Part III

Project Summaries

Mathematical Knowledge Management

Digital Library of Mathematical Functions

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http://dlmf.nist.gov/

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

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

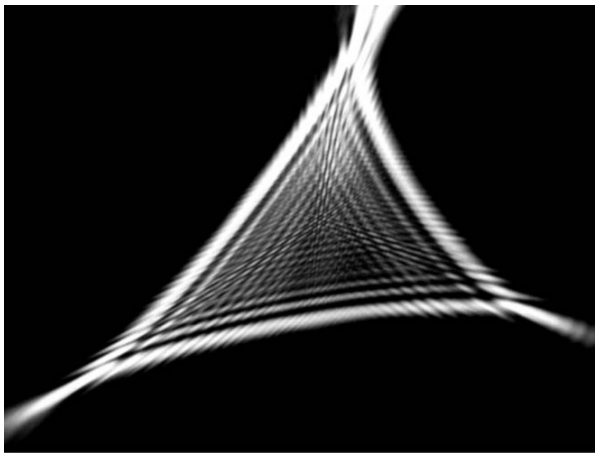

Figure 24. *A thin beam of light refracted by an irregularity in bathroom-window glass produces this image on a distant screen. The bright sharp-edged triangle is a caustic, that is, a line of focused light. The oscillating intensity of the interference fringes across the caustic is described by the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

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

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

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

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

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

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

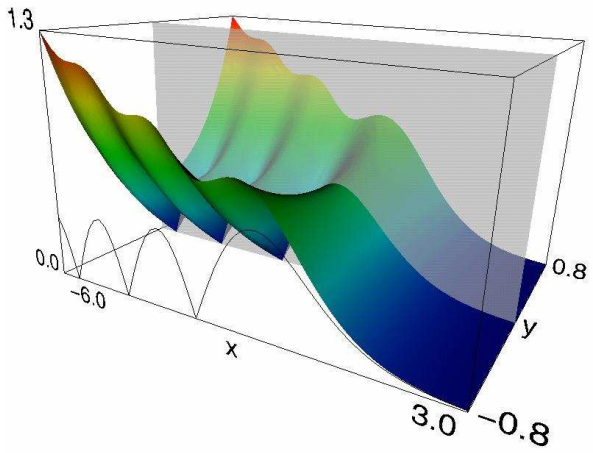

Figure 25. *The absolute value of the Airy function as a function of a complex variable. The interference fringes in Fig. 24 correspond to the oscillating behavior of the function when the variable is restricted to the negative real line.*

Representation and Exchange of Mathematical Data

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

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

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

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

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

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

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

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

Fundamental Mathematical Software Development and Testing

Sparse BLAS Standardization

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

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

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

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

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

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

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

Roldan Pozo
Bruce Miller

http://math.nist.gov/scimark

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

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

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

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

TNT: Object Oriented Numerical Programming

Roldan Pozo

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

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

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

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

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

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

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

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

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Geoffrey McFadden
James Filliben (NIST ITL)
Hung-kung Liu (NIST ITL)
Emil Simiu (NIST BFRL)
Howard Baum (NIST BFRL)
Kuldeep Prasad (NIST BFRL)
Roland deWit (NIST MSEL)
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As part of a 5-year joint competence project entitled "Complex System Failure Analysis: A Computational Science Based Approach," ITL staff formulated and began to address the following three questions on the computer simulation and analysis of complex structural system failures.

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

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

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

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

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

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

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

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

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

Mathematical Software Reference Databases

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Joyce Conlon
Marjorie McClain
Bruce Miller
Roldan Pozo

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

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

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

High Performance Computing

Computation of Atomic Properties with the Hy-CI Method

James Sims
Stanley Hagstrom (Indiana University)

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

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

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

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

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

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

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

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

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

Computation of Nano-structures and Nano-optics

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

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

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

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

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

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

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

Computational Modeling of the Flow of Concrete

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Nicos Martys (NIST BFRL)

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

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

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

The following two presentations were made to describe this code.

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

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

Interoperable MPI

William George
John Hagedorn
Judith Terrill

http://impi.nist.gov

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

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

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

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

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

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

Screen Saver Science

William L. George
Justin Haaheim
Thomas Bugnazet

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

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

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

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

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

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

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

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

Virtual Measurement Laboratory

Creating Visual Models of Nanoworlds

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

See feature article, page 35.

Measurement Science in the Virtual World

John Hagedorn
Adele Peskin
John Kelso
Steve Satterfield
Judith Terrill
Andrew Dienstfrey
Joy Dunkers (NIST MSEL)
Lori Henderson (NIST MSEL)

See feature article, page 37.

Tissue Engineering

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

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

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

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

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

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

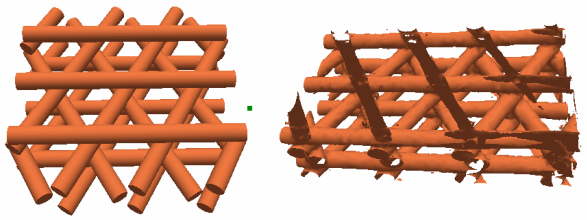


Figure 26. *Left: synthetically constructed scaffold based on the design specifications. Right: 3D reconstruction of a real scaffold made by solid freeform fabrication.*

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

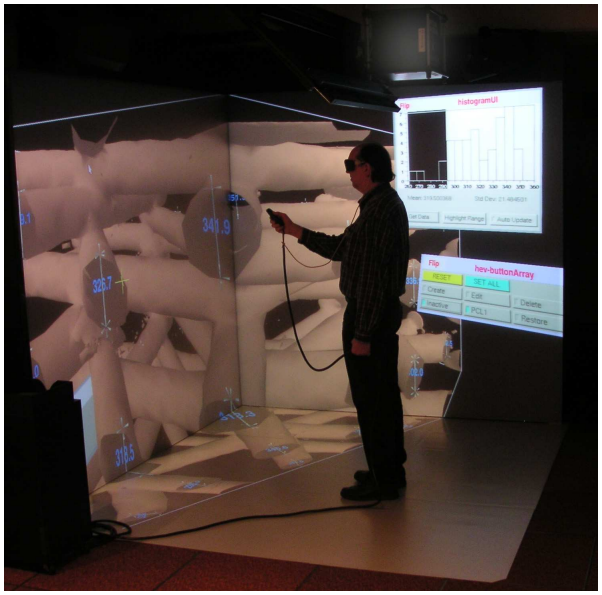
1. The user collects a set of linear measurements.
2. A simple statistical analysis is made.
3. The analysis, including the distribution of measurements, is presented to the user.
4. The user can interact with the measurement distribution in order to highlight measurements (back in the immersive environment)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

All of these tasks are performed in real-time.

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

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

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



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

3D Chemical Imaging at the Nanoscale

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

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

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

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

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

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

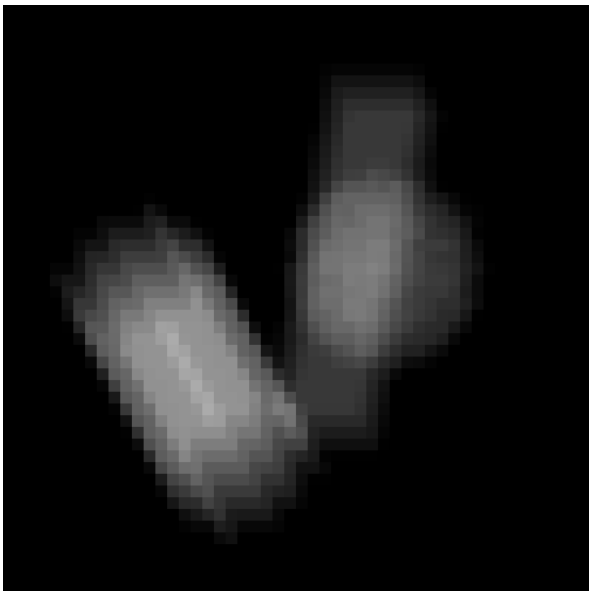


Figure 27. *This image demonstrates part of the functionality of the projection software. It simulates the projection of a volume containing a sphere, a cylinder, and a box onto a 2D sensor array at a specific orientation. Such an image would be generated experimentally as one of a tilt series that would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

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

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

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

Virtual Cement and Concrete Testing Laboratory

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

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

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

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

Visualization of Cement Hydration Models

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

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

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

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

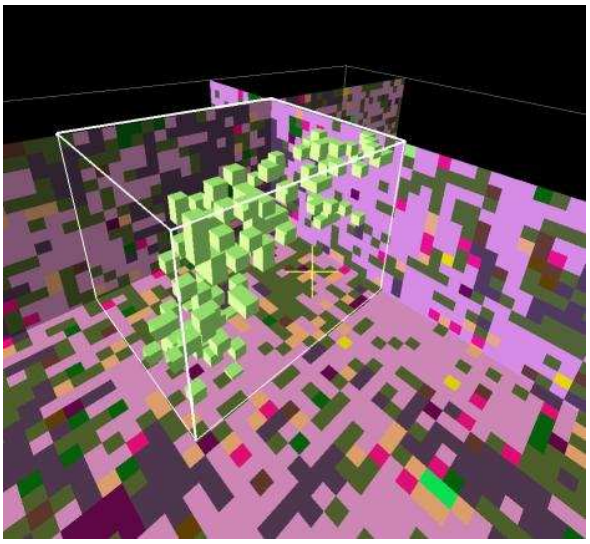


Figure 28. *A portion of the cement hydration data set output from CEMHYD3D. The user has interactively specified a region of interest (the small box) and the software is showing only the subset of the 3D data that is within that box, while simultaneously displaying orthogonal cross-sections based on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

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

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

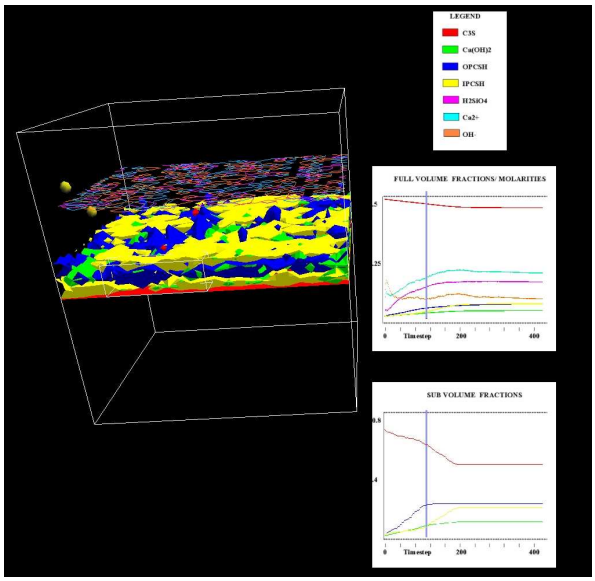


Figure 29. *Isosurfaces and isolines of selected phases of hydrating cement output from HydratiCA. The vertical line in the graphs on the right side shows the current state of the molarities for the volume.*

Visualization of Stress in Aggregate Flow

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

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

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

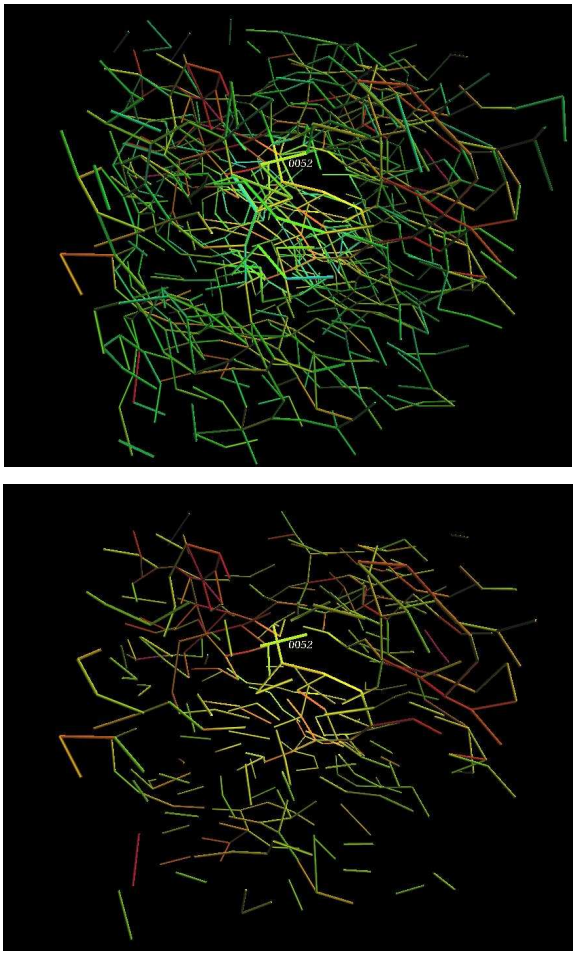


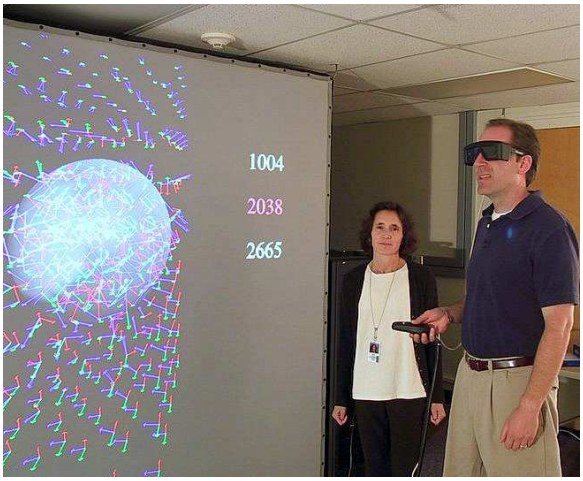
Figure 30. *The stress relationships between the spheres are represented as color coded sticks between the sphere positions shown in the top figure. The blue/green colors represent lower stress values while the yellow/red colors represent higher stress. Ranges of stress can be interactively selected.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

Visualization of Resonant Optical Scattering by Metamagnetic Materials

Adele Peskin
Andrew Dienstfry

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

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



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

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

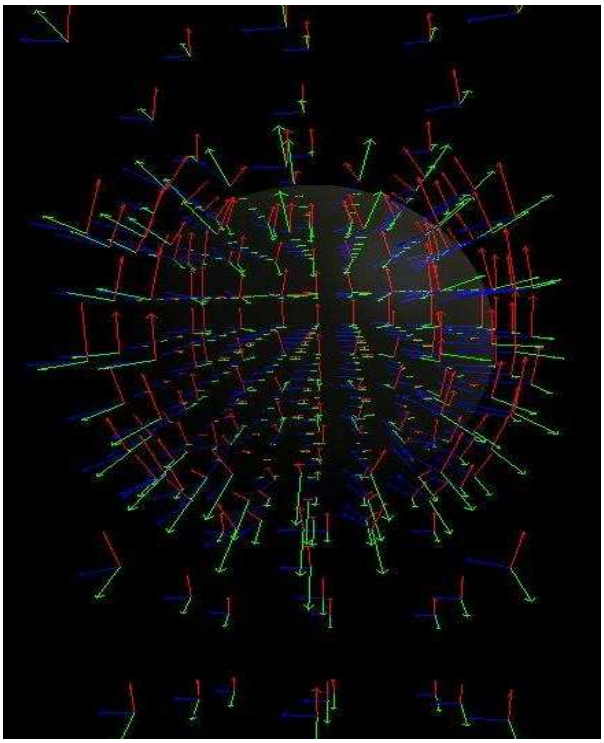


Figure 31. *A single time step in the simulation of this system at a frequency of 1004 hertz. The blue vectors represent the electric field, green vector the magnetic field, and red vectors the energy field.*

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

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

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

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

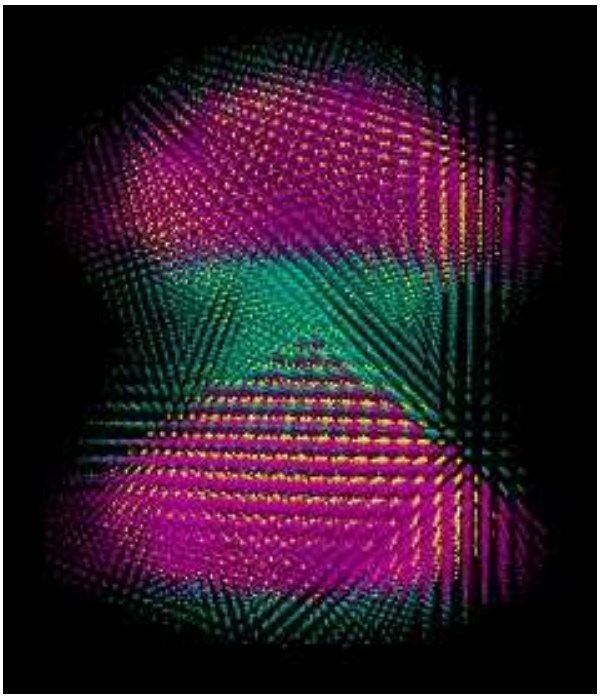


Figure 32. *Visualization of the S-orbitals of two individual quantum dots. The presence of significant S-orbitals between the dots indicates that tunneling is probable between the structures. While the structures are not connected physically, they are connected via quantum tunneling. They also created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

Visualization of Nano-structures and Nano-optics

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

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

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

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

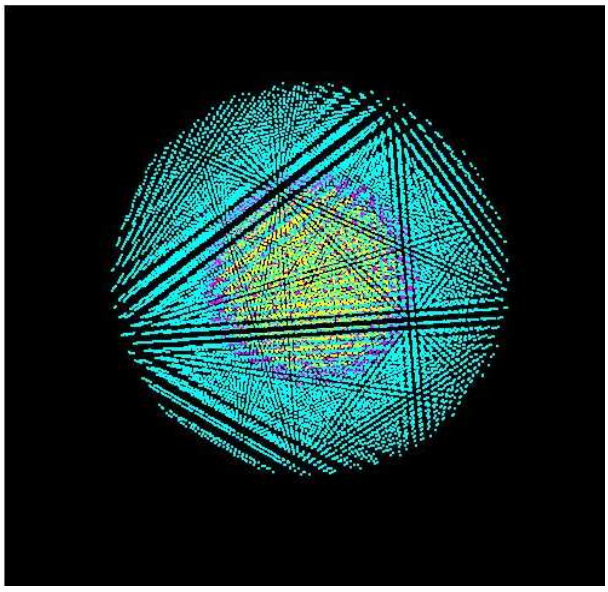


Figure 33. *Atomic lattice of a CdS/HgS/CdS core/well/clad nanohetero-structured nanocrystal (also known as a quantum do tquantum well). Atoms in the core are indicated by yellow, those in the HgS well by blue and the remaining atoms are in the clad.*

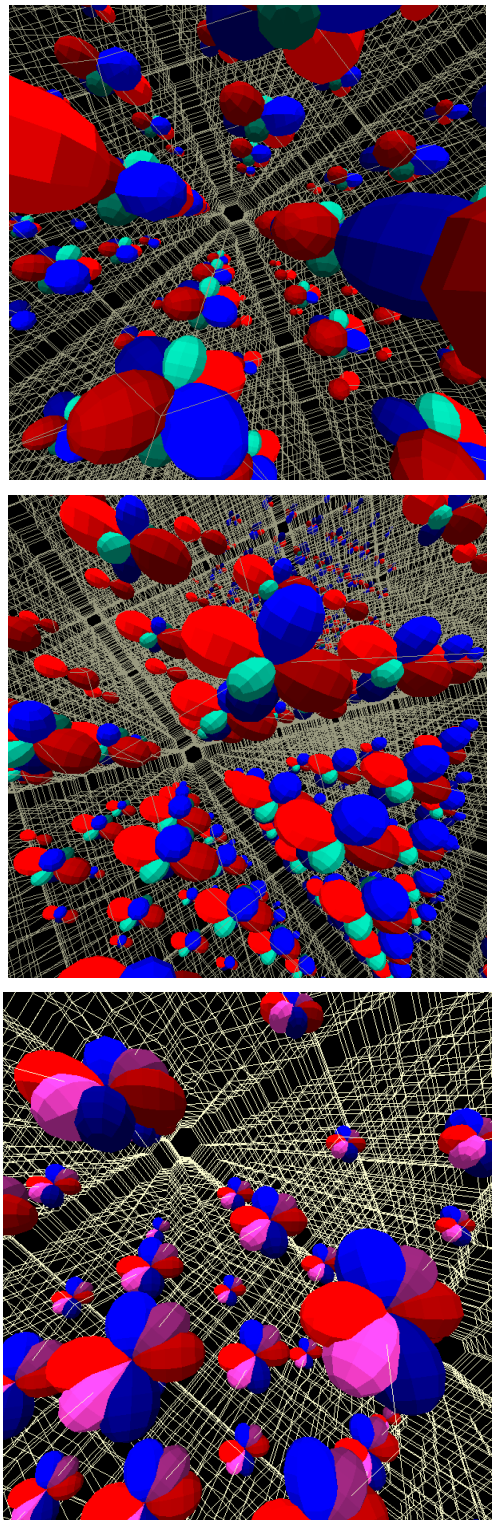


Figure 34. *Visualization of a quantum dot of GaAs. These three figures show the py orbital in dark blue, the px orbital in red, and a linear combination of px py pz. The line intersections indicate the nearest atom location.*

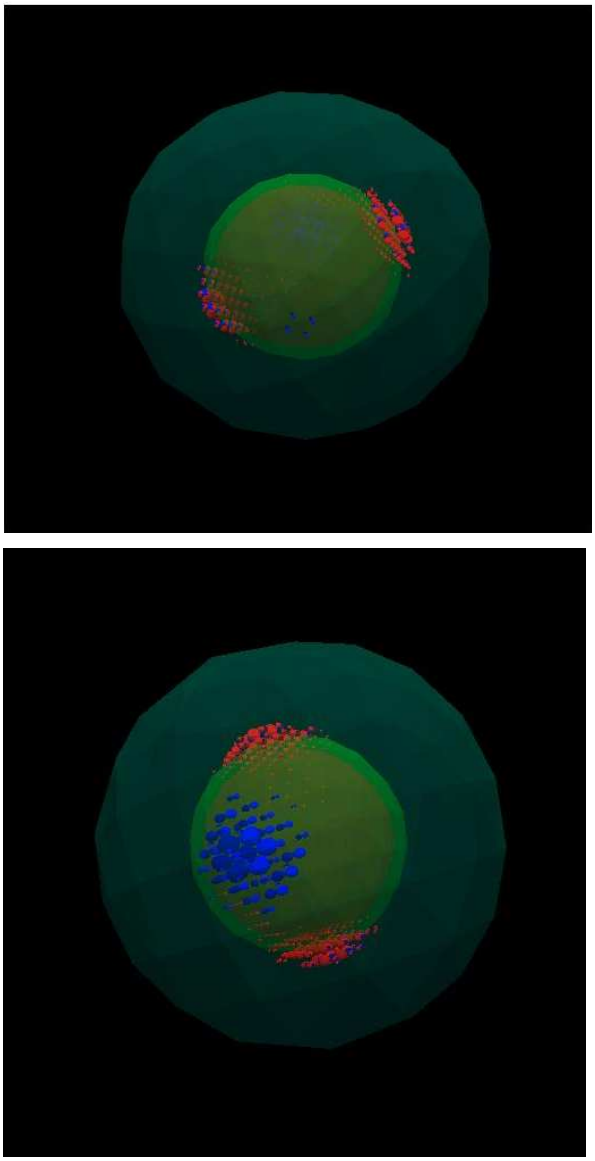


Figure 35. *Atomic scale charge density of a electronic state trapped in the well region of a CdS/HgS/CdS core/well/clad nanoheterostructured nanocrystal.*

Mathematical Modeling of Mechanical Systems and Processes

Stability of Nanowires

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

See feature article, page 31.

OOF: Finite Element Analysis of Material Microstructures

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

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

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

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

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

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

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

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

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

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

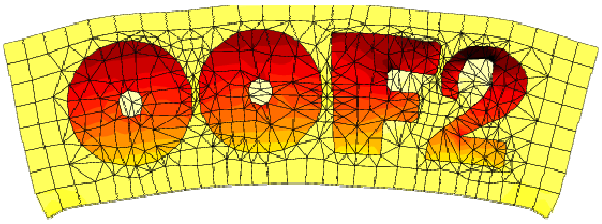


Figure 36. *Results of a calculation performed with OOF2. The lower corners of the sample are fixed in place and a temperature gradient has been applied from bottom to top. Thermal expansion of the letters has led to elastic deformation.*

Work began this year on the following future OOF2 features.

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

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

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

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

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

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

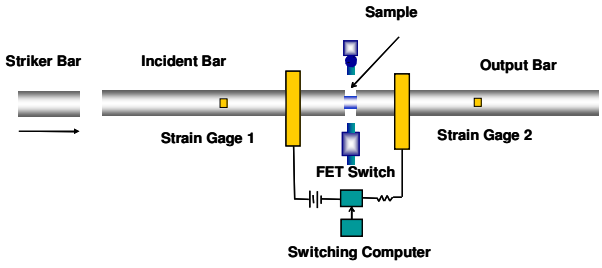


Figure 37. *Schematic drawing of the NIST pulse-heated Kolsky bar.*

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

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

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

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

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

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

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

Modeling and Simulation of High-Speed Machining Operations

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

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

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

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

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

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

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

Phase-Field Modeling of Solidification under Stress

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

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

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

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

Modeling Fluid Flow and Materials Processing

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

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

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

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

Modeling Nonequilibrium Boundary Condition at a Liquid-Liquid Interface

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

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

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

A Stochastic Approach to Modeling of Contact Dynamics of Silicon Cantilevers

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

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

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

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

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

Complex System Failure Analysis: A Computational Science Based Approach

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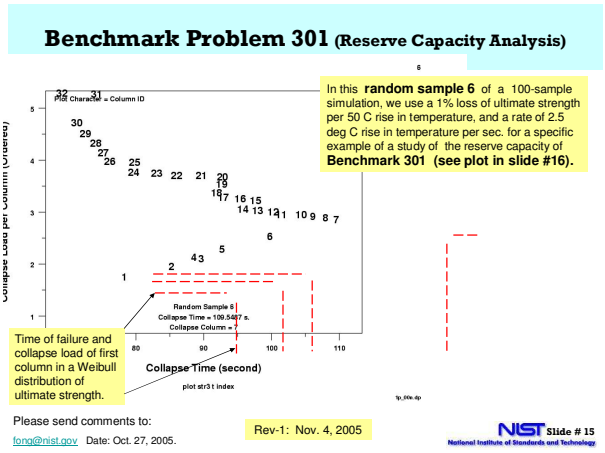
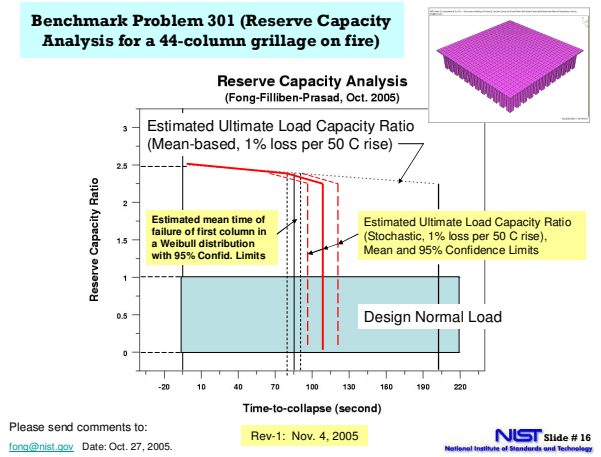
James Filliben
Hung-kung Liu.
Emil Simiu (NIST BFRL)
Dat Duthinh (NIST BFRL)
Therese McAllister (NIST BFRL)
Howard Baum (NIST BFRL)
Kuldeep Prasad (NIST BFRL)
Roland deWit (NIST MSEL)
Richard Fields (NIST MSEL)
Barry Bernstein (Illinois Institute of Technology)

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

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

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





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

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

Modeling the Behavior of Cryocoolers

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

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

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

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

Mathematical Modeling of Electromagnetic Systems

Mathematical Modeling of Nanomagnetism

Michael Donahue
Donald Porter
Robert McMichael (NIST MSEL)

See feature article, page 29.

High-Speed Waveform Metrology

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

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

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

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

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

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

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

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

Micromagnetic Modeling

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

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

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

M. Donahue and D. Porter in MCSD have developed a widely used public domain computer code for doing computational micromagnetics, the Object-Oriented Micromagnetic Modeling Framework (OOMMF). OOMMF serves as an open, well-documented environment in which algorithms can be evaluated on benchmark problems. OOMMF also provides a fully functional micromagnetic modeling system, handling both two and three-dimensional problems, with sophisticated extensible input and output mechanisms. OOMMF has become an invaluable tool in the magnetics research community. In fiscal year 2005 alone, the software was downloaded more than 3000 times, and use of OOMMF was acknowledged in 79 peer-reviewed journal articles.

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

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

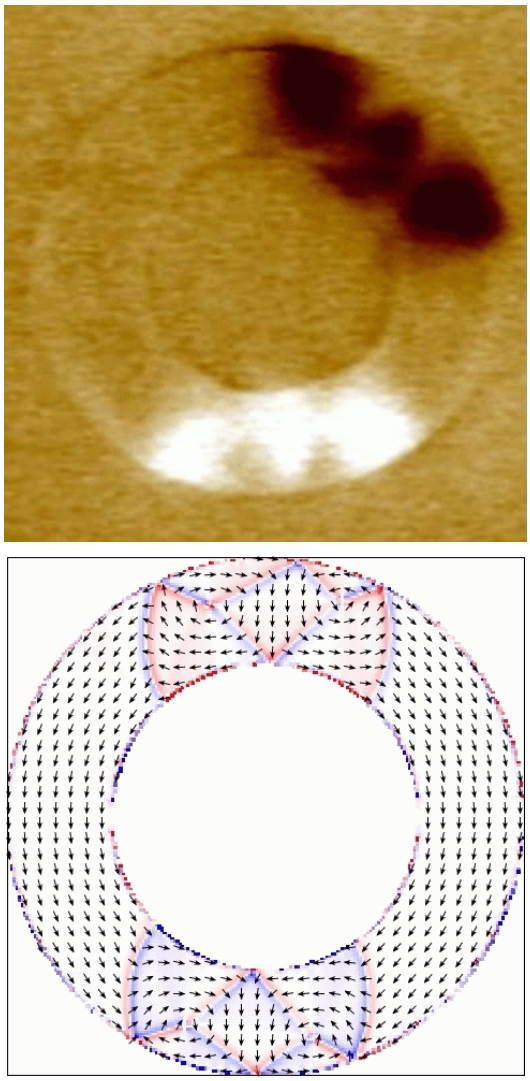


Figure 38. *Top: Image of 2000 nm diameter ring of ferromagnetic material produced by a magnetic force microscope. Bottom: Magnetization pattern computed by OOMMF based on known parameters chosen to match the experimental work.*

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

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

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

Time-Domain Algorithms for Computational Electromagnetics

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

http://math.nist.gov/AlgoCEM

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

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

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

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

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

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

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

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

Quantum Dot Identification and Characterization

Bradley Alpert
Alexana Roshko (NIST EEEL)

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

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

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

Terahertz Band Device Modeling

Bradley Alpert
Eyal Gerecht (NIST EEEL)

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

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

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

Physics Models for Transport in Compound Semiconductors

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

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

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

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

Quantum Information

Architectures for Fault-Tolerant Quantum Computing

Emanuel Knill

See feature article, page 23.

Quantum Circuit Synthesis

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

See feature article, page 25.

Adaptive Finite Element Modeling of Two Confined and Interacting Atoms

William Mitchell
Eite Tiesinga (NIST PL)

See feature article, page 27.

Realizing Quantum Information Processors

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

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

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

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

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

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

Optical Quantum Metrology and Quantum Computing

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

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

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

Mathematics of Metrology

Improving Image Resolution in Nanotechnology

Alfred Carasso
Andras Vladár (NIST MEL)

See feature article, page 33.

Identifying Objects in LADAR Scanning Data

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

See feature article, page 39.

Phase Modulation Measurements of Fluorescent Lifetimes

Fern Y. Hunt
Adolfas Gaigalas (NIST CSTL)

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

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

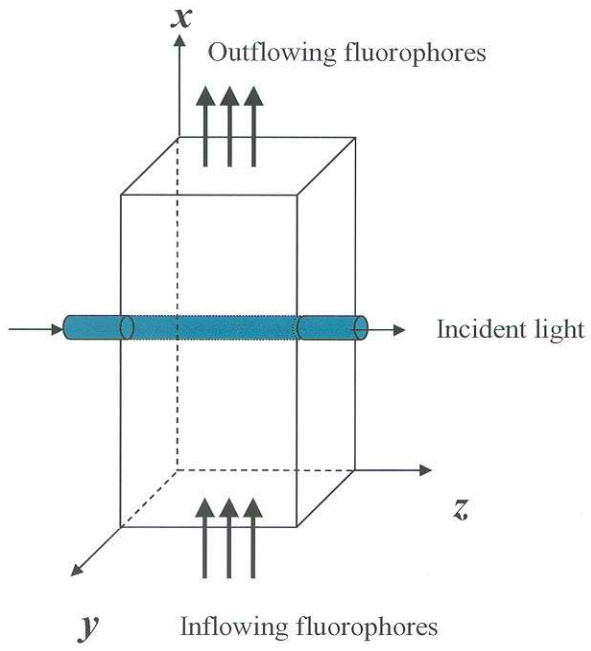

Figure 39. *Schematic of apparatus for performing phase modulation measurements with a lock-in amplifier*

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

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

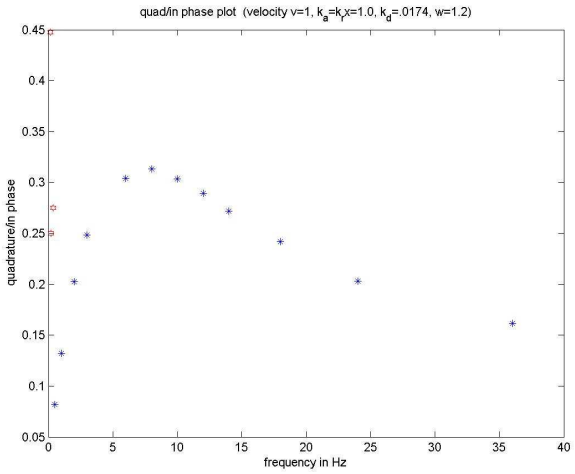

Figure 40. *Values of tan(φ) as a function of the laser frequency as computed from the model.*

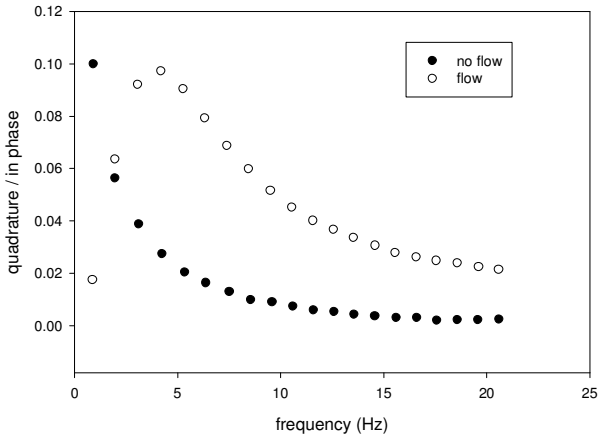

Figure 41. *Values of tan(φ) as a function of the laser frequency as measured by experiment.*

APEX Blind Deconvolution of Color Imagery

Alfred Carasso

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

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

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

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

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

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

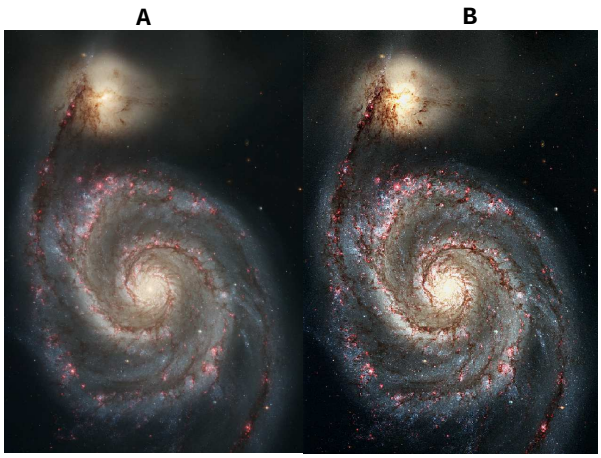

Figure 42. *(A) Hubble image of Whirlpool Galaxy M51. (B) The result of APEX sharpening.*

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

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Simulation of Bioregulatory Networks Involved in Cell Cycle Control

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

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

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

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

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

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

Computing Surface and Volume Estimates of 3-D Objects

Javier Bernal

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

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

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

Systems Identification and Parameter Estimation

Bert W. Rust

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

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

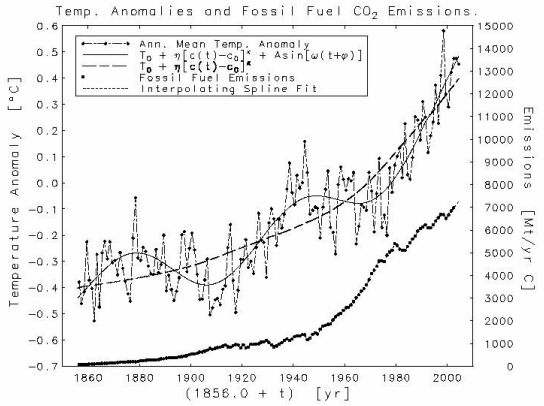

Figure 43. *The small diamonds are annual global average temperature anomalies. The solid curve is the fit of the new T(t) equation, and the long-dashed curve is the power law baseline for that fit. The small circles are annual global total fossil fuel emissions, measured in megatons of carbon, and the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

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

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

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

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

Technology Transfer of Monte Carlo Strategies

Isabel Beichl
Francis Sullivan (IDA Center for Computing Sciences)

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

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

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

Voting Systems

Peter Ketcham

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

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

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

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