust verification of the provider of the SSS Jini service. More work is needed to complete the security framework for SSS before this system can be fully deployed.

W. George and J. Devaney collaborated with Ray Mountain, of the Physical and Chemical Properties Division (838) of the Chemical Science and Technology Lab to develop a Monte Carlo style simulation for the study of the clustering of water molecules. R. Bohn and W. George, have ported a Fortran Monte Carlo simulation to Java as a first step in creating this SSS application. After some performance tuning, initial testing has shown that the Java version performs as well as the optimized Fortran version, with respect to speed, on our SGI and Sun workstations. Because this application depends heavily on input and output of large files, the completion of this SSS application awaits the completion of the SSS Secure Remote File Service.

W. George presented an invited talk on SSS at Bowie State University on Feb. 26, 2004.

Interoperable MPI (IMPI)

William George
John Hagedorn
Judith Devaney

http://impi.nist.gov/

The Interoperable Message Passing Interface (IMPI) project supports the vendors of MPI, as they implement the IMPI 0.0 protocols, by maintaining the NIST IMPI conformance tester, managing the IMPI mailing list (interop@nist.gov), maintaining the IMPI specification document and its errata, and in general promoting the implementation of IMPI by the current MPI vendors.

This year J. Devaney and W. George consulted with Andrew Lumsdaine and Jeff Squires of the University of Indiana Open Systems Lab concerning the support of IMPI in the new "Open MPI" library, which will be replacing LAM/MPI and several other open source MPI implementations in 2005. IMPI is seen as an important capability for this new MPI implementation. LAM/MPI supports IMPI and we expect Open MPI to support IMPI also.

The company MPI Software Technology, Inc. completed its NIST Phase II SBIR project and submitted their final report on "Collective, Performance-Oriented Algorithms for Interoperable MPI. This research helped advance and improve their implementation of IMPI within their commercial product MPI/Pro.

IMPI has begun to have impact in the Grid computing research community. This year W. George consulted with Yutaka Ishikawa, from the University of Tokyo, regarding the use of Interoperable MPI (IMPI) in a Grid computing environment they are developing. Additionally NSF is considering funding the development of IMPI support within one or more MPI research groups.

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

Finally, an article on IMPI was developed which appeared in Dr. Dobb's Journal: W.L. George, J.G. Hagedorn, and J.E. Devaney, "Parallel Programming with Interoperable MPI," *Dr. Dobb's Journal* **357** (Feb. 2004), pp 49-53.

Special Projects

Digital Library of Mathematical Functions

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30 authors under contract

http://dlmf.nist.gov/

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

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

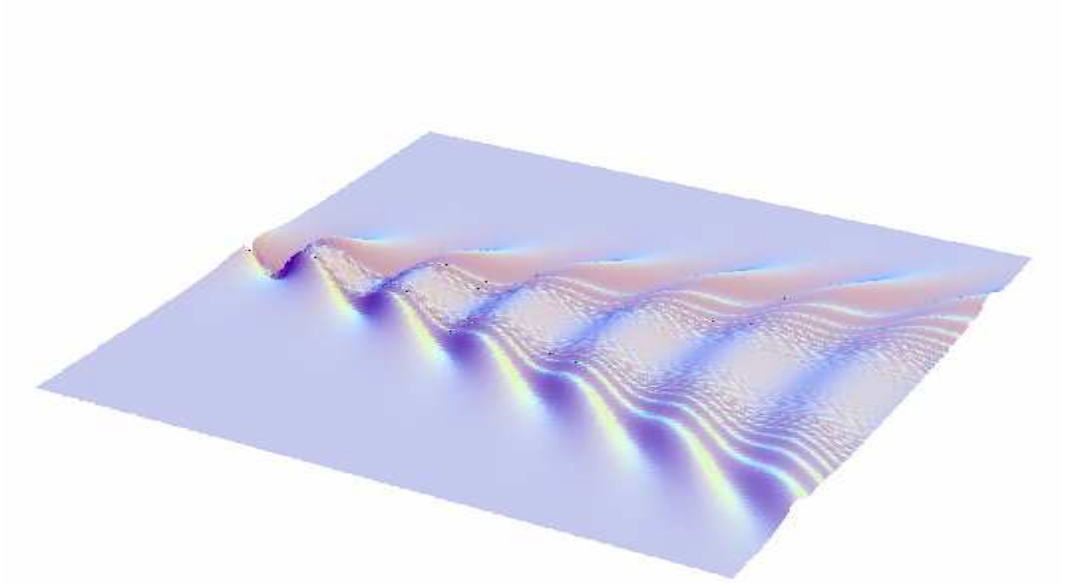
The Digital Library of Mathematical Functions has two main goals. First, to review the published literature on special functions, select the properties most relevant to current applications, and publish an up-to-date handbook of the traditional sort. The most recent comprehensive handbook was published in 1964 by the 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, to disseminate the same information, with important 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.

Substantial progress was made on both fronts in the past year. Complete drafts of all but two of the 38 planned handbook chapters have been received from authors outside NIST who are being compensated by funds from the National Science Foundation. Several chapters have been sent to

similarly compensated independent validators, and the remaining ones are scheduled for validation in the immediate future. The original plan to use HTML with GIF images for equations for the Web site has been superseded by the recent availablity of the new XML family of standards and the emerging development of tools that can put Web content into XML formats. This will yield rich improvements for math-aware search (via XQUERY) and semantic representation of mathematics in computer databases (via MathML). A major accomplishment was the project's successful construction of a translator that takes LaTeX, the mathematics word processor being used for the handbook edition, into XML/MathML. This achievement, which is at the forefront of a worldwide research effort in MKM (Mathematical Knowledge Management), was described in a keynote address and supporting technical talk at the North American MKM Workshop in January 2004, and also in an invited talk at a related workshop in Helsinki in May 2004.

Within the next year a contract with an outside publisher will be established to print, advertise and sell the handbook. The initial release of the Web site for public usage will occur simultaneously. Feedback from users is expected to suggest many avenues of enhancement for the Web site, which will continue to be an effective basis for MCSD participation in future MKM research and development activities.

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



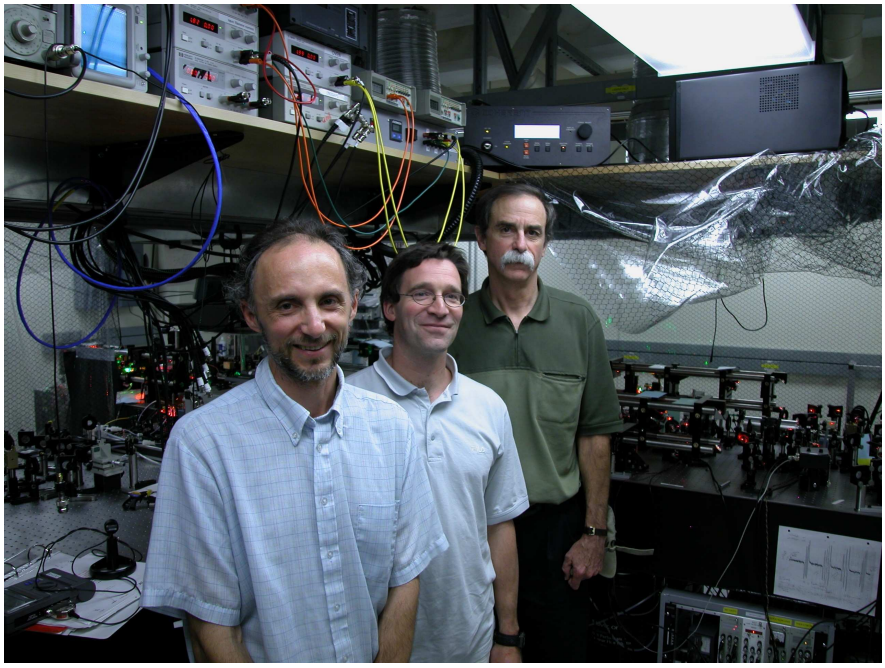
Kelvin's ship wave pattern. Many physical phenomena can be modeled very accurately with special functions. In this case the familiar wake behind a moving ship has been modeled in terms of the canonical integral associated with the cuspoid catastrophe. Catastrophe theory, begun in the 1960s, is a field of mathematics that studies and classifies phenomena characterized by sudden shifts in behavior arising from small changes in circumstances. Canonical integrals associated with different types of catastrophes are the subject of a chapter in the DLMF.

Quantum Information Theory Program

Since the mid-1960s the dimensions of transistors on microchips have halved approximately every 18 months. It is estimated that logic capacity and speed are doubling, and memory capacity is quadrupling, every three years. These rapid developments have fueled the explosive growth in information technology we have witnessed in the last 20 years. Projecting this progression into the future, a transistor will be charged with a single electron in about 15-20 years. At that point, the laws of quantum rather than classical physics will begin to dominate, requiring fundamental changes in the physical basis for computer technology if increases in computing power are to be sustained. An intriguing idea is the use of quantum states of atoms, ions, or photons themselves to store, process, and communicate information. The sometimes counterintuitive properties of quantum mechanics have led to the discovery of information processing capabilities which exceed those known classically. Among these are (a) the solution in polynomial time for problems considered exponentially difficult, such as factoring and discrete logarithms, the bases of common public-key encryption systems, and (b) communication channels secure against eavesdropping.

The NIST Physics Laboratory (PL) has a mature experimental program in quantum computing, and ITL and PL have a well established experimental program in quantum communication. MCSD is developing a program in quantum information theory to complement these efforts. This work is supported by the DARPA Quantum Information Science and Technology (QuIST) program, as well as by the NIST Competence program project entitled *Quantum Information Theory and Practice*. Work on this project centers on the development and analysis of architectures and algorithms for quantum information processing. The research being undertaken by MCSD staff is summarized below.

This work was supported in part by the NIST Competence Program and the Quantum Information Science and Technology (QUIST) Program of the Defense Advanced Projects Agency (DARPA).



Manny Knill (left) of MCSD collaborates closely with the ion trapping team led by Dave Wineland (right) of PL.

Realizing Quantum Information Processors

Emanuel Knill *David Wineland (NIST PL)*
Scott Glancy *Alan Mickelson (University of Colorado)*

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

- characterizing and benchmarking quantum devices, particularly those based on ion traps and linear optics, and
- investigating fault-tolerant architectures with the goal of improving error tolerance and reducing resource requirements.

Characterization and Benchmarking. Benchmarking quantum devices involves implementing procedures and making measurement to determine how well the procedures worked. For quantum information processing, the procedures should demonstrate the functioning of fundamental algorithmic techniques used in quantum algorithms and establish the error behavior of the devices used. The most advanced scalable quantum information processors available are based on the ion trap. This year Manny Knill has collaborated closely with Dave Wineland's group in the NIST Physics Lab's Time and Frequency Division to realize three three-qubit benchmarks:

1. *Quantum teleportation*, which is one of the most versatile and useful subroutines in quantum information processors (see *Nature* v429 p737 2004);
2. *Quantum error correction*, essential for scalability (*Nature* v432 p602); and
3. Measured *quantum Fourier transform*.

The three benchmarks establish the desired quantum behavior, and provide a baseline for error behavior to be improved in future experiments. Future work includes development of procedures that provide device error information with a resolution below that implied by the error of a single measurement.

Optical quantum information processors are not sufficiently well developed to implement benchmarks with the complexity of the ion trap experiments. Therefore, the main goal in this facet of our work is to characterize the different possible approaches to implementing non-trivial tasks with optical elements. Scott Glancy recently joined the project as a NIST NRC Postdoctoral Fellow, and he and Manny Knill are now investigating how different approaches can be combined to take better advantage of the strengths of optical devices, for example, the high efficiency possible with homodyne detection. There are presently three main approaches to optical quantum computing with primarily linear optical devices: LOQC (or the KLM proposal) is based on postselection and error correction without using non-linearities; CatQC uses cat states (superpositions of two displaced Gaussian states) as a resource for computing; and the GKP proposal involves states stabilized by discrete subgroups of the quadrature displacement group. They are collaborating with Alan Mickelson at the University of Colorado, who is planning on performing experiments in optical quantum computing.

Fault-tolerant Architectures. Effective error management is the key to building practical quantum computing devices. Up to now, the most capable fault-tolerant quantum computer architectures required physical devices with error probabilities below 0.2 %. This is a difficult level for experimentalists to obtain; the best quantum devices for which error information is available have error probabilities of 3%. Manny Knill of ITL has very recently succeeded in closing this gap by designing a simple fault-tolerant architecture that can operate with devices having error probabilities above 3%. His architecture requires too large a resource overhead at such high error probabilities, but becomes relatively practical below 1%. He used several innovations to achieve this goal, most notably error-correcting teleportation, which greatly simplifies the fault-tolerant architecture while reducing the effects of errors. The error tolerance improves if the devices are able to detect their failure. There is still work to be done to reduce the resource overheads for fault-tolerant quantum information processing.

Quantum Circuit Design

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

Practical Top-down Approach to Quantum Circuit Synthesis. Igor Markov and Vivek Shende of the University of Michigan, working in collaboration with Stephen Bullock of ITL, have developed a new universal quantum circuit capable of implementing any unitary operator. It has a top-down structure which concentrates the circuit on the less significant qubits, and the parameters for a given unitary may be computed using standard matrix analysis software. The number of controlled-not's is only half the number of matrix coefficients. The circuit is half as large as prior art developed at the Helsinki University of Technology and for three-qubits and is half as large as a competing circuit developed at JPL. Moreover, a theoretical lower bound shows that this new universal circuit may be improved by at most a factor of two. The circuit adapts well to architectures in which only nearest-neighbor interactions are possible, i.e. spin chains. See V.V. Shende, S.S. Bullock, and I.L. Markov, quant-ph/0406176.

Constrained QR Factorization Enabling Quantum Circuit Design. Any matrix of dimension m by n can be reduced to upper triangular form by multiplying by a sequence of $mn-n(n+1)/2$ appropriately chosen rotation matrices. In this work we address the question of whether such a factorization exists when the set of allowed rotation planes is restricted. Applications to the design of 3-qubit circuits as well as to the design of quantum multi-level logics (qudits) have been studied (see below). We introduce the rotation graph as a tool to devise elimination orderings in QR factorizations. Properties of this graph characterize sets of rotation planes that are sufficient (or sufficient under permutation) and identify rotation planes to add to a deficient set. We also devise a constructive way to determine all feasible rotation sequences for performing the QR factorization using a restricted set of rotation planes. A paper by D.P. O'Leary and S. Bullock has been submitted to the *Electronic Transactions on Numerical Analysis*.

Quantum Circuits for Multi-level Logics. Dianne O'Leary and Stephen Bullock, joint with Gavin Brennen (PL), have adapted QR orthonormalization techniques from numerical linear algebra to the construction of quantum logic circuits for multi-level logics. In the usual model of quantum computing, a computation is a unitary matrix applied to a complex vector space of dimension 2^n, when n is the number of qubits. This loosely corresponds to one component per n-bit string. In a d multi-level logic, bits are replaced by dits, taking on values $0, 1, \ldots d-1$, and n quantum dits (qudits) admit computations that are $d^n \times d^n$ unitary matrices. Building a qudit quantum circuit corresponds to

splitting the unitary matrix into factors which are simple Kronecker (tensor) products. Physically, a qudit quantum system could correspond to encoding quantum data into all the hyperfine states of an atom or electron rather than simply two.

Work on qudit circuits by the group has produced three major results. First, a variant QR decomposition allows for optimal construction of one-qudit ($d \times d$) unitaries in terms of the minimum number of possible laser pulses. Second, QR arguments allow for a bootstrap argument, producing all n-qudit unitaries given one-qudit unitaries and a simple two-qudit interaction. Third, the first asymptotically optimal quantum circuit for qudits has been produced. Meaning, dimensionality arguments prove that building an n-qudit unitary requires $C\ d^{2n}$ quantum gates in a circuit. Prior circuits however required $C\ n^2\ d^{2n}$, which is asymptotically worse. Using a delicate argument involving the structure of Kronecker products, the NIST group created the first explicit quantum circuit for a $d^n \times d^n$ unitary costing only $C\ d^{2n}$ gates. This circuit is also a variant of the QR decomposition.

Small quantum circuits are hoped to make quantum computing more feasible by driving down the number of physical operations required to manipulate quantum data. In this vein, quantum multi-level logics are thought to be more efficient for packing quantum data than quantum bits in certain applications, e.g. dit-wise Fourier transforms.

See quant-ph/0410116 and quant-ph/0407223.

Entanglement Dynamics of n-qubit Computations

Stephen Bullock *Anthony Kearsley*
Dianne O'Leary *Gavin Brennen (NIST PL)*

Stephen Bullock, Gavin Brennen (PL), Dianne O'Leary, and Anthony Kearsley have been studying the entanglement dynamics of n-qubit computations. Entanglement is a quantum phenomenon which in the context of quantum computing allows a computer to manipulate superpositions (vector sums) of all n-bit strings, given the device operates on n-qubits. Prior work shows that a quantum computer incapable of creating an entangled state can never outperform a classical emulator, although how entanglement allows for quantum computer-outperformance is poorly understood.

Concurrence is one measure of entanglement, itself defined in terms of the qubit spin-flip. A quantum state which is invariant under the spin flip must be entangled. Work at NIST has discovered a new matrix decomposition of the unitary group, the concurrence canonical decomposition (CCD), which splits any quantum computation (i.e., a $2^n \times 2^n$ unitary matrix) into three factors $U = K_1 A K_2$. Only the middle factor a may alter the concurrence, so that the matrix decomposition is a tool for studying how U entangles the quantum states it processes. Results arising from this tool include the following:

- Most quantum computations produce a lot of concurrence, carrying some state with no concurrence to a state of maximal concurrence.
- Specific examples may be treated numerically in up to *10* qubits using numerical matrix analysis software. Note that *10* qubits corresponds to $2^{10} \times 2^{10} = 1024 \times 1024$ matrices.
- If the unitary has a special CCD with $K_2 = K_1^{-1}$, then eigenstates of U either have multiplicity greater than or equal to 2 or have maximal concurrence. In particular, one might envision exploiting such a Kramer's' nondegeneracy to produce highly entangled states by freezing a quantum system into such an eigenstate.
- An explicit matrix decomposition computing u exists in all cases. When the number of qubits is odd, this relies on work of Dongarra on diagonalizing Hermitian matrices with time-reversal symmetry.

See quant-ph/0309104 and quant-ph/0402051.

Other Work in Quantum Information Theory

Isabel Beichl
Stephen Bullock
David Song
Ronald Boisvert
Eite Tiesinga (NIST PL)
Francis Sullivan (IDA/CCS)

New QKD Protocols Based Upon Entanglement Swapping. David Song has developed two new cryptographic key distribution schemes based on swapping quantum entanglement. Using two Bell states, two bits of secret key can be shared between two distant parties that play symmetric and equal roles. The protocols have been shown to be robust against common eavesdropping attacks. See D. Song, *Phys. Rev. A* **69** (March 2004), p. 034301.

Optimality in Projective Measurement for Entanglement Swapping. In two partially entangled states, entanglement swapping by Bell measurement will yield the weaker entanglement of the two. This scheme is optimal because the average entanglement cannot increase under local operation and classical communication. However, for more than two states, this scheme does not always yield the weakest link. In work completed this year, David Song considered projective measurements other than Bell-type measurement and showed, numerically, that while Bell measurement may not be unique, it is indeed optimal among these projective measurements. See D. Song, *Journal of Optics B: Quantum and Semiclassical Optics* **6** (January 2004) L5-L7

Generalization to Deutsch's Algorithm Detecting Concentrated Maps. We consider an arbitrary mapping $f: \{0,\ldots,N-1\} \rightarrow \{0,\ldots,N-1\}$ for $N=2^n$. Using N calls to a classical oracle evaluating $f(x)$ and an N-bit memory, it is possible to determine whether $f(x)$ is one-to-one. For some radian angle $0 \leq \theta \leq \pi/2$ we say $f(x)$ is θ-concentrated if and only if $e^{2\pi i f(x)/N} \subset e^{i[\psi-\theta,\psi+\theta]}$ for some given ψ and any $0 \leq x \leq N-1$. We have developed a quantum algorithm that distinguishes a θ-concentrated $f(x)$ from a one-to-one $f(x)$ in $O(1)$ calls to a quantum oracle function U_f with high probability. For $0 \leq \theta \leq 0.3301$ radians, the quantum algorithm outperforms the obvious classical algorithm on average, with maximum outperformance at $\theta = (1/2)\sin^{-1}(1/\pi) \approx 0.1620$ radians. Thus, the constructions generalize Deutsch's algorithm, in that quantum outperformance is robust for (slightly) nonconstant $f(x)$. A paper by I. Beichl, S. Bullock, and D. Song has been submitted to the *NIST Journal of Research*.

A Simple Proof of the Kochen-Specker Theorem. Contextuality in a quantum mechanical system is the idea that the value of one variable depends on the context in which it is observed. Isabel Beichl and Francis Sullivan have conducted research advancing the understanding of contextuality, which has resulted in a new and simple proof of the Kochen Specker theorem, a fundamental theorem at the foundation of quantum mechanics. Their proof is understandable and hence makes one of the most fundamental ideas of quantum mechanics accessible to more researchers.

Modeling of Qubits in Optical Traps. William Mitchell is collaborating with Eite Tiesinga and other NIST PL staff using Mitchell's PHAML package to solve the Schroedinger equation for eigenvalues and eigenstates relevant to optical traps for neutral atoms. In a quantum computer, arrays of such atoms will correspond to arrays of qubits, and interactions of adjacent atoms will be used to implement elementary quantum gates. PHAML is a parallel hierarchical basis finite element solver for partial differential equations with adaptive grid refinement and multigrid linear equation solution. The computational problems in question are particularly challenging due to the large-scale variations of the eigenfunctions in small portions of the domain. Because of this, PHAML's adaptive grid refinement capabilities are critical.

This year PHAML was modified to solve equations of this form, using ARPACK as the eigensolver. The potential for the 30-node solution computed last year did not have a deep enough

well, since the physics suggests there should be about 50 nodes in the wave. At Eite's suggestion, Mitchell changed the depth of the well to one that gives a 48-node solution. This requires more processors and a longer computation time. The first attempts at solving this problem failed. Initially the 30-node solution required 1.5 million vertices and took 6 hours on 8 processors. Mitchell made several improvements to PHAML so that this now takes 7 minutes on 8 processors, a 50-fold speedup. With these improvements we are now able to produce the 48-node solution using 4.5 million vertices in 35 minutes on 32 processors.

QITAP Seminar Series. A seminar associated with the competence project Quantum Information Theory and Practice was initiated this year. The following presentations were made.

1. T. Nakassis, "Bit String Reconciliation for QKD," October 10, 2003.
2. S. Lomonaco, "Continuous Quantum Algorithms," October 30, 2003.
3. D. Song, "A QKD Protocol Based on Entanglement Swapping," November 6, 2003.
4. G. Brennen, "Universal Computation with Qudits with Applications to Multi-level Atoms," December 4, 2003.
5. S. Bullock, "Concurrence Canonical Decomposition," December 18, 2003.
6. Igor Markov (University of Michigan), Automatic Synthesis and Simulation of Quantum Circuits, January 30, 2004.
7. I. Beichl, Limits of Quantum Computation, February 5, 2004.
8. Anocha Yimsiriwattana (UMBC), Distributed Quantum Factoring Algorithm
9. Dennis Lucarelli (JHU APL), Control Theoretic Aspects of Holonomic Quantum Computation, Match 24, 2004.
10. S. Bullock, Time Reversal and the CCD Matrix Decomposition, March 25, 2004.
11. James Clemens (University of Arkansas), Partially correlated noise and quantum error correction, May 11, 2004.
12. Yaakov Weinstein (Naval Research Lab), Pseudo-Random Operators for Quantum Information Processing, September 23, 2004
13. Scott Glancy, Quantum Computation with Optical Coherent States, October 7, 2004
14. Trey Porto and Jamie Williams, Quantum Information Processing in lattices, October 21, 2004
15. S. Bullock and G. Brennen, Quantum Circuits for d-level Systems, November 7, 2004.

A Finite-Element-Analysis Code Translation Methodology for Applications in NIST World Trade Center Investigation

Jeffrey Fong
Barry Bernstein
William Mitchell
James Filliben (ITL SED)
John Gross (NIST BFRL)
Terri McAllister (NIST BFRL)
Fahim Sadek (NIST BFRL)
Monica Starnes (NIST BFRL)
Howard Baum (NIST BFRL)
Kuldeep Prasad (NIST BFRL)
Ronald Rehm (NIST BFRL)
Roland deWit (NIST MSEL)
Richard Fields (NIST MSEL)

Ala Tabiei (University of Cincinnati)
Jun Tang (University of Iowa)
Ume. Herron (Computers & Structures, Inc.)
Bob Morris (Computers & Structures, Inc.)
Iqbal Suharwardy (Computers & Structures, Inc.)
Bradley Maker (Livermore Software Tech.)
Willem Roux (Livermore Software Tech.)
Nielen Stander (Livermore Software Tech.)
Abed Khaskia (Mallet Technology)
Matt Mehalic (Mallet Technology)
Bob Rainsberger (XYZ Scientific Apps.)

Beginning on Aug. 21, 2002, NIST undertook, at the request of the Congress, a 3-part response to the Sep. 11, 2001 World Trade Center (WTC) disaster: (1) A building and fire safety investigation into the probable causes of the WTC buildings collapse; (2) A multiyear R&D program to provide the technical basis for improved building and fire codes, standards, and practices; and (3) An industry-led and NIST-assisted program to disseminate practical guidance and tools to help building owners, contractors, and designers, as well as emergency responders and regulatory authorities to better respond to future disasters.

Some of the key engineering design and analysis documents of the WTC twin towers were transmitted to NIST in the form of four computer text files, each about 100MB long, which were only executable in a commercially-available finite element analyis (FEA) software package named SAP2000. Since SAP2000 is limited in its analysis capability because it was designed to model the linear elastic response of a framed structure, NIST saw a need to translate those four text files into executables in two other software languages, namely, ANSYS and LS-DYNA, with simulation capabilities for nonlinear impact, thermal-structural interactions, buckling, creep, fracture and ultimate collapse of complex structures.

During a period of four months (Oct. 2003 - Jan. 2004), MCSD worked with researchers in NIST (BFRL and MSEL) and academia, and mathematical software developers of ANSYS, LS-DYNA, SAP2000, and a parametric FEA translator code named TrueGrid, to develop a two-option translation and verification methodology: Option-a is for a translation of SAP2000 beam elements into ANSYS (beam type 44) without cross section details. Option-b goes further by capturing all of the SAP2000 beam details into ANSYS (beam type 188). For translation from SAP2000 into LS-DYNA, only option-a was implemented, because most of the FEA analysis work by NIST and its contractors used ANSYS.

A five-criteria verification specification and a test suite of five benchmarks for the newly-developed translation methodology were introduced to facilitate the application of this methodology to WTC investigation. A MCSD working document with 22 appendices containing the results of the translation of two full floors (96A and 75B) of the WTC twin towers was completed in Jan. 2004. For further information, contact fong@nist.gov.

Part III

Activity Data

Publications

Appeared

Refereed Journals

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3. G.K. Brennen and S.S. Bullock, "Stability of Global Entanglement in Thermal States of Spin Chains," *Physical Review A* **70** (2004), 052303.
4. S. Bullock "Note on the Khaneja Glaser Decomposition," *Quantum Information and Computation* **4** (5) (2004), pp. 396-400.
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11. S. Bullock and G.K. Brennen, "Two-qubit Quantum Logic Circuits with Measurement Gates," *Proceedings of the Design Automation Conference 2004*, (see http://www.dac.com .)
12. S. Bullock, V.V. Shende, and I.L. Markov, "Recognizing Small-Circuit Structure in Two-Qubit Operators and Timing Hamiltonians to Compute Controlled-Not Gates," *Physical Review*.
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14. S.S. Bullock, G.K. Brennen, and D.P. O'Leary, "Time Reversal Symmetry and n-Qubit Canonical Decompositions," *Journal of Mathematical Physics*.
15. D. Cotrell and A. Kearsley, "Optimal Topography for Flow in a Cylinder," *Optimization and Engineering*.
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18. D.E. Gilsinn, M. McClain, and C. Witzgall, "Using Nonoscillatory Splines to Model Urban Environments," *Proceedings SIAM Conference on Geometric Design and Computing*.
19. D. E. Gilsinn, G. S. Cheok, A. M. Lytle, "Pose of I-beams for Construction Site Automation," *Proceedings 21st International Symposium on Automation and Robotics in Construction*, Jeju, Korea, September 21-25, 2004.
20. M.A. Hamstad and A. O'Gallagher, "Modal-Based Identification of Acoustic Emission Sources in the Presence of Electronic Noise," *Journal of Acoustic Emission*.
21. F.Y. Hunt, A. O'Gallagher, A.J. Kearsley," A Tutorial on Multiple Sequence Alignment of Biological Sequences"
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27. A.J. Kearsley, L.A. Melara, Jr., and R.A. Tapia, "Numerical Experiments with Total Variation Denoising Problems," *Journal of Optimization Theory and Applications*.
28. A. Kearsley, "Optimization Algorithms for Optimal Signal Set Design," *Optimization Methods and Software*.
29. W.F. Mitchell, "Hamiltonian Paths Through Two- and Three-Dimensional Grids," *SIAM Journal of Scientific Computing*.
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33. L. Viola, E. Knill, "Random Decoupling Schemes for Quantum Dynamical Control and Error Suppression," *quant-ph* and *Physical Review Letters*.
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2. I. Beichl and F. Sullivan, "Grover's Algorithm: Lower Bounds on Quantum Complexity".
3. I. Beichl, M. Robinson, D. Song, and F. Sullivan "A Quantum Algorithm for Determining If a Function is One to One."
4. I. Beichl and F. Sullivan, "Contextuality and Its Relation to Quantum Computing."
5. B. Bernstein, J.T. Fong, J. Tang, and H.F. Brinson, "Adiabatic Tensile Creep Test of a Nonlinearly Visco-elastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 327-336..
6. M. D. Bowdrey, J. A. Jones, E. Knill, R. Laflamme, "Compiling Gate Networks on an Ising Quantum Computer."
7. H.F. Brinson, J.T. Fong, and B. Bernstein, "Adiabatic Tensile Stress Relaxation Test of a Linearly Visco-elastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 317-326.
8. D.L. Cotrell and G.B. McFadden, "Axial Flow Effects on the Linear Stability of Circular Couette Flow with Viscous Heating."
9. R. Davis, T. Bur, M. Nyden, and R. Kacker, "Polymer Nano-composite composition."
10. R. deWit, R., and J.T. Fong, "Bending of a Cantilever Beam," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 287-296.
11. R.J. Fields, J.T. Fong, J. Tang, and B. Bernstein, "Adiabatic Tensile Creep Test of a Visco-plastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 347-356.
12. J.T. Fong, "A Finite Element Analysis Code Translation Methodology for Applications in NIST World Trade Center (WTC) Investigation," internal consulting report for NIST Building and Fire Research Laboratory.

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14. J.T. Fong, B. Bernstein, J.J. Filliben, and R.F. Fields, "A Stochastic Time-to-Failure Model of the Deformation, Progressive Local Damage, and Ultimate Collapse of a Single-Floor Steel Grillage on Fire," *ASCE Journal of Structural Engineering*.
15. J.T. Fong, R. Rainsberger, and R. deWit, "On the Validation of Nonlinear Finite Element Analysis Results by a "Comparable Simulation" Method," *ASME Mechanical Engineering Magazine*.
16. J.T. Fong, J. Filliben, and H.K. Liu, "An ISO-compliant Reference Benchmark Approach to Verification and Validation of Models in Computational Physics, Applied Mechanics, and Structural Engineering," *NIST Journal of Research*.
17. J.T. Fong, R. deWit, R.J. Fields, J. Filliben, and H.K. Liu, "A Strong-sense Benchmark Problem for Testing the Feasibility of a Five-step Process of Verification and Validation of Computational Models," NIST Workshop, Nov. 8-9, 2004.
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19. J.T. Fong, A. Tabiei, M.H. Koebbe, and J.J. Filliben, "Collapse Failure of a 7-story Box Impacted at 6th Floor," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 387-396.
20. J. T. Fong and R. deWit, eds., *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*.
21. W.L. George, "Constructing a Distributed Parallel Computing Environment Using Jini and JavaSpaces," *Computing in Science and Engineering*.
22. W.L. George, A. Lumsdaine, J. Squyres, and J. Devaney "Interoperable MPI," *IEEE Transactions on Parallel and Distributed Systems.*
23. D.E. Gilsinn, "Integral Equation Methods of Estimating Characteristic Multipliers for Linear DDEs with Periodic Coefficients."
24. D.E. Gilsinn, G.S. Cheok, "Estimating Location and Pose of Objects on Construction Sites," NISTIR.
25. D. E. Gilsinn, G. S. Cheok, and A. M. Lytle, "Pose of Objects on Construction Sites."
26. K.F. Gurski, G.B. McFadden, M.J. Miksis, "The Effect of Contact Lines on the Rayleigh Instability with Anisotropic Surface Energy."
27. K. Irikura, R. Johnson, and R. Kacker, "Fractional Uncertainties in Computational Chemistry Models."
28. R. Kacker and R. Dersimonian, "Quantification of Uncertainty in Meta-analysis."
29. R. Kacker and I. Olkin, "Abstracts of Tables of Probability Distributions."
30. R. Kacker, B. Toman, and W. Guthrie, ""Application of the ISO Guide, Bayesian Statistics, and Numerical Simulation to Simple Linear Calibration."
31. A.J. Kearsley, L.A. Melara, Jr., "Computational Simulation of Twinned-Martensite Using Symmetric P_2 Finite Element Mesh.
32. A.J. Kearsley and L.A. Melara, Jr., "An Equality Constrained Optimization Approach to Simulating Twinned Martensite."
33. A.J. Kearsley and L.A. Melara Jr., "Optimization and Homotopy Methods in Multidimensional Scaling."
34. A. Kearsley, "Projections onto Ordered Simplexes and the Isotonic Regression Problem."
35. R. Kessel and R. Kacker, "Uncertainty Index."
36. M.H. Koebbe, J.T. Fong, and J.J. Filliben, "Compressive Failure of a Two-Floor Grillage on Fire," *Proc. of a NIST Workshop on V&V of Computer Models*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 377-386. Also to appear as an internal document of the NIST-ITL Mathematical and Computational Sciences Division, Oct. 2004.
37. T. Litorja and R. Kacker, "Analysis of Aperture Data."
38. Z.K. Liu, L.Q. Chen, P. Raghavan, Q. Du, J.O. Sofo, S.A. Langer, and C. Wolverton, "An Integrated Framework for Multi-Scale Materials Simulation and Design," *Journal of Computer-Aided Material Design*.
39. D. Matheu, C. Gonzalez, and R. Kacker, "Uncertainty Associated with Reaction Barrier of Transition State in Bi-molecular Reactions."
40. W.F. Mitchell, "A Refinement-tree Based Partitioning Method for Dynamic Load Balancing with Adaptively Refined Grids."

41. C. Negrevergne, R. Somma, G. Ortiz, E. Knill and R. Laflamme, "Liquid State NMR Simulations of Quantum Many-body Problems."
42. B. Rust and D. Donnelly, "The Fast Fourier Transform for Experimentalists Part I – Concepts," *Computing in Science & Engineering*.
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44. B. Rust and B. Thijsse, "Fitting Nature's Basic Functions Part V: Freestyle Data Fitting," *Computing in Science and Engineering*.
45. B. Rust and D. O'Leary, "A Truncated Singular Component Method for Ill-Posed Problems."
46. J.S. Sims and S.A. Hagstrom, "Math and Computational Science Issues in High Precision Hy-CI Variational Calculations II. Four-electron Integrals."
47. J. Slutsker, A.L. Roytburd, W.J. Boettinger and J.A. Warren, G.B. McFadden, K. Thornton, P. Voorhees, "Phase-field Modeling of Solidification Under Stress."
48. R.W. Swindeman, J.T. Fong, B. Bernstein, and R.J. Fields, "Adiabatic Tensile Stress Relaxation Test of a Visco-plastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 357-366.
49. A. Tabiei, J.T. Fong, H.F. Brinson, and B. Bernstein, "Adiabatic Tensile Creep Test of a Linearly Visco-elastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 307-316.
50. J. Tang, J.T. Fong, R.J. Fields, and B. Bernstein, "Adiabatic Tensile Test of an Elastic-plastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 297-306.
51. D.C. Venerus, J.T. Fong, B. Bernstein, and H.F. Brinson, "Adiabatic Tensile Stress Relaxation Test of a Nonlinearly Visco-elastic Material," *Proceedings of a NIST Workshop on Verification and Validation of Computer Models for High Consequence Engineering Systems*, Nov. 8-9, 2004, J. T. Fong and R. deWit, eds., pp. 337-346.
52. Q. Wang and B. Saunders, "Web-Based 3D Visualization in a Digital Library of Mathematical Functions," NISTIR.

Visualizations Published

1. S. Satterfield, Animation of Smart Gel, Opening video of the SC (Supercomputing) 2003 Conference, Phoenix Arizona, November, 2003.
2. D. Feder and P. Ketcham, Three Bose-Einstein Condensate images, p. 22, "Networking and Information Technology Research and Development: Advanced Foundations for American Innovation," Oct 2003 Supplement to the President's FY 2004 budget.

R. Boisvert giving a presentation on the Digital Library of Mathematical Functions Project at the Symposium on Software Environments for Numerical Problems held in Gent, Belgium, in November 2004.

Presentations

Invited Talks

International

1. R. Boisvert, "A Handbook of Special Functions for the Digital Age," Department of Computer Science Distinguished Lecture, University of Toronto, Toronto, Canada, October 7, 2003.
2. R. Boisvert, "A Handbook of Special Functions for the Digital Age," Symposium on Software Environments for Numerical Problems, University of Gent, Belgium, November 18, 2004.
3. Bruce R. Miller, "Digital Library of Mathematical Functions: LaTeX, MathML and ... OpenMath?" 10 Years of OpenMath Workshop, Helsinki, Finland, May 21-22, 2004.
4. R. Pozo, "The Role of Virtual Machines in Scientific Computing," Cluster and Computational Grids for Scientific Computing (CCGSC 2004) Conference, Faverges de la Tour, France, Sept. 26-29, 2004.

Domestic

5. B. Alpert, "Nonreflecting Boundary Conditions for Time-Domain Acoustic and Electromagnetic Wave Propagation," Computational and Applied Mathematics Seminar, Purdue University, West Lafayette, Indiana, September 17, 2004.
6. S. Bullock, "Time Reversal and n-qubit Canonical Decompositions," Gordon Conference on Quantum Computing, Ventura, CA, February 25, 2004.
7. S. Bullock, "Cartan Involutions and Entanglement Dynamics," Cornell University Department of Mathematics Lie Theory Seminar, Ithaca, NY, March 5, 2004.

8. J. Fong, "A SAP-to-LSDYNA Translator," Applied Research Associates, Mountain View, California, Nov. 10, 2003.
9. J. Fong, "From Kane to World Trade Center: A 40-Year Journey in Computational Mechanics and Applied Physics," SMAC-Stanford Symposium on Topics in Analytical Dynamics and Applied Mechanics, Stanford University, Stanford, CA, March 5, 2004.
10. J. Fong, "The Role of Metrological Research and the Application of Design of Experiments in Verification and Validation of Computer Solutions," Applied Research Associates, Inc., Littleton, CO, Aug. 2, 2004.
11. J. Fong, "The Role of Metrological Research and the Application of Design of Experiments in Verification and Validation of Computer Solutions," Sandia National Laboratories, Albuquerque, NM, Aug. 5, 2004.
12. D. Gilsinn, M. McClain, and C. Witzgall, "Using Nonoscillatory Splines to Model Urban Environments," SIAM Conference on Geometric Design and Computing, Seattle, WA, November 10-13, 2003.
13. F. Hunt, "Constructing Sequence Alignments from a Markov Decision Model with Estimated Parameter Values," Biological Language Conference, University of Pittsburgh, Pittsburgh, PA., November 21, 2003.
14. F. Hunt, "Markov Decision Processes and a Potential Application to Biological Sequence Alignment," American Mathematical Society Southeastern Section meeting, Tallahassee, FL, March 13, 2004.
15. A. Kearsley "Managing Explicit Nuclear Magnetic Resonance (NMR) Nonlinear Constraints on the Interatomic Distances"', DIMACS Working Group on New Algorithms for Inferring Molecular Structure from Distance Restraints, Rutgers University, New Brunswick, New Jersey, January 19, 2004.
16. E. Knill, "Postselected Quantum Computation," Quantum Information and Control Conference, Toronto, Ontario, Canada, July 22, 2004.
17. E. Knill, "Quantum Computing with Linear Optics," SPRC Annual Meeting, Stanford University, Stanford, CA, Sept 13, 2004.
18. D. Lozier, "MKM and the NIST Digital Library of Mathematical Functions," 2nd North American Workshop on Mathematical Knowledge Management, Phoenix, AZ, January 6, 2004.
19. G. McFadden, "Phase-Field Models of Solidification and Electrochemistry," Department of Materials Science and Engineering Seminar, Rensselaer Polytechnic Institute, Troy, NY, October 30, 2003.
20. G. McFadden, "Phase-Field Modeling of Electrochemistry," Department of Mathematical Sciences Department Seminar, New Jersey Institute of Technology, Newark, NJ, November 14, 2003.
21. G. McFadden, "Phase-Field Modeling of Elastic Effects During Phase Transitions," 3rd Annual Workshop on the Evolution and Self-Assembly of Quantum Dots, Northwestern University, Evanston, IL, August 16-17, 2004.
22. L. Melara, "Computational Modeling of Austenite-twinned-Martensite Interface," Department of Mathematical Sciences, University of Delaware, Newark, DE, November 11, 2003.
23. L. Melara, "Introduction to the Finite Element Method," Department of Mathematics, Colorado College, Colorado Springs, CO, January 26, 2004.
24. L. Melara, "Computational Modeling of Austenite-twinned-Martensite Interface," Colloquium, Department of Mathematics, Colorado College, Colorado Springs, CO, January 27, 2004.
25. L. Melara, "Introduction to the Finite Element Method," Department of Mathematics, Union College, Schenectady, NY, February 9, 2004.
26. L. Melara, "Simulation of an Austenite-Twinned-Martensite Interface, a PDE Optimization Problem," Computational Sciences and Mathematics Research, Sandia National Laboratories, Livermore, CA, June 7, 2004.
27. W.F. Mitchell, "A Parallel Adaptive Multilevel Method for Elliptic Boundary Value and Eigenvalue Problems, Rensselaer Polytechnic Institute, Troy, NY, February 4, 2004.

Local Area

28. I. Beichl, "Fast Methods for Sampling from a Dynamic PDF Part I: Fast Methods, Some Up-Front Cost," University of Maryland, Oct. 16, 2003.
29. I. Beichl, "Approximate Counting with Stratified Sampling: the 3D Hard Sphere Entropy Constant," Mathematics Research Division, NSA, Fort Meade, MD, April 7, 2004.
30. I. Beichl, "Counting, the Monte Carlo Way," NIST SURF Summer Seminar Series, July 3, 2004.
31. S. Bullock, "Time Reversal Symmetry and Concurrence Dynamics," NIST Quantum Information and Bose Einstein Condensate Seminar (QIBEC,) April 21, 2004.
32. S. Bullock and G. Brennen, "Time Reversal Symmetry and Entangled Eigenstates," Quantum Information and Coherence Seminar, University of Maryland, College Park, MD, May 4, 2004.

33. S. Bullock, "Matrix Decompositions and Quantum Circuit Design," Second Feynman Festival, University of Maryland College Park Physics Department, August 21, 2004.
34. S. Bullock, "Some Results on Quantum Circuits Design," UMBC Electrical Engineering and Computer Science Seminar, Sept. 17, 2004.
35. A. Carasso, "Singular Integrals and Recovery of Texture in Image Deblurring," Department of Mathematics, University of Maryland, College Park, MD, February 5, 2004.
36. J. Devaney, "Science at the Speed of Thought," The Coalition for Academic Scientific Computation Meeting, Washington, DC, March 4, 2004.
37. M. J. Donahue, "Standard Problems and Public Code for Micromagnetics," IFIP Workshop on the Changing Face of Mathematical Software, Washington, DC, June 3, 2004.
38. J. Fong, "An ISO-compliant Reference Benchmark Approach to Verification & Validation of Virtual Prototyping," DOD Defense Modeling & Simulation Office, Arlington, VA, July 15, 2004.
39. J. Fong, "The Role of Metrological Research and the Application of Design of Numerical Experiments (DNEX) in Verification and Validation of Virtual Prototyping," Office of Nuclear Regulatory Research, U. S. Nuclear Regulatory Commission, Rockville, MD, Sept. 13, 2004.
40. W. George, "A Java Based Parallel and Distributed Computing Environment," Bowie State University, Feb 26, 2004.
41. F. Hunt, "Visualizing the Frequency Patterns of DNA sequences," 4th Virtual Bioinformatics Research Conference, Ballston, VA, Sept. 21, 2004.
42. A. Kearsley, "An Infeasible Point Method for Solving a Class of Multidimensional Scaling Problems," University of Maryland, College Park, MD, Sept. 21, 2004.
43. J. Kelso, "Virtual Environments Using DIVERSE," Virginia Tech, Blacksburg, VA, August 16, 2004.
44. E. Knill, "Linear Optics Approaches," Quantum Information Science, Engineering, and Technology Workshop, Boulder, CO, April 30, 2004.
45. S. Langer, "Object Oriented Modeling of Microstructural Physics," Workshop on Nonequilibrim Interface Dynamics: Theory and Simulation from Atomistic to Continuum Scales, Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park, MD, October 27, 2003.
46. S. Langer, "OOF: Object-Oriented Finite Element Analysis for Materials Scientists," Physics Colloquium, Georgetown University, Washington DC, February 17, 2004.
47. S. Langer, "Object Oriented Modeling of Microstructural Physics," Mechanical Engineering Colloquium, University of Maryland Baltimore Country, April 9, 2004.
48. S. Langer, "OOF: Object Oriented Modeling of Material Microstructure," IFIP Workshop on the Changing Face of Mathematical Software, Washington, DC, June 3, 2004.
49. D. Lozier and B. Miller, "A Handbook of Special Functions for the Digital Age," SIMA Technical Seminar, NIST, Gaithersburg, MD, February 24, 2004.
50. G. McFadden, "Interfacial Boundary Conditions and Phase-field Models of Solidification, Nonequilibrium Interface Dynamics: Theory and Simulation from Atomistic to Continuum Scales," Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park, MD, October 20, 2003.
51. B. Miller, "Representing Mathematical Knowledge in the Digital Library of Mathematical Functions," IFIP Workshop on the Changing Face of Mathematical Software, Washington DC, June 4, 2004.
52. R. Pozo, "The Role of Java in High Performance Computing," IFIP Workshop on the Changing Face of Mathematical Software, Washington DC, June 3, 2004.
53. A. Youssef, Search in Mathematical Databases, IFIP Workshop on the Changing Face of Mathematical Software, Washington DC, June 4, 2004.

Conference Presentations

International

1. S. Bullock, "Quantum Circuit Design and the Word Problem on the Unitary Group," Conference on Locally Symmetric Spaces, Mathematisches Forschungsinstittut Oberwolfach, Oberwolfach Germany, Oct. 1, 2003.
2. S. Bullock, "Gaussian Weighted L_2 Cohomology of Locally Symmetric Spaces," Conference on Locally Symmetric Spaces, Mathematisches Forschungsinstittut Oberwolfach, Oberwolfach Germany, Oct. 1, 2003.

3. T .J. Burns (with M.A. Davies, R.L. Rhorer, D. Basak, H.W. Yoon, R.J. Fields, L.E. Levine, E.P. Whitenton, M.D. Kennedy, and R. Ivester), "Influence of Heating Rate on Flow Stress in High-Speed Machining Processes," *7th CIRP International Workshop on Modelling of Machining Operations*, Cluny, France, May 4, 2004.
4. J. Devaney (with S. Satterfield and J. Hagedorn), "Science at the Speed of Thought" at the Workshop on Ambient Intelligence for Scientific Discovery, Vienna, Austria, April 25, 2004.

Domestic

5. B. Alpert, "Successes and Sticky Issues for Nonreflecting Boundary Conditions," International Conference on Spectral and High-Order Methods (ICOSAHOM), Providence, RI, June 22, 2004.
6. I. Beichl, "Approximate Counting with Stratified Sampling: the 3D Hard Sphere Entropy Constant," SIAM Workshop on Combinatorial Scientific Computing (CSC04), San Francisco, CA, February 28, 2004.
7. S. Bullock, "Entanglement Capacity of n-qubit Quantum Computations," SPIE Symposium, Orlando, FL, April 14, 2004.
8. A. Carasso, "Singular Integrals and Recovery of Texture in Image Deblurring," SIAM Conference on Imaging Science, Salt Lake City, UT, May 5, 2004.
9. D. Cotrell and A. J. Pearlstein, "Computation of Flow between a Rotating Screw and a Coaxial Circular Cylinder," American Physical Society Division of Fluid Dynamics Meeting, Rutherford, NJ, November 23-25, 2003.
10. J. Devaney, "Cement and Concrete: Parallel Computing, Scientific and Information Visualization," VCCTL (Virtual Cement and Concrete Testing Laboratory) Annual Meeting, November 20-21, 2003.
11. M. Donahue, "OOMMF: Where Is It, Where Is It Going?" muMAG meeting, Anaheim, CA, January 7, 2004.
12. M. Donahue, "Motion of Magnetic Domain Walls in Thin, Narrow Strips," SIAM Conference on Mathematical Aspects of Materials Science, Los Angeles, CA, May 23, 2004.
13. D. Gilsinn, M. McClain, C. Witzgall., "Experiences Using L_1 Splines in Modeling Urban Environments," SIAM Geometric Design and Computing Conference, Seattle, WA, Nov. 12-14, 2003.
14. D. Gilsinn, "Integral Equation Methods of Estimating Characteristic Multipliers for Linear DDEs with Periodic Coefficients" 2004 SIAM Annual Meeting, Portland, OR, July 10-16, 2004.
15. K. Irikura, R. Johnson, and R. Kacker, "Uncertainty Associated with Virtual Measurements from Computational Chemistry Models," Measurement Science Conference 2004, Anaheim, CA, Jan. 15-16, 2004.
16. R. Kacker, "Penal Discussion: ISO Guide to the Expression of Uncertainty in Measurement: Conventional vs. Bayesian Statistical Methods," National Conference of Standards Laboratories International, Salt Lake City, UT, July 11-15, 2004.
17. R. Kacker, "Statistical Interpretation of Key Comparison Reference Value and Degrees of Equivalence," National Conference of Standards Laboratories International, Salt Lake City, UT, July 11-15, 2004.
18. R. Kacker, "Combining Information from Interlaboratory Evaluations using Random Effects Model," National Conference of Standards Laboratories International, Salt Lake City, UT, July 11-15, 2004.
19. J. Kelso and S. Satterfield, "DIVERSE: Open-Source VR and Simulation API," Birds of a Feather Session, SIGGRAPH '04, Los Angeles, CA, August 12, 2004.
20. D. Lozier, "Digital Library of Mathematical Functions: A Project Report," AMS-SIAM Special Session on Classical and Nonlinear Special Functions, Joint Mathematics Meetings, Phoenix, AZ, January 8, 2004.
21. L. Melara, "Simulation of Twinned-Martensite as a PDE Optimization Problem," Sixth Joint AMS-SMM International Meeting, Houston, TX, May 15, 2004.
22. B. Miller, "Authoring Mathematical Knowledge," 2nd North American Workshop on Mathematical Knowledge Management, Phoenix, AZ, January 6, 2004.
23. W. Mitchell, "Adaptive Grid Refinement for a Model of Two Confined and Interacting Atoms," Adaptive Methods for Partial Differential Equations and Large-Scale Computation Conference, Troy NY, October 12, 2003.
24. W. Mitchell and E. Tiesinga, "On Preconditioners for Interior Eigenvalues of Schroedinger's Equation," 2003 International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications, Napa, CA, October 28, 2003.

25. W. Mitchell and E. Tiesinga, "A Parallel Multigrid Method Applied to Schroedinger's Equation," The Eleventh Conference on Parallel Processing for Scientific Computing, San Francisco, CA, February 26, 2004.
26. A. Pearlstein and D. Cotrell, "Computation of Pressure-Driven Flow between a Nonrotating Screw and an Outer Coaxial Circular Cylinder," American Physical Society Division of Fluid Dynamics Meeting, Rutherford, NJ, November 23-25, 2003.
27. D. Porter, "OOMMF 1.1b2 Release," MicroMagnetic Modeling Activity Group Meeting, Anaheim, CA, January 8, 2004.
28. D. Porter and M.J. Donahue, "Velocity of Tranverse Domain Wall Motion Along Thin, Narrow Strips," 9th Joint MMM/Intermag Conference, Anaheim, CA, January 6, 2004.
29. B. Saunders and Q. Wang, "Mesh Generation for Effective 3D Visualizations in a Digital Library of Mathematical Functions," 13th International Meshing Roundtable, Williamsburg, VA, September 19-22, 2004.
30. D. Song, "Entanglement Swapping Based Quantum Key Distribution," DARPA Quantum Information Science and Technology (QuIST) Review Meeting, Chicago, IL, May 4-6, 2004."

Local Area

31. R. Kacker, "Combining Information from Interlaboratory Studies Using Random Effects Model," Eleventh Spring Research Conference on Statistics in Industry and Technology, American Statistical Association and the Institute of Mathematical Statistics, NIST, Gaithersburg, MD, May 19-21, 2004.

Software Released

1. M. Donahue and D. Porter, OOMMF 1.1.1.2, January 15, 2004.
2. D. Porter contributed to Tcl/Tk releases 8.4.5 (November 24, 2003), 8.4.6 (March 1, 2004), 8.5a1 (March 3, 2004), and 8.4.7 (July 29, 2004).
3. J. Kelso, visualization DSOs and utilities: tim.2 (Things In Motion, version 2), xwand, printScenegraph, smallFeatureCull DSO, dtk-writeShm, lodScale DSO, sgb (Scene Graph Builder) file loader, ifl (Instancing File loader), lod (Level Of Detail) file loader, m4 pseudo loader, flatten pseudo loader, clean" pseudo loader.
4. S. Langer, OOF2 version 2.0.b2.
5. A. Peskin, ABCDswitch DSO.
6. R. Pozo, Sparse Basic Linear Algebra Subprograms (BLAS) in ANSI C, preliminary version.
7. R. Pozo, SparseLib++ Version 1.6.
8. R. Pozo, Matrix Market Matlab input/output code update.
9. R. Pozo, Template Numerical Toolkit (TNT), Version 1.2.1 and Version 1.2.2.

Conferences, Minisymposia, Lecture Series, Shortcourses

MCSD Seminar Series

1. D. Gilsinn (ITL), "Approximating Limit Cycles of an Autonomous Delay Differential Equation," September 28, 2004.
2. S. Bullock (ITL), "Matrix Decompositions and Quantum Circuit Design," September 15, 2004.
3. K. Mills (ITL), "Considering Emergence in Global Information Systems," July 27, 2004.
4. E. Shirley (PL), "Intrinsic Birefringence in Cubic Crystalline Optical Materials," June 10, 2004.
5. A. Sandu (Virginia Polytechnic Institute and State Univ.), "KPP: A Software Environment for Modeling Chemical Kinetics," May 25, 2004.
6. T. Schulze (Univ. of Tennessee), "Some New Tools for Simulating Nano-Scale Crystal Growth," May 10, 2004.

7. R. Nochetto (Univ. of Maryland), "Finite Element Methods for Surface Diffusion and Applications to Stressed Epitaxial Films," May 4, 2004.
8. K. Irikura, R. Johnson (CSTL) and R. Kacker (ITL), "Uncertainty from Bias in Virtual Measurements and the NIST Computational Chemistry Comparison and Benchmark Database," April 20, 2004.
9. J. Hubbard (CSTL), "Hydrodynamics, Electrostatics, and Brownian Motion: Some Rigorous, Tight Bounds," April 6, 2004.
10. C. Williams (PL), "An Introduction to Quantum Computing," March 23, 2004.
11. H. Elman (Univ. of Maryland), "Preconditioning Strategies for Models of Incompressible Flow," March 15, 2004.
12. R. Mountain (CSTL), "Molecular Dynamics Simulations and Sources of Uncertainty in Virtual Measurements," February 24, 2004.
13. T. Wanner (George Mason Univ.), "Pattern Formation in Cahn-Hilliard-Type Models," February 17, 2004.
14. A. Rukhin (ITL and UMBC), "Balanced Randomization Designs and Classical Probability Distributions," February 3, 2004.
15. K. Prasad (BFRL), "Coupled Fire Dynamics and Thermal Response of Complex Building Structures," January 20, 2004.
16. A. Carasso, "Singular Integrals, Image Smoothness, and the Recovery of Texture in Image Deblurring," December 16, 2003.
17. V. Torczon, "Generating Set Search for Nonlinear Programming," December 9, 2004.
18. R. Rainsberger, "Mesh Generation for Non-linear Finite Element Analysis," December 4, 2003.
19. L. Melara, "Computational Modeling of Austenite-twinned-Martensite Interface" November 18, 2003.
20. D.L. Cotrell, "Linear Stability of Spiral Poiseuille Flow and Comparison to Experiments," November 4, 2003.
21. L. Giraud, "Sparse Iterative Techniques for the Solution of the 3D Maxwell Equations in Boundary Element Formulation," October 31, 2003.
22. T. Burns, "Subcritical Flip Bifurcation in High-Speed Machining," October 22, 2003.
23. B. Schneider, "The Discrete Variable Method for the Time Dependent and Time Independent Schroedinger Equation, Part II," October 15, 2003.
24. B. Schneider, "The Discrete Variable Method for the Time Dependent and Time Independent Schroedinger Equation, Part I," October 14, 2003.
25. M. Mascagni, "Computational Infrastructure for Parallel, Distributed, and Grid-based Monte Carlo Computations," October 9, 2003.

Local Events Organized

1. R. Boisvert, Organizing Committee, NIST Workshop on Metrology and Instrumentation for Nanotechnology, Gaithersburg, January 27-28, 2004.
2. R. Boisvert, Organizer, Workshop on the Changing Face of Mathematical Software, International Federation for Information Processing (IFIP) Working Group 2.5 (Numerical Software), Washington, DC, June 3-4, 2004.
3. J. Fong, Chair, Organizing Committee, NIST Workshop on the Verification and Validation of Computer Models of High-Consequence Engineering Systems, Nov. 8-9, 2004.
4. D. E. Gilsinn, Organizer, Symposium on Topics in Operations Research, NIST Gaithersburg, May 13, 2004. Held in honor of the retirement of Christoph Witzgall.

IFIP Working Group 2.5 on Numerical Software meets in Washington in June 2004. From left to right: Wayne Enright, Bill Gropp, Bo Einarsson, Michael Thune, Craig Douglas, Ian Gladwell, Mladen Vouk, Brian Ford, Jim Pool, Ulrich Kulisch, and Mo Mu.

External Events Organization

1. R. Boisvert, Program Committee, *International Symposium on Symbolic and Algebraic Computation*, Beijing, China, July 2005, http://www.mmrc.iss.ac.cn/~issac2005.
2. R. Boisvert, Co-chair, Program Committee, *Symposium on Scientific Computing and Mathematical Software in Emerging Sciences and Technology*, Hong Kong, China, June 2005, http://www.math.ust.hk/~mamu/IFIP/Announce.html.
3. A. Carasso, Co-Organizer, Minisymposium on Loss and Recovery of Fine Structure in Image Processing, SIAM Image Science Conference, Salt Lake City, May 2004.
4. J. Devaney, Program Committee, Government and Industrial Track, Knowledge Discovery in Databases Conference.
5. M. Donahue, Program Committee, 49th Conference on Magnetism and Magnetic Materials, Washington DC, July 18-19, 2004.
6. J. Fong, Co-Chair, Symposium on Topics in Analytical Dynamics and Applied Mechanics, Stanford University, March 5, 2004.
7. D. E. Gilsinn, Chair, Minisymposium on Recent Developments in Methods of Solving Delay Differential Equations, SIAM 2004 Annual Meeting, Portland, OR, July 12-16, 2004.
8. D.W. Lozier, Organizing Committee, AMS-SIAM Special Session on Classical and Nonlinear Special Function, Joint Mathematics Meetings, Phoenix, AZ, January 7-10, 2004.
9. D.P. O'Leary, Organizing Committee, 2004 SIAM National Meeting.

Other Professional Activities

Internal

1. I. Beichl, Co-coordinator, ITL Summer Undergraduate Research Fellowship (SURF) Program
2. R. Boisvert and Abbie O'Gallagher, ITL Diversity Committee.

3. R. Boisvert, NIST People Council.
4. R. Boisvert, NIST Nanotechnology Strategic Working Group.
5. R. Boisvert, NIST Scientific Computing Steering Group.
6. D. Porter, ITL Awards Committee.
7. 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, Editorial Board, *Computing in Science & Engineering*.
3. I. Beichl, Associate Editor, *Journal of Numerical Analysis and Computational Mathematics*
4. R. Boisvert, Editor-in-Chief, *ACM Transactions on Mathematical Software*.
5. M. Donahue, *Journal of Computational Methods in Science and Engineering*
6. E. Knill, *IEEE Transactions on Information Science*
7. D. Lozier, Associate Editor, *Mathematics of Computation*.
8. G. McFadden, Associate Editor, *Journal of Crystal Growth.*
9. G. McFadden, Associate Editor, *Interfaces and Free Boundaries.*
10. G. McFadden, Associate Editor, *SIAM Journal on Applied Mathematics.*
11. W. Mitchell, Associate Editor, *Journal of Numerical Analysis and Computational Mathematics*
12. D. O'Leary, Editorial Board, *Computing in Science & Engineering*.
13. D. O'Leary, Editorial Board, SIAM Book Series on Fundamentals of Algorithms.
14. R. Pozo, Associate Editor, *ACM Transactions on Mathematical Software*

Boards and Committees

1. R. Boisvert, ACM Publications Board.
2. R. Boisvert, Chair, International Federation for Information Processing Working Group 2.5 (Numerical Software)
3. R. Boisvert, Technical Review Committee, Institute for Defense Analysis Center for Computing Sciences.
4. J. Devaney, High End Computing Group, National Coordination Office for Information Technology Research and Development.
5. J. Devaney, High End Computing Revitalization Task Force.
6. F. Hunt, Executive Committee, Association for Women in Mathematics.
7. D. Lozier, Chair, SIAM Activity Group on Orthogonal Polynomials and Special Functions.
8. D. O'Leary, SIAM/AMS/ASA/AWM/IMS/MAA/NCTM Joint Committee on Women
9. D. Porter, Tcl Core Team.
10. B. Saunders, External Advisory Council, School of Computer, Mathematical and Natural Sciences, Morgan State University.

Reviewing

1. Division staff members referee manuscripts for a wide variety of journals including

American Mathematical Monthly
ASME Journal of Manufacturing Science and Engineering
Computers and Mathematics with Applications
Computers in Engineering
IEEE Transactions on Antennas and Propagation
IEEE Transactions on Computer Aided Design (TCAD)
IEEE Transactions on Electromagnetic Compatibility
IEEE Transactions on Instrumentation and Measurement
IEEE Transactions on Magnetics

IEEE Transactions on Parallel and Distributed Computing
International Journal of Numerical Methods in Engineering
International Journal of Plasticity
Journal of Computational and Applied Mathematics
Journal of Computational Physics
Journal of Computational Statistics
Journal of Magnetism and Magnetic Materials
Journal of Physics A: Mathematical and General Physic
Journal of Physics B: Atomic, Molecular, and Optical Physics
Journal of Rheology
Metrologia
Physical Review A
Physical Review B
Physical Review Letters
Precision Engineering
Radio Science
SIAM Journal on Applied Mathematics
SIAM Journal on Numerical Analysis
SIAM Journal on Optimization
SIAM Journal of Scientific Computing
Theoretical Computer Science
Total Quality Management and Business Excellence

2. Staff members review proposals for the following research programs: Kentucky Science and Engineering Foundation (KSEF), Civilian Research and Development Foundation, University of California Microelectronics Innovation and Computer Research Opportunities (MICRO) Program, Dutch National Science Foundation (NWO), and the National Science Foundation (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

Absoft Corporation
Altera Corporation
American Hydro Corp.
Applied Research Associates, Inc.
Atrenta, Inc.
Cisco Systems
Computers and Structures, Inc.
Cray, Inc.
Delta Add-Power Systems
Ether Media
Fuji Electric Advanced Tech., Co., Ltd.
General Electric Research Labs
Institute for Electronic Design Automation
Integral Systems, Inc.
Integrity Applications, Inc.
Intel Corporation
Invensys Systems, Inc.
Lick Observatory
Livermore Software Technology Corp.
Lucent Technologies
Mallett Technology, Inc.
Open Tech Inc.
Optimization Partner Stockholm AB
Raytheon
Rockwell Collins
SAC Capital
SIGOS
Superior Methods
System Planning Corp.
Targacept
Well Code Software
XYZ Scientific Applications, Inc.

Government/Non-profit Organizations

Association for Computing Machinery (ACM)
American Mathematical Society (AMS)
Air Force Office of Scientific Research
Army Research Office
DARPA
European Southern Observatory
FBI
IDA Center for Computing Sciences
Japan Aerospace Exploration Agency
Jet Propulsion Laboratory
Los Alamos National Laboratory
Mayo Clinic
National Institutes of Health
National Coordination Office for IT R&D
NASA
National Security Agency
NOAA
National Science Foundation (NSF)
Office of Naval Research
Office of Science and Technology Policy (OSTP)
Ohio Supercomputer Center
Research Org. for Info. Science & Tech. (Japan)
Sandia National Laboratory
Senate Appropriations Committee
Society for Industrial and Applied Mathematics (SIAM)
The Canadian Space Agency
U.S. Army Night Vision Laboratory
U.S. Department of Energy
U.S. Department of Defense
U.S. Joint Forces Command
U.S. Nuclear Regulatory Commission
Walter Reed Army Institute of Research

Universities

Abilene Christian University
American University
American University of Beruit Medical Center
Boston University
Bowie State University
Brown University
Cachan University (France)
Chinese Academy of Sciences
Colorado College
Coppin State University
Cornell University
Delaware State University
Drexel University
Duke University
George Mason University
George Washington University
Georgetown University
Graz University (Austria)
Illinois Institute of Technology
Innsbruck University (Austria)
Instituto Nazionale per las Fisica della Materia (Spain)
International University of Bremen (Germany)
Iowa State University
Jackson State University
New Mexico State University
Millersville University
Mississippi State University
MIT
Morgan State University
Northwestern University
Penn State University
Princeton University
Purdue University
Rensselaer Polytechnic Institute
Saarland University (Germany)
San Jose State University
Sienna College
Stanford University
Technion (Israel)
Tel-Aviv University (Israel)
Union College
University of Alaska
University of California
University of Cambridge
University of Cincinnati
University of Erlangen-Nurenberg (Germany)
University of Houston
University of Idaho
University of Illinois
University of Indiana
University of Iowa
University of Kentucky
University of Maryland
University of Minnesota
University of Mons (Belgium)
University of New Mexico
University of North Carolina
University of Puerto Rico
University of San Diego
University of Southhampton (United Kindom)
University of Tokyo
University of Valparaiso (Chile)
University of Verlangen (Germany)
University of Washington
University of Wisconsin

Utrecht University (The Netherlands)
Virginia Tech
Williams College

Part IV

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 and appointments. The following list reflects the status at the end of FY 2004.

Division Staff

Ronald Boisvert, *Chief* , Ph.D. (Computer Science), Purdue University, 1979
Robin Bickel, *Secretary*
Joyce Conlon, B.A. (Mathematics), University of Maryland Baltimore County, 1979
Jeffrey Fong, Ph. D. (Applied Mechanics and Mathematics), Stanford University, 1966
Roldan Pozo, Ph.D. (Computer Science), University of Colorado at Boulder, 1991

Mathematical Modeling Group

Geoffrey McFadden, *Leader* , Ph.D. (Mathematics), New York University, 1979
Bradley Alpert (Boulder) , Ph.D. (Computer Science), Yale University, 1990
Timothy Burns, Ph.D. (Mathematics), University of New Mexico, 1977
Alfred Carasso, Ph.D. (Mathematics), University of Wisconsin, 1968
Andrew Dienstfrey (Boulder), Ph.D. (Mathematics), New York University, 1998
Michael Donahue, Ph.D. (Mathematics), The Ohio State University, 1991
Fern Hunt, Ph.D. (Mathematics), New York University,
Raghu Kacker, Ph.D. (Statistics), Iowa State University, 1979
Anthony Kearsley, Ph.D. (Computational and Applied Mathematics), Rice University, 1996
Peter Ketcham. M.S. (University of Minnesota), 1997
Stephen Langer, Ph.D. (Physics), Cornell University, 1989
Agnes O'Gallagher (Boulder), M.S. (Applied Math), University of Colorado at Boulder, 1991
Donald Porter, Ph.D. (Electrical Engineering), Washington University, 1996

Postdoctoral Fellows
David Cotrell, Ph.D. (Mech. Engineering), University of Illinois at Urbana-Champaign, 2003

Faculty Appointees
Richard Braun (University of Delaware)
Dianne O'Leary (University of Maryland College Park)
Florian Potra (University of Maryland Baltimore County)

Guest Researchers
Daniel Anderson (George Mason University)
Katharine Gurski (George Washington University)
Seung-Ill Haan (University of Maryland Baltimore County)

Students
Eric Baer (Carnegie Mellon University)
Christopher Copeland (Vanderbilt University)

Mathematical Software Group

Daniel Lozier, *Leader,* Ph.D. (Applied Mathematics), University of Maryland, 1979
Marjorie McClain, M.S. (Mathematics), University of Maryland College Park, 1984
Bruce Miller, Ph.D. (Physics), University of Texas at Austin, 1983
William Mitchell, Ph.D. (Computer Science), University of Illinois at Urbana-Champaign, 1988
Bert Rust, Ph.D. (Astronomy), University of Illinois at Urbana-Champaign, 1974
Bonita Saunders, PhD (Mathematics), Old Dominion University, 1985

Faculty Appointees
Bruce Fabijonas (Southern Methodist University)
G.W. Stewart (University of Maryland College Park)
Abdou Youssef (George Washington University)

Guest Researchers
Leonard Maximon (George Washington University)
Frank Olver (University of Maryland College Park)

Students
Elaine Kim (Stanford University)

Optimization and Computational Geometry Group

Ronald Boisvert, *Acting Leader*
Isabel Beichl, Ph.D. (Mathematics), Cornell University, 1981
Javier Bernal, Ph.D. (Mathematics), Catholic University, 1980
David Gilsinn, Ph.D. (Mathematics), Georgetown University, 1969
Emanuel Knill (Boulder), Ph.D., (Mathematics), University of Colorado at Boulder, 1991

Postdoctoral Fellows
Stephen Bullock, Ph.D. (Mathematics), Cornell University, 2000
Scott Glancy (Boulder), Ph.D. (Physics), University of Notre Dame, 2004

Faculty Appointees
Saul Gass (University of Maryland College Park)
James Lawrence (George Mason University)

Guest Researchers
David Song
Francis Sullivan (IDA Center for Computing Sciences)
Christoph Witzgall
Anoka Yimsiriwattana (University of Maryland Baltimore County)

Scientific Applications and Visualization Group

Judith Devaney, *Leader*, Ph.D. (Information Technology), George Mason University, 1998
Yolanda Parker, *Office Manager*
Robert Bohn, Ph.D. (Physical Chemistry), University of Virginia, 1991

William George, Ph.D. (Computer/Computational Science), Clemson University, 1995
Terence Griffin, B.S. (Mathematics), St. Mary's College of Maryland, 1987
John Hagedorn, M.S. (Mathematics), Rutgers University, 1980
Howard Hung, Ph.D. (Operations Research), University of Massachusetts, 1973
John Kelso, M.S. (Computer Science), George Washington University, 1984
Adele Peskin (Boulder), Ph.D. (Chemical Engineering), University of Colorado at Boulder, 1985
Steven Satterfield, M.S. (Computer Science), North Carolina State University, 1975
James Sims, Ph.D. (Chemical Physics), Indiana University, 1969

Staff Leaving the Division During FY 2004

Postdoctoral Fellows
Luis Melara

Guest Researchers
Alan Goldman
Bruce Murray
Eduardo Martinez-Vecino

Students
Whitney Austin
Shauntia Burley
Angel Villalain-Garcia
Michael Huber
Brandon Smith

Acronyms

ACM	Association for Computing Machinery
AMS	American Mathematical Society
ANSI	American National Standards Institute
API	application programming interface
APS	American Physical Society
ATP	NIST Advanced Technology Program
AWM	Association for Women in Mathematics
BFRL	NIST Building and Fire Research Laboratory
BLAS	Basic Linear Algebra Subprograms
CAD	computer-aided design
CARB	NIST Center for Advanced research in Biotechnology
CCCBDB	NIST Computational Chemistry Comparison and Benchmark Database
CCD	concurrence canonical decomposition
CCS	Center for Computing Sciences
CEM	computational electromagnetics
CG	conjugate gradient
CSTB	Centre Scientifique et Technique du Batiment
CSTL	NIST Chemical Science and Technology Laboratory
CTCMS	Center for Theory and Computation in Materials Science
CWI	Centrum voor Wiskunde en Informatica (National Research Institute for Mathematics and Computer Science in the Netherlands)
DARPA	Defense Advanced Research Projects Agency
DIVERSE	Device Independent Virtual Environments — Reconfigurable, Scalable, Extensible (visualization software)
DLMF	Digital Library of Mathematical Functions (MCSD project)
DOD	Department of Defense
DOE	Department of Energy
DPD	dissipative particle dynamics
DSO	distributed shared object
ECG	explicitly correlated Gaussian
EEEL	NIST Electronics and Electrical Engineering Laboratory
EM	electromagnetic
EPA	Environmental Protection Agency
ESRF	European Synchrotron Radiation Facility
FY	fiscal year
GAMS	Guide to Available Mathematical Software
GMR	giant magneto-resistance
GMRES	generalized minimal residual
HECRTF	High End Computing Revitalization Task Force
Hy-Cl	Hylleraas-Configuration Interaction
IDA	Institute for Defense Analysis
IMPI	Interoperable MPI
IT	information technology
ITL	NIST Information Technology Laboratory
IFIP	International Federation for Information Processing
ISO	International Organization for Standardization
JAMA	Java Matrix package
JVM	Java virtual machine

LADAR	Laser Distance and Ranging
LOQC	linear optics quantum computation
LP	linear programming
MatCASE	Materials Computation and Simulation Environment
MCSD	ITL Mathematical and Computational Sciences Division
MEL	NIST Manufacturing Engineering Laboratory
MKM	mathematical knowledge management
MPI	Message Passing Interface
MRAM	magnetic random access memory
MSEL	NIST Materials Science and Engineering Laboratory
Mspec	mass spectrometry
NAG	Numerical Algorithms Group
NASA	National Aeronautics and Space Administration
NBS	National Bureau of Standards (former name of NIST)
NIH	National Institutes of Health
NIJ	National Institute of Justice
NIRT	NSF Nanoscale Interdisciplinary Research Team
NIST	National Institute of Standards and Technology
NOAA	National Oceanographic and Atmospheric Administration
NRC	National Research Council
NSA	National Security Agency
NSF	National Science Foundation
ODE	ordinary differential equation
OLES	NIST Office of Law Enforcement Standards
OMB	Office of management and Budget
OOF	Object-Oriented Finite Elements (software package)
OOMMF	Object-Oriented Micromagnetic Modeling Framework (software package)
OSTP	Office of Science and Technology Policy
PDE	partial differential equation
PHAML	Parallel Hierarchical Adaptive Multi Level (software)
PL	NIST Physics Laboratory
QDPD	quarternion-based dissipative particle dynamics
QKD	quantum key distribution
QMR	quasi-minimal residual
quant/ph	quantum physics report archive at www.arXiv.org
RAVE	Reconfigurable Automatic Virtual Environment
SAVG	MCSD Scientific Applications and Visualization Group
SEM	scanning electron micrograph
SIAM	Society for Industrial and Applied Mathematics
SMS	smart machining system
SSS	Screen Saver Science
SURF	Student Undergraduate Research Fellowship
SVD	singular value decomposition
TIN	triangulated irregular network
TNT	Template Numerical Toolkit
TOMS	Transactions on Mathematical Software
VCCTL	Virtual Cement and Concrete Testing Laboratory
VRML	Virtual Reality Modeling Language
WTC	World Trade Center