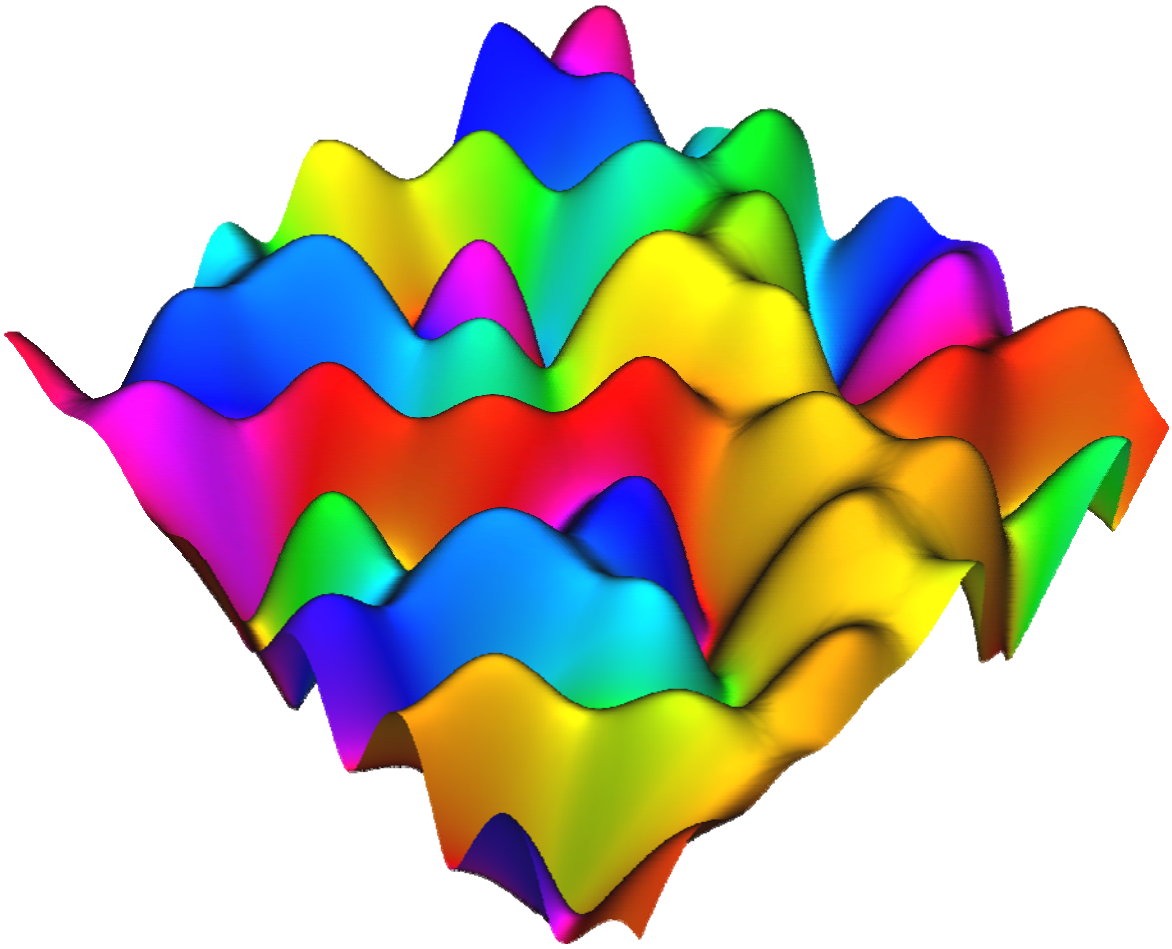
NISTIR 7762

Applied and Computational Mathematics Division

Summary of Activities for Fiscal Year 2010



National Institute of Standards and Technology
U.S. Department of Commerce

NISTIR 7762

Applied and Computational Mathematics Division

Summary of Activities for Fiscal Year 2010

Ronald F. Boisvert, Editor
Applied and Computational Mathematics Division
Information Technology Laboratory

February 2, 2011

U.S. Department of Commerce
Gary Locke, Secretary

National Institute of Standards and Technology
Patrick D. Gallagher, Director

Abstract

This report summarizes the technical work of the Applied and Computational Sciences Division of NIST's Information Technology Laboratory. Part I (Overview) provides a high-level overview of the Division's activities, including highlights of technical accomplishments during the previous year. Part II (Features) provides further details on ten projects of particular note this year. This is followed in Part III (Project Summaries) by brief synopses of all technical projects active during the past year. Part IV (Activity Data) provides listings of publications, technical talks, and other professional activities in which Division staff members have participated. The reporting period covered by this document is October 2009 through December 2010.

For further information, contact Ronald F. Boisvert, Mail Stop 8910, NIST, Gaithersburg, MD 20899-8910, phone 301-975-3812, email boisvert@nist.gov, or see the Division's web site at http://www.nist.gov/itl/math/index.cfm.

Cover Visualization: The modulus of the Riemann theta function $\hat{\theta}(i\,x, i\,y|\mathbf{\Omega}), 0 \le x, y \le 5$, where $\mathbf{\Omega}$ is the matrix defined in http://dlmf.nist.gov/21.4. Surface colors correspond to phase angle. This image, which originates in the NIST Digital Library of Mathematical Functions (http://dlmf.nist.gov/), was developed by Brian Antonishek, Qiming Wang, and Bonita Saunders.

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

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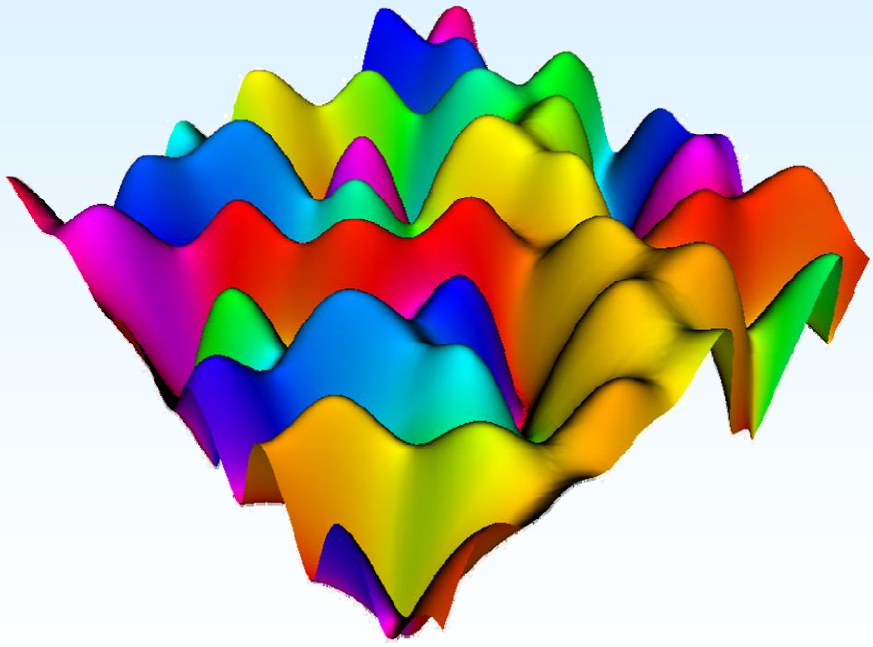
Overview



Introduction

Founded in 1901, NIST is a non-regulatory federal agency within the U.S. Department of Commerce. NIST's mission is to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life. The NIST Laboratory program is broad-ranging, with research efforts in physics, electrical engineering, materials science, chemistry, bioscience, engineering, fire research, and information technology.

The Information Technology Laboratory (ITL) is one of six major laboratories at NIST. ITL seeks to (a) accelerate the development and deployment of information and communication systems that are reliable, usable, interoperable, and secure; (b) advance measurement science through innovations in mathematics, statistics, and computer science; and (c) conduct research to develop the measurements and standards infrastructure for emerging information technologies and applications.

The Applied and Computational Mathematics Division (ACMD) is one of six technical Divisions in ITL. ACMD provides leadership within NIST in the use of applied and computational mathematics to solve science and engineering problems arising in measurement science and related applications. In that role Division staff members

- perform research and development in applied mathematics and computer science and engineering, including analytical methods, numerical and symbolic algorithms, advanced computing and communications architectures and applications, and high performance scientific visualization;
- engage in peer-to-peer collaborations in the application of mathematical and computational technologies to NIST problems;
- develop and disseminate mathematical reference data, software, and related tools; and
- work with internal and external groups to develop standards, test procedures, reference implementations, and other measurement technologies for advanced scientific computation on current and future architectures.

Division staff is organized into four groups:

Mathematical Analysis and Modeling Group (*Timothy Burns, Leader*)

Performs research and maintains expertise in applied mathematics, mathematical modeling, and numerical analysis for application to measurement science.

Mathematical Software Group (*Daniel Lozier, Leader*)

Performs research and maintains expertise in the methodology and application of mathematical algorithms and software in support of computational science within NIST as well as in industry and academia.

Computing and Communications Theory Group (*Ronald Boisvert, Acting Leader*)

Performs research and maintains expertise in fundamental mathematics, physics, and measurement science necessary to enable the development of future computing and communications systems.

High Performance Computing and Visualization Group (J*udith Terrill, Leader*)

Performs research and maintains expertise in the methodologies and tools of high performance scientific computing and visualization for use in measurement science.

The technical work of the Division is organized into six thematic areas; these are described in the sidebar. In Part III of this document we provide outlines of most ongoing technical projects of the Division. These are organized by thematic area.

For the past three years, ITL has managed its technical work in a matrix-management structure built on a set of Laboratory-wide programs. During FY 2010 the ITL Programs were:

Division Thematic Areas

Mathematics of Metrology. Mathematics plays an important role in the science of metrology. Mathematical models are needed to understand how to design effective measurement systems, and to analyze the results they produce. Mathematical techniques are used to develop and analyze idealized models of physical phenomena to be measured, and mathematical algorithms are necessary to find optimal system parameters. Finally, mathematical and statistical techniques are needed to transform the resulting data into useful information. The goal of this work is to develop fundamental mathematical methods and analytical tools necessary for NIST to continue as a world-class metrology institute, and to apply them critical measurement science applications.

Scientific Software. Modern science and engineering in general, and modern measurement science in particular, requires a wide variety of software tools for scientific discovery, exploration, and analysis. As scientific inquiry becomes deeper and more specialized, so must the supporting software tools. The goal of this work is to develop critical software tools that support measurement science at NIST, as well as computational science and engineering at large.

Foundations of Measurement Science for Information Systems. Modern information systems are astounding in their complexity. Software applications are built from thousands of interacting components. Computer networks interconnect millions of independently operating nodes. Large-scale networked applications provide the basis for services of national scope, such as financial transactions and electrical power distribution. In spite of our increasing reliance on such systems, our ability to build far outpaces our ability to secure. Protocols controlling the behavior of individual nodes lead to unexpected macroscopic behavior. Local power anomalies propagate in unexpected ways leading to large-scale outages. Computer system vulnerabilities are exploited in viral attacks resulting in widespread loss of data and system availability. The long term stability of our critical infrastructure is simply unknown. Measurement science has long provided a basis for the understanding and control of physical systems. Similar types of deep understanding and insight are lacking for complex information systems. We seek to develop the mathematical foundations needed for the emergence of a true measurement science for complex networked information systems.

High Performance Computing and Visualization. Computational capability is advancing rapidly. This means that modeling and simulation can be done with greatly increased fidelity (e.g., higher resolution, more complex physics). However, developing large-scale parallel applications remains highly challenging, requiring expertise that application scientists rarely have. In addition, the hardware landscape is changing rapidly so new algorithmic techniques must constantly be developed. We are developing and applying facilities and expertise of this type for application to NIST problems. Large scale computations and laboratory experiments invariably produce large volumes of scientific data, which cannot be readily comprehended without some form of visual analysis. We are developing the infrastructure necessary for advanced visualization of scientific data, including the use of 3D immersive environments and applying this to NIST problems. One of our goals is to develop the 3D immersive environment into a true interactive measurement laboratory.

Digital Library of Mathematical Functions. The special functions of applied mathematics are fundamental tools enabling modeling and analysis in all areas of science and engineering. To make effective use of such functions, practitioners must have ready access to a reliable source of information on their properties. The goal of this work is the development and dissemination of definitive reference data on the special functions of applied mathematics. The centerpiece of this effort is the DLMF, a freely available interactive and richly linked online resource.

Quantum Information. An emerging discipline at the intersection of physics and computer science, quantum information science (QIS) is likely to revolutionize science and technology in the same way that lasers, electronics, and computers did in the 20th century. By encoding information into quantum states of matter, one can, in theory, exploit the seemingly strange and counter-intuitive behavior of quantum systems to enable phenomenal increases in information storage and processing capability, as well as communication channels with extremely high levels of security. Although many of the necessary physical manipulations of quantum states have been demonstrated experimentally, scaling these up to enable fully capable quantum computers remains a grand challenge. We are engaged in (a) theoretical studies to understand the true power of quantum computing, (b) collaborative efforts with the multi-laboratory experimental quantum science program at NIST to characterize and benchmark specific physical implementations of quantum information processing, and (c) the development and assessment of technologies for quantum communication.

*Complex Systems**
Cyber and Information Security
Enabling Scientific Discovery
*Health Care Information Technology**
Identity Management Systems
Information Discovery, Use and Sharing
*Pervasive Information Technology**
*Quantum Information**
Trustworthy Information Systems
*Virtual Measurement Systems**

* Programs continuing into FY 2011

Late in 2010 ITL changed its program management structure, maintaining only five of these programs (the starred ones), and transitioning the remainder to Division-level management. The project summaries in Part III of this report indicate ITL program affiliations during FY 2010.

NIST itself underwent a significant organizational realignment effective October 1, 2010. The new structure includes two measurement labs, two technology labs, and two user facilities:

Physical Measurement Laboratory (PML)
Material Measurement Laboratory (MML)
Engineering Laboratory (EL)
Information Technology Laboratory (ITL)
Center for Nanoscale Science and Technology (CNST)
National Center for Neutron Research (NCNR)

When identifying our collaborators from other NIST Laboratories in this report we use the new organizational structure.

Highlights

In this section we identify some of the major accomplishments of the Division during the past year. We also provide news related to ACMD staff.

Technical Accomplishments

ACMD has made significant technical progress on many fronts during the past year. Here we highlight a few examples. Further details are provided in Part II (Features) and Part III (Project Summaries).

Digital Library of Mathematical Functions. The NIST Digital Library of Mathematical Functions (DLMF), the 21st century successor to the classic *Handbook of Mathematical Functions* (Abramowitz and Stegun, eds., NBS, 1964), was released in May 2010. The DLMF is a free interactive web service provided by NIST. Most of the mathematical content is also be available in book form as the *NIST Handbook of Mathematical Functions* which has been published by Cambridge University Press. The DLMF is the result of a 12 year effort managed by four NIST editors: F. W. J. Olver, D. W. Lozier, and R. F. Boisvert of the ACMD, and C. W. Clark of the NIST PML. In all, the project has had some 50 participants worldwide, serving as editors, authors, validators, and consultants. The web site, which includes innovative presentation, search, and interactive graphics, was designed and executed by ACMD staff. Reception of the new resources has been quite positive. The web site and book were officially launched at a workshop on the Numerical Solution of the Painlevé Equations on May 12 in Edinburgh, Scotland. The web site was "slashdotted" a few days after it was released, resulting in a single day with nearly 25,000 user visits. In the first four months of operation, the site has registered more than 157,000 user visits accounting for more than 620,000 page views. Flattering reviews have appeared in the September issue of the *SIAM News* and the October issue of *Optics and Photonics News*. [See page 25.]

Mathematics of Metrology. We continue to make critical contributions to the measurement science program at NIST via the application of our expertise in mathematical analysis and modeling. Our collaborative modeling efforts are highly diverse, ranging from studies of reactive wetting of metals to the magnetic properties of nanostructures. We also continue to develop new analysis techniques. For example, Alfred Carasso of ACMD has developed an innovative technique for removing noise from images while preserving fine-scale details. Existing techniques for removing noise typically wash out fine detail in the process. Carasso's techniques employ extremely sophisticated mathematics, including fractional diffusion, low exponent Lévy stable laws, and "slow motion" solution of parabolic equations. Carasso's tests demonstrate that the new method is superior to the best of existing methodologies based on the split Bregman iteration and on the curvelet transform. The new method has been applied to the denoising of state-of-the-art Helium Ion Microscope nanoscale imagery in collaboration with András Vladár of NIST PML. A paper describing the new method has been submitted for publication. [See page 47.]

High Performance Computing and Visualization. ACMD leads NIST in the application of parallel computing to problems in measurement science. For example, due to ACMD involvement, NIST's ability to perform high fidelity simulations of the flow of complex suspensions has achieved best-in-the-world status. Armed with substantial awards of computer time on Argonne National Laboratory's Blue Gene supercomputer from DoE's INCITE program, William George and his colleagues in ACMD and the NIST EL have significantly enhanced our understanding of the flow of fresh concrete, a dense suspension composed of cement, water, sand, and rocks. Novel visual analysis techniques have also been critical to generating insights from the voluminous simulation output. This work, performed under the aegis of the Virtual Cement and Concrete Testing Lab Consortium, is a critical step in transforming the design of concrete materials from an art to a science, which is expected to have significant impact on this $100B US industry whose products are the foundation of much of the Nation's physical infrastructure. This work was recognized with the Department of Commerce's Silver medal in 2009. [See pages 19 and 34.]

Scientific Software. ACMD has three major software systems under active development: OOMMF, a system for micromagnetic modeling, OOF, a system for modeling of materials with complex microstructure based on the analysis of real or simulated material imagery, and PHAML, a finite element partial differential equations solver implementing parallel hierarchical adaptive multigrid methods. Each has made significant strides this year. OOMMF, originally designed as reference software for the testing of solution algorithms, continues to be the solver of choice in the nano-magnetic modeling community, this year surpassing the milestone of 1,000 cited uses in refereed publications. [See page 70.] OOF was downloaded more than 1,600 times this year, and saw considerable usage via Purdue University's nanoHUB portal. A 3D version of OOF, a significant undertaking, is now at the beta stage. [See page 71.] Finally, PHAML is being used at NIST as both the platform for a comprehensive study of *hp*-adaptive solution strategies, and for the study of the eigenstates of optical traps for neutral atoms for application in quantum information processing. [See page 72.]

Quantum Information. ACMD continues to be the principal focus at NIST for quantum information theory, providing the theoretical underpinnings for a wide variety of experimental efforts being undertaken in the NIST Laboratories. For example, Scott Glancy and Manny Knill of ACMD were part of a team of NIST researchers who this year created "quantum cats" made of photons (particles of light), boosting prospects for manipulating light in new ways to enhance precision measurements as well as computing and communications based on quantum physics. The experiments repeatedly produced light pulses that each possessed superpositions of two exactly opposite properties—specifically, opposite phases—a so-called optical Schrödinger's cat. This quantum state was the first to be realized by detecting three photons at once and was one of the largest and most well-defined cat states ever made from light. Glancy developed a survey of methods for producing optical cats that was the basis for the experiment. Glancy and Knill developed techniques for quantum state tomography that were used in the analysis of experimental results. A paper describing the accomplishment appeared in *Physical Review A* in September 2010; Glancy was second author of ten. The accomplishment was subsequently highlighted in *Nature Photonics*. [See page 80.]

Also this year, in an effort to consolidate ITL's quantum information research program within a single Division, ACMD gained a group of scientists specializing in quantum optics experimentation. This team, lead by Xiao Tang, has been developing and evaluating quantum communication technologies and systems. One of their recent accomplishments, a spin-off of highly successful efforts to demonstrate high-speed quantum key distribution systems, has been the development of a highly sensitive (i.e., single-photon-level) near-infrared spectrometer based on photon upconversion technology. This year the team used this device in a collaboration with physicists in the NIST CNST on a first-time demonstration of the conversion of near-infrared 1,300 nm wavelength single photons emitted from a true quantum source, a semiconductor quantum dot, to a near-visible wavelength of 710 nm. The ability to change the color of single photons makes them much easier to detect, thus aiding in the development of quantum systems for applications in quantum communication, computation and metrology. A paper describing this achievement was published in *Nature Photonics* in October 2010. [See page 42.]

Foundations of Measurement Science for Information Systems. A major new focus of ACMD, bolstered by a significant infusion of cybersecurity funding during the last three years, is the quest to de-

velop the mathematical foundations of measurement science for information systems. It is hoped that this will begin to provide a solid science base to inform ITL's efforts to improve computer and communication systems security and reliability within government and industry. Our early efforts in this area have primarily focused on developing an understanding of how the structure and dynamics of interconnected systems, i.e., abstract networks, relate to overall system performance. For example, a fundamental measure of the reliability of a network is its reliability polynomial. This function gives the probability that a network will remain connected given that each edge can fail independently with a probability p. One definition for the reliability polynomial R of a connected graph G with m edges and for the edge failure probability p is

$$R(G;p) = \sum_{j=1}^{m} a_j (1-p)^j p^{m-j}$$

where a_j is the number of distinct connected subgraphs of G with exactly j edges. The problem in using the reliability polynomial for network analysis has been the fact that computing the polynomial itself is computationally intractable. (Technically, the problem is #P complete.) Thus the best we can expect to do in general is to approximate the polynomial. Brian Cloteaux and Isabel Beichl of ACMD have developed a new and highly efficient method to do this. Their approach has two advantages. First, while there are several algorithms that provide pointwise approximations of the polynomial, they approximate the polynomial coefficients themselves. Secondly, their method has shown much faster rate of convergence than previously proposed methods. A paper describing this work appeared in the March 2010 issue of the journal *Congressus Numerantium*. [See page 40.]

Game theory is another important mathematical tool for modeling the dynamics of computer network attacks. This year, Vladimir Marbukh of ACMD, working with Daniel Genin and Anastase Nakassis of ITL's Advanced Networking Technologies Division, used game-theoretic methods to demonstrate that proposed user-directed ("selfish") Internet routing strategies are particularly vulnerable, in the sense that an agile attacker of very limited power can inflict significant damage on overall network performance. Their paper on this result was cited with a best contribution award at the 2010 International Conference of Information Security and Internet Engineering. [See page 85.]

Software testing can also be greatly improved with fundamental mathematical insights. ACMD mathematicians are part of an ITL team making significant advances to a technology known as combinatorial testing. This is a black box testing approach in which combinations of inputs are selected in order to ensure that all 2-way, 3-way, 4-way, etc. combinations of input parameters appear in a test suite. This approach is notable because it ensures that the most likely sources of errors – interactions among small numbers of parameters – are exercised in a minimal number of tests. Raghu Kacker of ACMD and Rick Kuhn of the ITL Computer Security Division, working with colleagues from the University of Texas at Arlington have recently applied combinatorial testing to the detection of buffer overflow vulnerabilities. Such coding lapses are among the most common used by hackers to infect and exploit computer systems. The team has built a prototype tool, called Fugai, which implements this approach. Empirical results of applying Fugai to several open source programs show that it may be quite effective in detecting buffer overflows. [See page 90.]

Technology Transfer and Professional Activities

The volume of technical output of ACMD remains high. During the last 18 months, Division staff members were (co-)authors of 38 articles appearing in peer-reviewed journals, two books, three book chapters, 36 papers in conference proceedings, and eight other formal publications. Fourteen additional papers have been accepted for publication, while 28 others are undergoing review. Division staff members gave 26 invited technical talks and presented 35 others in conferences and workshops.

ACMD continues to maintain an active Web site with a variety of information and services, including the Digital Library of Mathematical Functions, the Guide to Available Mathematical Software, the Matrix Market, and the SciMark Java benchmark. During calendar year 2010, the division web server

Table 1. *Downloads of Selected Division Software Packages During CY 2010*

Package	Description	Downloads
JAMA	Linear algebra in Java	25,995
TNT	Linear algebra using C++ templates	6,085
SparseLib++	Sparse linear algebra in C++	4,645
OOMMF	Modeling of nano-magnetic phenomena	4,500
LAPACK++	Linear algebra in C++	4,190
OOF	Modeling materials with complex microstructure	1,663
f90gl	Fortran 90 interface to OpenGL graphics	1,424
spblas	Sparse basic linear algebra components	1,185
REGEN	Modeling of cryocoolers	569
PHAML	Parallel adaptive solution of partial differential equations	506

satisfied more than 9.3 million requests for pages from more than 68,000 distinct hosts. In total, there have been more than 272 million "hits" on ACMD Web servers since they went online as NIST's first web servers in 1994. The individual software packages that we produce and distribute also continue to see very high usage. Table 1 lists download counts for some of our most popular ones. Another indication of the successful transfer of our technology is references to our software in refereed journal articles. For example, our OOMMF software for nano-magnetic modeling was cited in 96 such papers which were published in 2010 alone (more than 1,000 such papers have been identified since 2001).

Members of the Division are also active in professional circles. Isabel Beichl began a second term as Editor-in-Chief of *Computing in Science & Engineering* in January 2011. Staff members hold a total of ten additional editorial positions in peer-reviewed journals. They are also active in conference organization, serving on nine organizing/steering/program committees. Staff members organized three minisymposia at technical conferences in 2010.

Service within professional societies is also prevalent among our staff. For example, Ronald Boisvert serves as Co-Chair of the Publications Board of the Association for Computing Machinery (ACM) and is a member of the ACM Council, the association's board of directors. Daniel Lozier served as Secretary of the Society for Industrial and Applied Mathematics (SIAM) Activity Group on Orthogonal Polynomials and Special Functions. Staff members are also active in a variety of working groups. For example, Ronald Boisvert serves as Chair of the International Federation for Information Processing (IFIP) Working Group 2.5 on Numerical Software, Donald Porter is a member of the Tcl Core Team, and Bruce Miller is a member of W3C's Math Working Group. Judith Terrill represents NIST on the High End Computing Interagency Working Group of the Federal Networking and Information Technology Research and Development (NITRD) Program.

For further details, see Section IV, Activity Data.

Administrative News

The Division undertook a significant reorganization this past year in an attempt to align our structure to current activities and goals. Three of our four groups underwent name changes, and all had their mission statements updated. Nine staff members moved between groups. Also at midyear six staff members and associates from ITL's quantum communications project were moved to ACMD in an effort to consolidate ITL's quantum information research in one Division. The past year also saw many additional staffing changes. Among these are the following.

- *Geoffrey McFadden* stepped down as Leader of the Mathematical Analysis and Modeling Group after serving 10 years in that position to devote his energies to his appointment as a NIST Fellow. *Timothy Burns*, a NIST research mathematician for 25 years, was named the new Group Leader.
- Two new National Research Council (NRC) Postdoctoral Associates joined MCSD this year. The first, *Elizabeth Moseman*, has a PhD in Mathematics from Dartmouth (2007), with a thesis on the

combinatorics of coordinate percolation. She comes to ACMD most recently from the US Military Academy (West Point) where she had a faculty appointment. At NIST she is working with Isabel Beichl on methods for determining robustness in infrastructure networks. The second, *Howard Cohl*, comes to ACMD from the University of Auckland, New Zealand, where he completed a thesis on Fourier and Gegenbauer expansions for fundamental solutions of the Laplacian and powers in R^d and H^d. Cohl is working with Daniel Lozier on rotationally-invariant expansions for solving linear inhomogeneous partial differential equations.

- Three of ACMD's NRC Postdoctoral Associates completed their terms this year. *Bryan Eastin*, who worked with Manny Knill on quantum information theory, took a position with Northrop Grumman; he remains a guest researcher with ACMD in Boulder. *Aaron Lott*, who worked with Geoffrey McFadden on techniques for solving partial differential equations important in materials modeling, moved to Lawrence Livermore National Laboratory. Finally, *Valerie Coffman*, who worked with Stephen Langer on our OOF system for modeling materials with complex microstructure, was awarded a two-year term appointment in ACMD to complete the development of OOF3D.
- *Sandy Ressler* came to ACMD this year from ITL's Information Access Division after a 3-year detail as Manager of ITL's Complex Systems Program. An expert in computer graphics, including 3D web technologies, Ressler will be working on information visualization techniques and applications in ACMD's High Performance Computing and Visualization Group.
- *Andrew Reid*, a long time guest researcher and contractor in ACMD, was given a regular staff appointment by the NIST Materials Measurement Laboratory. Half his support will come from ACMD, where he continues to be a principal developer in our OOF project.
- Three ACMD staff members spent part of the year on detail to other organizations. *Robert Bohn* returned to ACMD in September 2010 after a long stint working in the National Coordination Office of the National Information Technology Research and Development (NITRD) program. Bohn is now working on ITL's Cloud Computing Program, which is providing leadership and guidance to catalyze the use of cloud computing within industry and government. *Anthony Kearsley* returned to ACMD in late 2010 after a successful three-year detail as Manager of ITL's Enabling Scientific Discovery Program. Finally, *Jeffrey Fong* spent the year on detail in NIST's Technology Innovation Program as a TIP Associate.
- *David Gilsinn* of ACMD retired from NIST at the end of 2010 after 40 years of Federal service. Gilsinn, an expert in nonlinear dynamics, contributed to a wide variety of projects at NIST, including studies of the dynamics of high speed machining, assessments of surface roughness, the modeling of construction sites from LIDAR data, and the identification of features in cell imagery.

Figure 1. *David Gilsinn retired from NIST in 2010 after 40 years of Federal service.*

During FY 2010 ACMD was able to support the work of 20 student interns, including six in the Student Undergraduate Research Fellowship (SURF) program, three graduate students in Boulder's Professional Research Experience Program (PREP), and three high school volunteers. We also hosted five graduate students from French universities, which was facilitated by a Memorandum of Understanding signed in late 2009 between ITL and the Institut Supérieur d'Informatique, de Modélisation et de leurs Applications (ISIMA) at the University of Clermont-Ferrand. See Table 2 for a complete list.

Table 2. *Student Interns in MCSD*

Name	Institution	Level	Program	Mentor	Project Title
Styvens Belloge	ISIMA (France)	G	Guest Researcher	J. Terrill	Visualization and analysis of the National Vulnerability Database
Guillaume Bousquet	ISIMA (France)	G	Guest Researcher	F. Hunt	Applied mathematics and computational science
Luis Catacora	Montgomery Blair HS	HS	SHIP	J. Terrill	Gestures that cause actions in the Immersive Visualization Environment
Amanda Crawford	University of Colorado	U	SURF	I. Beichl	Sequential importance sampling for computing entropy
Matthew Du	Thomas Wootton HS	HS	SHIP	J. Terrill	Glass breakage using bullet physics engine, and a logic-based approach to machine learning
Mark Girard	Trinity University	U	SURF	S. Glancy	Quantum state estimation.
William Hess	Purdue University	U	STEP	J. Terrill	Lighting in the Immersive Visualization Environment
Marlene Hildebrand	Polytech (Nice)	G	Guest Researcher	J. Terrill A. Peskin	Visualization of medical images
Nathan Jacobson	Hood College	U	SURF	R. Kacker	Numerical simulation of coverage intervals
Adam Meier	University of Colorado	G	PREP	E. Knill	Quantum computer simulation
Michael Mullan	University of Colorado	G	PREP	E. Knill	Quantum computing theory
Kevin Rawlings	Carnegie Mellon University	U	STEP	J. Terrill	Visualization and analysis of the National Vulnerability Database
Clement Rey	ISIMA (France)	G	Guest Researcher	R. Pozo	Visualization of large complex networks
Anshu Rustagi	University of Illinois	U	STEP	W. George	Screen Saver Science
Poorva Singal	Franklin W. Olin College of Engineering	U	SURF	J. Terrill	Generating realistic patterns of glass breakage
Becky Song	Richard Montgomery HS	HS	SHIP	J. Terrill	Visualization and analysis of de- and re-mineralization of teeth
Armeen Taeb	University of Colorado	U	SURF	A. Peskin	Image processing and volumetric measurement
Jean-Loup Traore	Université Blaise Pascal, France	G	Guest Researcher	J. Terrill	Cement hydration modeling
Luis Valentin	The College of William and Mary	U	SURF	B. Cloteaux	Approximating the number of leaf nodes in trees.
Yanbao Zhang	University of Colorado	G	PREP	E. Knill	Tests of local realism

Legend G: Graduate student
U: Undergraduate student
HS: High school student
SURF: NIST Summer Undergraduate Student Fellowship Program.
PREP: NIST Professional Research Experience Program

Recognition

Division staff garnered a number of professional recognitions during the past year. These are described below.

Awards

o *Department of Commerce Silver Medal.* William George and Judith Terrill of ACMD were co-winners of a 2009 Silver Medal from the Department of Commerce for their work on the modeling and simulation of complex suspensions; see Figure 2. The Silver Medal recognizes "exceptional performance characterized by noteworthy or superlative contributions which have a direct and lasting impact within the Department." Dale Bentz, Jeffrey Bullard, Edward Garboczi, and Nicos Martys of EL were co-winners. The award citation credits the group with the creation of the virtual cement and concrete testing laboratory (VCCTL), "which uses intensive computer simulation to mimic a physical testing laboratory and has proven to be capable of revealing behavior beyond the limits of traditional testing instruments."

Figure 2. *DOC Silver Medal Award Recipients. William George and Judith Terrill (second and third from left) of ACMD with co-winners Edward Garboczi, Dale Bentz, Nicos Martys, and Jeffrey Bullard of the NIST Engineering Laboratory.*

o *NIST Allen V. Astin Measurement Science Award.* Andrew Dienstfrey of ACMD was a co-winner of NIST's 2009 Allen V. Astin Measurement Science Award for work in waveform metrology; see Figure 3. The award recognizes "outstanding achievement in the advancement of measurement science or in the delivery of measurement services". Paul Hale and Dylan Williams of PML and Jack Wang of ITL's Statistical Engineering Division were co-winners. The team was cited for "providing a world-first method for simultaneously calibrating high-speed electrical test equipment in both time and frequency domains with point-by-point uncertainty analysis, and for the first time making waveform calibrations traceable to fundamental physics." The citation goes on to explain "The new method improves accuracy in calibrations of oscilloscopes,

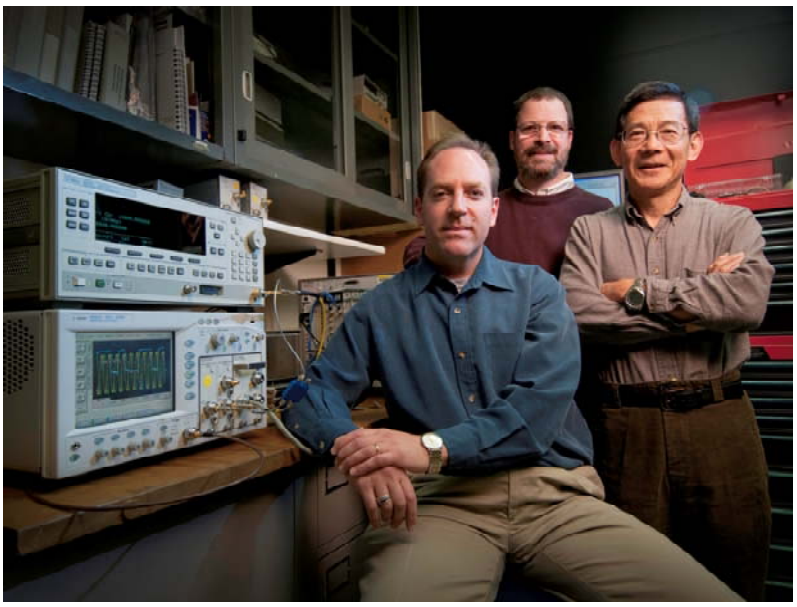


Figure 3. *Allen V. Astin Meaurement Science Award Winners: Andrew Dienstfrey (ACMD), Paul Hale (Physical Measurement Laboratory), Jack Wang (Statistical Engineering Division, Information Technology Laboratory).*

common test instruments that measure voltage in communications and electronic devices, and potentially could boost performance and save money in other fields ranging from medical testing to structural analysis and remote sensing."

Figure 4. *Ronald Boisvert won NIST's EEO/Diversity Award.*

- *NIST EEO/Diversity Award.* Ronald Boisvert of ACMD was the recipient of NIST's Equal Employment Opportunity / Diversity Award for 2010. He was cited for "leadership and continuous membership on the ITL Diversity Committee and his commitment to fostering diversity.
- *ITL Outstanding Journal Paper.* Bryan Eastin and Emanuel Knill of ACMD received the 2010 ITL Best Journal Paper Award for their article "Restrictions on Transversal Encoded Quantum Gate Sets," which appeared in *Physical Review Letters*, Volume 102, Article Number 110502 (March 20, 2009). The pair was cited "for exemplary scientific research and exposition in the field of fault-tolerant quantum computing." In their paper Eastin and Knill proved that the ability of a quantum code to detect arbitrary errors on component subsystems is incompatible with the existence of a universal, transversal, and unitary encoded gate set. This result completely settles this long standing fundamental question in quantum information theory, showing that the search for a universal transversally encoded quantum gate set is futile.
- *ITL Associate of the Year.* Qiming Wang, a guest researcher in ACMD was selected at the ITL Associate of the Year for 2010. Wang was recognized for her essential contributions to the Digital Library of Mathematical Functions project in the area of interactive 3D computer graphics. The ITL Associate of the Year Award recognizes one guest researcher each year for outstanding contributions to NIST programs.
- *NIST Alumni Portrait Gallery.* Cornelius Lanczos (1893-1974) was selected for recognition by the NIST Alumni Association as part of the NIST Portrait Gallery of Distinguished Scientists, Engineers and Administrators. The Gallery honors NIST alumni for outstanding career contributions to the work of the Institute. Portraits and biographies of those selected are displayed in the corridor of the NIST cafeteria in Gaithersburg. Lanczos was a NIST staff member in 1943-44 participating in the NBS Math Tables Project, and again in 1949-52 as a member of the NBS Institute for Numerical Analysis. A towering figure in applied mathematics and theoretical physics, Lanczos' best-known contribution to science, as measured by citations, was made while at NBS. The "Lanczos method" for calculating the eigenvalues of large matrices was published in the *Journal of Research of NBS* in 1950.

Figure 5. *Cornelius Lanczos' daughter-in-law Alice (Seattle, WA) and grandson Andrew (Tel Aviv, Israel) attended the Alumni Portrait Gallery induction ceremony held in Gaithersburg, MD on October 1, 2010. Lanczos' portrait is visible on the bottom row.*

Best Contribution Awards

- *Best Paper Award at Info Security Conference.* Vladimir Marbukh of the ACMD, along with Daniel Genin and Anastase Nakassis of the ITL Advanced Networking Technologies Division were awarded a Certificate of Merit for outstanding contribution to the 2010 International Conference of Information Security and

Internet Engineering, which was held in London on June 30 – July 2, 2010. The paper, *Vulnerability of Selfish Routing to Attacks: Game-theoretic Models and Initial Results*, presented a model of a potential strategic attack on a class of network packet routing algorithms. They demonstrated that even a weak attacker can inflict serious damage (as measured by degradation in system performance) in routing algorithms characterized by selfish user behavior. The paper was one of four cited as best papers at the conference. The conference was one of 12 co-located conferences comprising the World Congress on Engineering sponsored by the International Association of Engineers

Other Significant Recognition

- *Beichl Named Editor-in-Chief of Scientific Computing Magazine.* Isabel Beichl of ACMD was selected to serve a second term as Editor-in-Chief of *Computing in Science and Engineering* (CiSE), a joint publication of the IEEE Computer Society and the American Institute of Physics. CiSE is a bimonthly publication that combines peer-reviewed articles, columns, tutorials, and book reviews in a magazine format. According to its statement of purpose, CiSE "aims to support and promote the emerging discipline of computational science and engineering and to foster the use of computers and computational techniques in scientific research and education." Beichl's original appointment as Editor-in-Chief, which was made by the IEEE Computer Society Board of Governors, began in January 2009; her second term extends to December 2012.

- *Faculty Appointee G. W. Stewart's 70th Birthday Noted*. G. W. (Pete) Stewart, Professor Emeritus of Computer Science at the University of Maryland and long-time faculty appointee in ACMD, was honored by a conference, a book, and a special journal issue organized in commemoration of his 70th birthday. The conference, *Numerical Linear Algebra: Perturbation, Performance, and Portability*, which held July 19-20, 2010, in Austin, Texas, was attended by nearly 100 of Stewart's friends and colleagues from around the world. Birkhauser, in their Contemporary Mathematicians series, has also recently published *G. W. Stewart: Selected Works with Commentaries,* in Stewart's honor. Edited by Misha Kilmer of Tufts University and Dianne O'Leary of the University of Maryland (another faculty appointee in ACMD), the new book collects 44 of Stewart's papers, along with over 100 pages of essays putting his work in historical perspective. In addition, a special issue of the journal *Linear Algebra and Its Applications* is being organized in Stewart's honor. Stewart is a world-renowned expert in computational linear algebra. He has made fundamental and highly cited advances in the analysis of rounding error in numerical computations, perturbation of eigensystems, generalized inverses, least squares problems, and matrix factorizations. He has developed efficient algorithms for the singular value decomposition, updating and downdating matrix factorizations, and the eigenproblem that are widely used in applications. His six textbooks are models of exposition that have educated multiple generations of researchers. Stewart's contributions have led to numerous honors, including election to the National Academy of Engineering. Stewart was 70 years old on October 1, 2010.

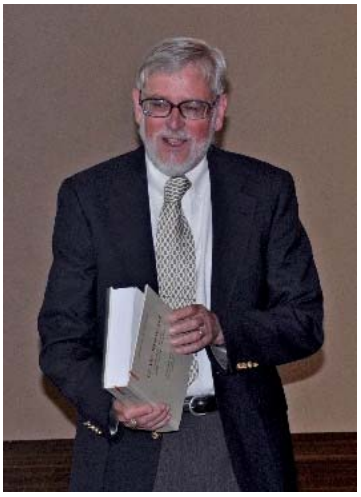
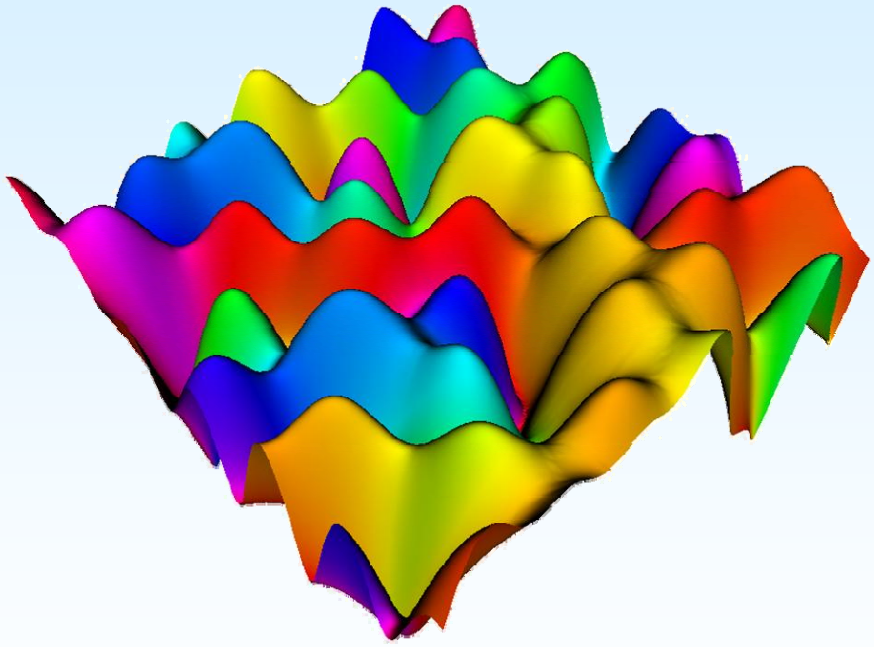


Figure 6. *Pete Stewart. (Photo by Eric de Sturler of Virginia Tech. Used with permission.)*

Part II

Features



A Special Functions Handbook for the Digital Age

In May 2010 NIST released the Digital Library of Mathematical Functions (DLMF), a free online repository of information on the special functions of applied mathematics. The culmination of a 12-year effort involving some 50 researchers from around the globe, the DLMF details the mathematical properties of some 33 classes of functions. The richly linked resource also includes interactive 3D graphics, a comprehensive index of available software, and a math-aware search engine. The DLMF is a successor to the enormously successful Handbook of Mathematical Functions *(M. Abramowitz and I. Stegun, eds.), which was published by NBS in 1964. A print companion, the* NIST Handbook of Mathematical Functions *has also been published by Cambridge University Press.*

Ronald F. Boisvert

With an estimated 40,000 citations[1], the classic NBS *Handbook of Mathematical Functions* [1] is among the most cited works in the mathematical literature. Edited by Milton Abramowitz and Irene Stegun and released in 1964, the Handbook was the result of a 10 year project to compile essential information on the special functions of applied mathematics (e.g., Bessel functions, hypergeometric functions, and orthogonal polynomials) for use in applications [2]. In spite of its enormous success, the NBS Handbook is also *old*: (a) more than half of its 1,046 pages are tables of function values whose use has largely been superseded by modern numerical software, (b) there have been enormous advances in the field of special function in the last 45 years, and (c) modern communications networks provide unique new opportunities for effectively conveying information.

Recognizing these problems and opportunities, in 1997 we undertook a project to update and modernize the Abramowitz and Stegun Handbook. Our main goals were to identify those mathematical functions and their properties that are most important in application, to present this information in a concise form accessible to practitioners, and to disseminate it to the widest possible audience. The culmination of that project was the release in May 2010 of the online and freely available NIST Digital Library of Mathematical Functions (DLMF) and its print companion, the *NIST Handbook of Mathematical Functions* [3].

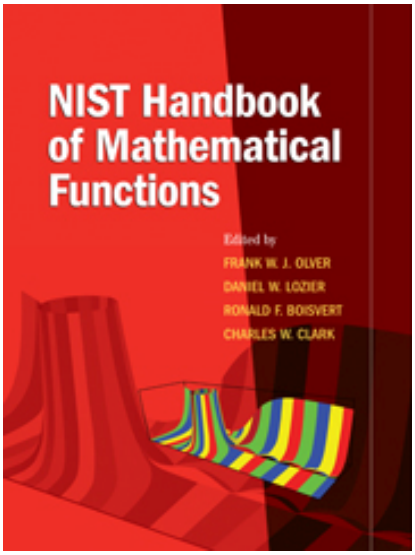


Figure 7. *The print companion to the NIST Digital Library of Mathematical Functions.*

Mathematical Content. The mathematical content of the DLMF[2] is organized into 36 chapters; see Table 3. The first three are methodological in nature, providing essential definitions and background needed for the analysis and computation of special functions. The remaining 33 chapters each address a particular class of functions. These each have a similar organization. The first section provides a brief description of the notation that is used and its relation to alternate notations.

Next comes an enumeration of the function's mathematical properties, such as the defining differential equation, special values, periods, poles, zeros, elementary identities, series representations, integral representations, transformations, relations to other functions, asymptotic expansions, derivatives, integrals, sums, and products. All of these are presented in the telegraphic style characteristic of the Abramowitz and Stegun Handbook. One noteworthy new feature of the DLMF is that references are provided that connects every formula to a proof. Not only is this a means of verification, but it allows researchers to learn proof techniques that may help them derive variations on the formulae.

In each function chapter a section entitled Graphics provides a set of 2D and 3D views of the functions designed to convey visually their essential features. Complex-valued functions are displayed by showing a 3D surface representing the modulus of the function; the surface is color coded to convey information about the phase (a 4D effect). Each function chapter also has a brief section pointing out mathematical and physical applications.

Finally, each chapter ends with a section on computation. Here the DLMF provides a set of hints on fruitful numerical approaches with references.

[1] This estimate was produced with the help of the Thomson Reuters *Web of Science*. It is an estimate because the Handbook was cited in hundreds of different ways, making a complete harvest of citations quite laborious.

[2] We use DLMF to refer to both the online handbook and its print companion.

Online-only Content. The online version of the DLMF provides additional technical content in comparison with its print counterpart. For example, in some cases additional instances in a series of formulae, such as weights and nodes of higher-order Gauss quadrature formulae, are available online. The online DLMF also has a much larger collection of visualizations, and all 3D visualizations there are interactive [4]. The DLMF provides its interactive 3D content in two separate formats: Virtual Reality Modeling Language (VRML) [5] and Extensible 3D (X3D) [6], a newer standard.

Another substantial collection of online-only content is information about software for the special functions. In each chapter, a Software section lists research articles describing software development efforts associated with functions covered in the chapter. In addition, a table of links is provided to help users identify available software for each function. Open source software, software associated with published books, and commercial software are all included.

The online DLMF also provides a rich set of tools which enhance its use as an interactive reference work. For example, each equation has a link providing the following additional information (metadata):

- The name of each symbol in the equation linked to its definition.
- Reverse links to places in the DLMF where the equation is cited.
- Alternate encodings of the equation: TeX, MathML, png (image).

The online references have a similarly rich set of links associated with them:

- Links to reviews in the AMS's MathSciNet and Zentralblatt's MATH database.
- Links to full text of articles online.
- Links to software associated with the reference.
- Reverse links to places in the DLMF where the reference is cited.

Table 3. *Chapters of the DLMF.*

1	Algebraic and Analytic Methods
2	Asymptotic Approximations
3	Numerical Methods
4	Elementary Functions
5	Gamma Function
6	Exponential, Logarithmic, Sine, and Cosine Integrals
7	Error Functions, Dawson's and Fresnel Integrals
8	Incomplete Gamma and Related Functions
9	Airy and Related Functions
10	Bessel Functions
11	Struve and Related Functions
12	Parabolic Cylinder Functions
13	Confluent Hypergeometric Functions
14	Legendre and Related Functions
15	Hypergeometric Function
16	Generalized Hypergeometric Functions and Meijer G-Function
17	q-Hypergeometric and Related Functions
18	Orthogonal Polynomials
19	Elliptic Integrals
20	Theta Functions
21	Multidimensional Theta Functions
22	Jacobian Elliptic Functions
23	Weierstrass Elliptic and Modular Functions
24	Bernoulli and Euler Polynomials
25	Zeta and Related Functions
26	Combinatorial Analysis
27	Functions of Number Theory
28	Mathieu Functions and Hill's Equation
29	Lamé Functions
30	Spheroidal Wave Functions
31	Heun Functions
32	Painlevé Transcendents
33	Coulomb Functions
34	3*j*, 6*j*, 9*j* Symbols
35	Functions of Matrix Argument
36	Integrals with Coalescing Saddles

Math Search. While the DLMF does have an extensive index, the main way in which one finds reference information online is through search engines. Existing search technology is largely based upon analysis of words in documents. As a mathematical reference written in a "telegraphic" style, there is not a wealth of words in the DLMF for a search engine to index. As a result, it was necessary to develop our own math-oriented search engine. The DLMF search engine is based on Lucene[3], an open-source text-based search engine maintained by the Apache project. To enable math search this tool was augmented with additional data and processing layers [7, 8].

The query interface is a single text box. Query terms can be English text or mathematical expressions. The latter can be expressed in a LaTeX-like form, or using notation used in common computer algebra systems. Examples are given in Table 4. To match mathematical expressions, the underlying search engine should understand elementary arithmetic rules like commutative and associative laws. It should also realize that a search for sin(x) should probably also return expressions with sin(y), etc. Providing a search engine with such mathematical smarts remains a challenge. Instead, we approximate this using query relaxation. If

[3] http://lucene.apache.org/

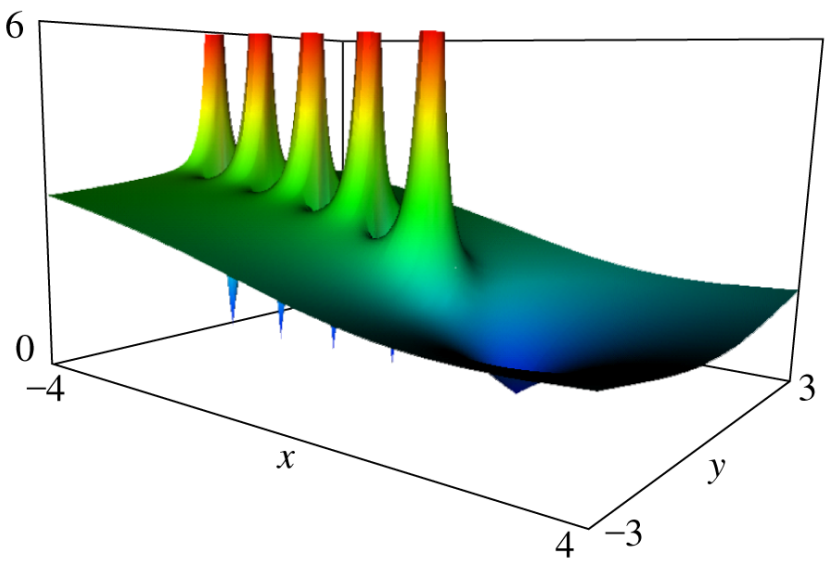


Figure 8. *| ψ(x + i y) | , the modulus of the complex psi function.*

Table 4. *Examples of DLMF queries.*

Query	Interpretation
`Gamma(?) = int`	$\Gamma(x) = \int$, for any x. ? is a single-character wildcard.
`int_$^$ BesselJ`	Any definite integral containing a *J* Bessel function. $ is a multi-character wildcard, which will match "infinity" and "pi/2" for example
`sum_infinity^infinity BesselJ`	Any sum with limits -∞ to ∞ containing the *J* Bessel function
`zeta contour integral`	Text search for contour integrals of the zeta function

a user's search does not result in any matches, the system will allow matches with successively larger numbers of intervening symbols or matches with symbols in any order.

The page of search results delivered by the DLMF is a list of matched objects, which can include displayed equations, figures, tables, section titles or text, and references. Matched portions of equations and text are highlighted to help the user understand why the item was matched. Clicking on any item follows a link to see the object in context.

Math on the Web. Displaying mathematical content on the web presents its own set of challenges. For the DLMF we have decided to embrace MathML[4], the open community standard for representing mathematics developed by the World Wide Web Consortium (W3C). MathML provides a number of advantages. It allows equations to be scaled automatically when one scales the text size in the browser. It enables accessibility features to be deployed. It also has the potential to support semantics-preserving exchange of mathematical content[5]. One example is cut-and-paste of equations between web pages, text editors, and computation systems, or other types of interoperability between computer algebra systems.

MathML presents some practical problems, however. First, it is not yet supported by all browsers. It is supported natively in Firefox, but in Internet Explorer only with a specialized (free) 3rd party plug-in. Because of this, the DLMF is delivered in two forms: with MathML and with equations as images. The DLMF server identifies the requesting browser and sends the most appropriate form.

The second issue is that MathML is a language for computers, not humans, and hence authoring in MathML is a challenge. Authors are more comfortable writing in LaTeX, and hence this was used as the input language for the DLMF. From this we wished to generate each of XHTML + MathML, HTML + images, and a traditional printed handbook. Generating MathML from LaTeX source is far from trivial, especially if one wants to represent mathematical semantics in the MathML. A LaTeX to MathML translator was developed at NIST to confront this problem. LaTeXML[6] is a Perl program that completely mimics the processing of TeX, but generates XML rather than DVI. A postprocessor converts the XML into other formats such as HTML or XHTML, with options to convert the math into MathML or images. The system relies on additional declarations and a variety of heuristics to perform the generation. While it was developed specifically for the DLMF project, LaTeXML is a general-purpose tool and has been applied to much broader collections of scientific publications [9].

Putting It All Together. No one institution has the resources and technical expertise to carry out a project like this one alone. NIST is fortunate to have had the

[4] http://www.w3.org/Math/

[5] MathML comes in two flavors: Presentation Markup and Content Markup. The former is focused only on proper display, while the latter includes some semantic-preserving markup. Most current implementations only support Presentation Markup.

[6] http://dlmf.nist.gov/LaTeXML/

Figure 9. *DLMF editors and developers at NIST included the following (l. to r.): Abdou Youssef, Brian Antonishek, Daniel Lozier, Marjorie McClain, Bruce Miller, Bonita Saunders, Charles Clark, Frank Olver, and Ronald Boisvert.*

cooperation of a large number of experts worldwide in the assembly of the technical information contained in the DLMF. The DLMF chapters were assembled by 29 external authors working under contract to NIST. NIST was responsible for editing the material so as to achieve the necessary depth and breadth of coverage and to ensure a uniform style of presentation. In addition, a set of 25 independent validators were enlisted to check the accuracy of the technical content. Development of the DLMF web site and its interactive content was performed by NIST staff.

A project as complex (both technically and organizationally) as this one takes time. The initial plans for the project were laid out at a workshop held at NIST in 1997. So, the DLMF has been some 12 years in the making. It is to their credit that NIST management had the patience to see these efforts through such a long and exacting process.

The Future. NIST is committed to the continued maintenance and development of the DLMF. We already have had suggestions for extensions. New chapters are under consideration. We are also considering bringing back tables, but, rather than static tables, tables generated on demand with certified correct values. We do hope that the DLMF provides a firm foundation for extending the legacy of Abramowitz and Stegun far into the 21st century.

References

[1] M. Abramowitz and I. Stegun, eds., *Handbook of Mathematical Functions, with Formulas, Graphs and Tables*, Applied Mathematics Series 55, National Bureau of Standards, Washington, DC, 1964.

[2] R. F. Boisvert and D. W. Lozier, Handbook of Mathematical Functions, in *A Century of Excellence in Measurements, Standards, and Technology – A Chronicle of Selected NBS/NIST Publications, 1901-2000* (D. Lide, ed.), NIST Special Publication 958, 2000, pp. 135-139.

[3] F. W .J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, eds., *NIST Handbook of Mathematical Functions*, Cambridge University Press, 2010.

[4] Q. Wang and B. Saunders, Web-based 3D Visualization in a Digital Library of Mathematical Functions, in *Proceedings of the 10th International Conference on 3D Web Technology*, Bangor, Wales, UK, 2005, 151-157.

[5] A. Ames, D. R. Nadeau, and J. L. Moreland, *VRML 2.0 Sourcebook*, Wiley, 1996.

[6] D. Brutzman and L. Daly, *X3D: Extensible 3D Graphics for Web Authors*, Morgan Kaufmann, 2007.

[7] A. Youssef, Information Search And Retrieval of Mathematical Contents: Issues And Methods, in *Proceedings of the ISCA 14th International Conference on Intelligent and Adaptive Systems and Software Engineering*, Toronto, July 20-22, 2005, pp. 100-105.

[8] A. Youssef, Methods of Relevance Ranking and Hit-content Generation in Math Search, in *Proceedings of the 6th International Conference on Mathematical Knowledge Management*, Hagenberg, Austria, June 27-30, 2007, pp. 393-406.

[9] H. Stamerjohanns, M. Kohlhase, D. Ginev, C. David, and B. Miller, Transforming Large Collections of Scientific Publications to XML, *Mathematics in Computer Science* **3** (2010), pp. 299-307.

Participants

Frank Olver, Daniel Lozier, Charles Clark (NIST PML), Ronald Boisvert, Bruce Miller, Bonita Saunders, Abdou Youssef, Marjorie McClain, Qiming Wang, Brian Antonishek (NIST ITL). In addition, the DLMF benefited from the active participation of some 50 external editors, authors, validators, and consultants. A complete list can be found on the DLMF website.

http://dlmf.nist.gov/

Linnik Densities, Logarithmic Diffusion Equations, and Blind Deconvolution of Hubble Space Telescope Imagery

An important mathematical construct involving Brownian motion in randomized time, and used extensively on Wall Street as a tool for pricing options, has been successfully applied at NIST to sharpen galaxy images obtained with the Hubble Space Telescope's ultra sophisticated Advanced Camera for Surveys, (ACS). This work is discussed in detail in a recently published paper in the SIAM Journal on Imaging Sciences [1]. In May 2009, the ACS camera and other vital instruments aboard the Hubble were refurbished and upgraded, in a heroic mission by Space Shuttle Atlantis astronauts. In private discussions at NIST in September 2010, Debra Elmegreen, President of the American Astronomical Society, praised NIST's Hubble image sharpening technology.

Alfred Carasso

Optical Transfer Functions and Blind Deconvolution. Images produced by scientific instrumentation are commonly blurred in such a way that important fine scale information is poorly reproduced. Many factors may contribute to this blur, including optical aberrations, scattering properties of the intervening medium, possible atmospheric effects, motion of the object, and the cumulative effect of various interfacing electronic acquisition devices, each with its own imperfect response. Mathematically, it is helpful to lump all of these various effects into a single optical transfer function (OTF) that describes how each Fourier harmonic in the unknown desired sharp image, is attenuated by the imaging process. The result of all these individually attenuated Fourier components is the recorded blurred image. In principle, knowledge of the OTF can be used to deblur the image. However, special precautions are necessary, as deblurring is an ill-conditioned problem which is prone to severe noise amplification.

Unfortunately, accurate knowledge of the OTF is seldom available. Over the last several years, Carasso has developed and refined a blind deconvolution approach that seeks to identify a plausible OTF from the asymptotic behavior in the Fourier transform of the blurred image. Brownian motion is pervasive in many branches of science, and the familiar bell-shaped Gaussian probability distribution is the DNA of Brownian motion. Naturally, Gaussian OTFs are ubiquitous in image science. A blind identification method might be based on appropriate curve-fitting of a Gaussian candidate OTF to the Fourier transform behavior in the given blurred image. Surprisingly, Gaussian OTFs turn out to be poor candidates for Hubble images, indicating

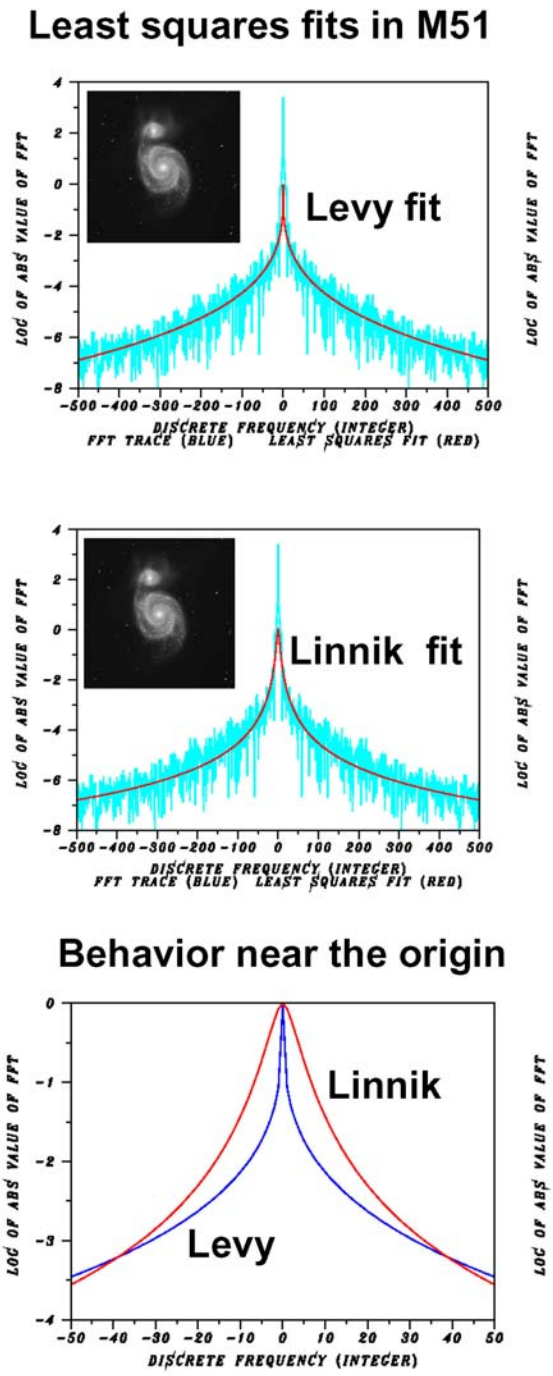


Figure 10. *Blurred M51 image data* $\log|\hat{g}(\xi,0)|$ *can be well-fitted with a Lévy stable OTF, as well as with a generalized Linnik OTF. Both OTFs have similar behavior away from the origin, but differ fundamentally near the origin. This difference plays a crucial role.*

Figure 11. *Pinwheel Galaxy NGC1309 (left). Linnik deblurred image (right) exhibits multitude of previously faint stars, scythe-shaped structure at eleven o'clock is more clearly defined, and outer spiral arms have been recovered.*

that the blurring is not the result of an underlying Brownian motion process.

Linnik OTFs and Brownian Motion in Randomized Time. As is now being increasingly recognized, many types of random processes that play significant roles in applied science, involve a fundamental modification of Brownian motion. This is the seminal notion of a subordinated process put forth by Princeton mathematician Salomon Bochner in 1949. This concept refers to the stochastic process obtained when Brownian motion is observed at an appropriate randomized operational time $T(t)$, rather than in standard clock time t. An analogous idea would be to record the values of the Dow Jones Industrial Average at intervals of 10 million shares traded (the trading clock), rather than at ten minute intervals. Commonly occurring Lévy stable motions are examples of subordinated Brownian motion, and Lévy stable OTFs were successfully applied by Carasso and his NIST collaborators in deblurring nanoscale scanning electron microscope imagery.

Generalized Linnik processes are obtained by evaluating Lévy stable motions at the stochastic time $\Gamma(t)$, where, for each $t > 0$, $\Gamma(t)$ obeys a gamma probability distribution on $u \geq 0$. This amounts to two consecutive, independent, subordinations of Brownian motion. The Variance Gamma process, a standard tool used on Wall Street for options trading, is a special case of such generalized Linnik processes. An important new NIST idea was to consider generalized Linnik characteristic functions as candidate OTFs in blind deconvolution of Hubble imagery. While Linnik processes are unknown in image science, Carasso was drawn to consider such OTFs because of their mathematical properties. As shown in Figure 10 for the Whirlpool galaxy, both Linnik and Lévy stable OTFs have the same desirable high frequency behavior, one that accords well with a large class of astronomical images. However, while Lévy stable OTFs exhibit non-differentiable cusps near the origin, Linnik OTFs are smoothly differentiable at the origin. It is this difference in behavior that enables Linnik OTFs to produce superior reconstruction of fine scale information.

Deblurring Hubble Imagery. Carasso's slow motion blind deconvolution procedure is based on solving an ill-posed logarithmic diffusion equation backwards in time. The defining parameters of the Linnik candidate OTF enter this diffusion problem. These are estimated directly from the blurred image by least squares curve fitting of the absolute value of the blurred image Fourier transform, as shown in Figure 10.

The Advanced Camera for Surveys (ACS) is Hubble's most powerful camera. However, in many cases, Linnik blind deconvolution can extend the range of that instrument by making faint background objects more visible, while the structure of foreground objects becomes more clearly defined. The first example, in Figure 11, is a February 2006 ACS image of the Pinwheel Galaxy NGC1309. Here, the Linnik deblurred image exhibits a multitude of previously faint stars, the scythe-shaped structure at eleven o'clock is now brighter and more clearly defined, and the previously barely visible outer spiral arms have been recovered. Within the galaxy's main body, the bluish star clusters along the spiral arms, and the dust lanes, are now much better resolved.

The second example, in Figure 12, is an April 2008 ACS image of NGC 6050, involving a collision between two spiral galaxies. As in Figure 11, the Linnik deblurred image is brighter and displays better resolution of the structural details in the two galaxies. Also, background galaxies have become more visible.

The last example, the barred spiral galaxy NGC6217 in Figure 13, is significant. This was the first celestial object imaged by Hubble using the upgraded ACS camera after the May 2009 refurbishing. Again, the Linnik deblurred image shows substantial sharpening of the dust lanes and other structural details. The outer spiral arms and background galaxies have also become more visible.

References

[1] A. Carasso, Bochner Subordination, Logarithmic Diffusion Equations, and Blind Deconvolution of Hubble Space Telescope Imagery and Other Scientific Data, *SIAM Journal on Imaging Sciences* **3** (2010), pp. 954-980.

Figure 12. *Colliding galaxies NGC6050 (left). Linnik deblurred image (right) is brighter and displays better resolution of the structural details in the two galaxies. Also, background galaxies have become more visible.*

Figure 13. *Barred spiral galaxy NGC6217. First celestial object imaged by Hubble using May 2009 upgraded ACS camera. Linnik deblurred image shows substantial sharpening of dust lanes and other structural details. Outer spiral arms and background galaxies have become more visible.*

Modeling Reactive Wetting

The term "wetting" usually refers to the tendency of a liquid to spread on a substrate; for example, a drop of oil will spread on the surface of water until it reaches atomic-level thicknesses ("complete wetting"). A water drop placed on a stainless steel surface will form a spherical cap with characteristic "contact angles" at the water-steel-air tri-junction that are determined by the surface energies of the three interfaces ("partial wetting"). On the other hand, a drop of mercury placed on glass surface beads up in an attempt to minimize its area of contact ("non-wetting"). The tendency of a fluid to wet a substrate is an important consideration for many technological applications, including coating flows, soldering, and electronic interconnects. We have developed mathematical and computational models of the process in order to improve our understanding of the complex dynamics involved in this process.

Geoffrey B. McFadden

Reactive wetting occurs when a liquid and substrate can interact chemically; for example, the substrate may dissolve in the liquid, or the liquid may diffuse into the substrate. In this case the understanding of the wetting process involves not only capillary considerations but also the thermodynamics of the components and their tendency to combine in order to minimize the free energy of the system. This results in a more complicated process, since the substrate plays an active, rather than a passive, role in establishing the system geometry, including the determination of the free surfaces and contact angles that appear in the system. An example of the resulting geometry during reactive wetting is shown in Figure 14.

An interesting aspect of wetting concerns the dynamics associated with the motion of the contact lines at the junction of the liquid, solid, and vapor phases. For the simpler problem of spreading on an inert planar substrate, it is well-known that the imposition of standard no-slip boundary conditions at the moving contact line leads to a non-physical singularity in the flow field at the contact line [1]. This is often alleviated by introducing a notion of "slip" as the fluid flows along the substrate [2]. Another approach [3], the one we adopt, involves the introduction of a diffuse interface description of the inter-phase boundaries, which also tends to relieve the hydrodynamic singularity. In the case of reactive wetting, another mechanism for dissipation is the diffusion of solute near the contact line, which introduces possible non-equilibrium effects ("solute trapping") in the dynamical description of the motion.

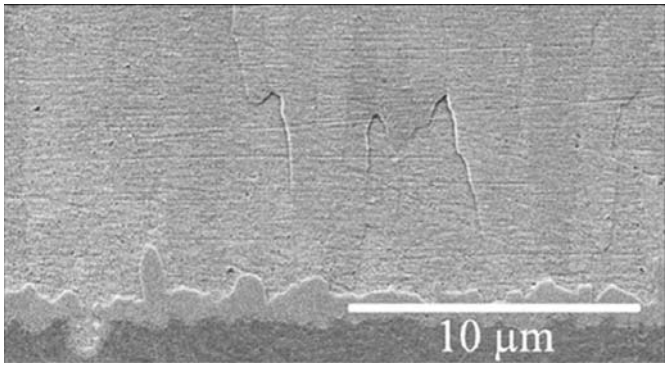


Figure 14. *Liquid tin (top) has coated a copper substrate (bottom), leading to the formation of a tin-copper compound ("intermetallic") near the solid-liquid interface; The image is taken after the liquid has been quenched to lower temperatures and become solid. The image focuses on the liquid-solid interface; a larger scale image would include the region surrounding the contact line, which would involve the vapor, liquid, solid, and intermetallic phases. The system components are binary alloy and the inert gas.*

The mechanisms of reactive wetting thus involve the interplay of fluid flow, heat and mass transport, capillary phenomena, and phase transformations. A mathematical model of reactive wetting in an isothermal, three-component, four-phase system is currently under development. To treat free surfaces and contact lines in the problem, a diffuse-interface ("phase-field") model is used [4], which involve the introduction of additional unknowns ("order parameters") that track the local phase at each point and incorporate the effects of capillarity and interfacial adsorption of solute [5].

In practice the model requires the numerical determination of surface energies that depend on phenomenological coefficients in the model. This can be done using a steady-state one-dimensional computation. An example of the phase field and solute profiles is shown in Figure 15, which illustrates that a form of wetting can also occur in the interfacial region as well as in the bulk; in this case, the solid-liquid interface is being wet by an intruding intermetallic phase localized to the interfacial region. This intermediary surface phase alters the interfacial surface energy considerably, which complicates the relation between the model's phenomenological coefficients and the surface energy.

Once the surface energies of the model are known, time-dependent, axisymmetric numerical simulations are performed to assess the dynamical behavior of the model (see Figure 16). The figure illustrates the nucleation and growth of intermetallic at the solid-liquid interface, and the spread of the intermetallic phase towards the region of the solid-liquid-vapor trijunction. The original trijunction then is replaced by two other trijunctions: liquid-vapor-intermetallic and solid-vapor-intermetallic. At an intermediate stage

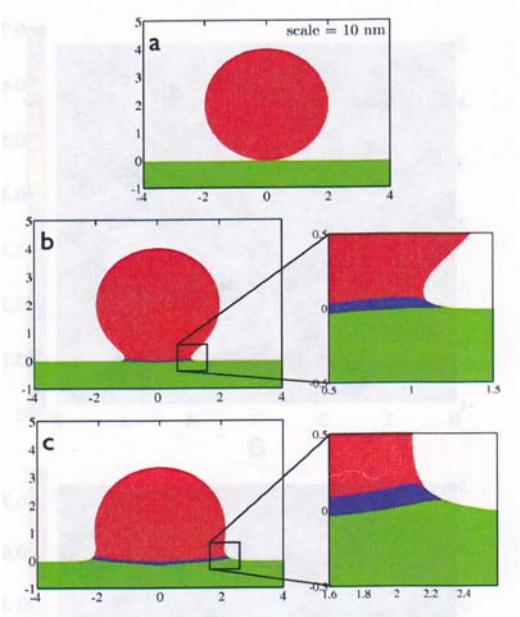


Figure 15. *Numerical simulation of the spreading of a molten metal drop (red) on a solid substrate (green) with the formation of intermetallic phase (blue) between the drop and the substrate.*

there is a transient quadrijunction where all four phases coexistence instantaneously. Thus, issues of existence and stability of quadrijuctions are also raised by the calculation, which are currently under consideration. We are also studying the control of intermetallic formulation by various parameters in the model. This can be approached by computing the size and shape of an axisymmetric lenticular "seed" of intermetallic placed at the solid-liquid interface to determine the seed's "critical radius" from a balance between surface and bulk energies. Seeds smaller than this size shrink as surface energy considerations dominate bulk energies and, conversely, larger seeds will grow as the dominance is reversed. Preliminary comparisons between the model's computation results and the analytical theory for the critical radius show good agreement.

These calculations are performed using an adaptive finite element code developed by W. Villanueva and colleagues. A manuscript describing the model appeared in recent conference proceedings [6], and another on the latest aspects of the research is currently in preparation.

References

[1] C. Huh and L. E. Scriven, Hydrodynamic model of steady movement of a solid/liquid/fluid contact line. *Journal of Colloid Interface Science* **35** (1971), pp. 85–101.

[2] E. B. Dussan, On the spreading of liquids on solid surfaces: Static and dynamic contact Lines, *Annual Review of Fluid Mechanics* **11** (1979), pp. 371–400.

[3] T. Qian, X. P. Wang, and P. Sheng, A variational approach to moving contact line hydrodynamics, *Journal of Fluid Mechanics* **564** (2006), pp. 333-360.

[4] D. M. Anderson, G. B. McFadden, and A. A. Wheeler, Diffuse-interface methods in fluid mechanics, A*nnual Review of Fluid Mechanics* **30** (1998), pp. 139-165.

[5] G. B. McFadden and A. A. Wheeler, On the Gibbs adsorption equation for diffuse interface models, *Proceedings of the Royal Society (London) A* **458** (2002), pp. 1129--1149.

[6] W. Villanueva, W.J. Boettinger, G.B. McFadden, and J.A. Warren, A Multicomponent and Multiphase Model of Reactive Wetting, *Proceedings of the 7th International Conference on Multiphase Flow*, 2010, pp. 1-8.

Participants

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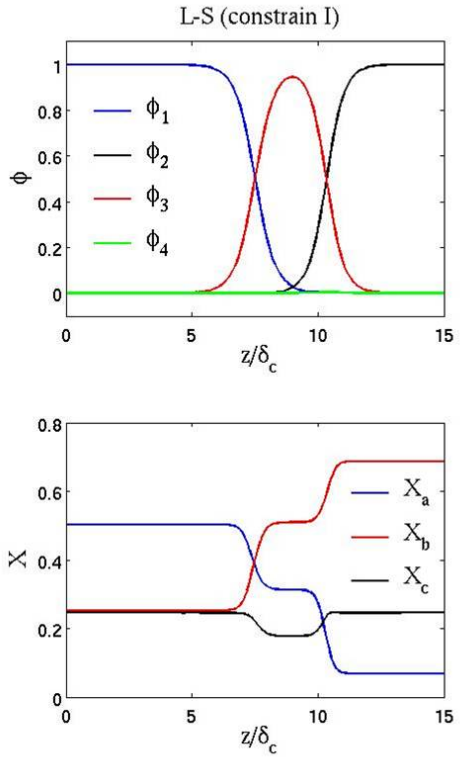

Figure 16. *One-dimensional profiles of the phase field (top) and solute field (bottom) for a diffuse interface model of a solid-liquid interface. The liquid phase field parameter is in blue, and the solid is in black. The red curve shows the intrusion of intermetallic phase which "wets" the solid-lquid interface and altering its surface energy (the green curve represents the vapor phase).The solute profiles for the three components of the ternary system assume values in the intermediate region which can be understood using thermodynamic concepts from "nucleation theory" which can be applied to the intruding phase.*

Large-scale Simulation of Suspensions

Understanding the mechanisms of dispersion or agglomeration of particulate matter in fluids, such as suspensions, is of technological importance in many industries such as pharmaceuticals, coatings, and concrete. These fluids are disordered systems consisting of a variety of components with disparate properties that can interact in complex ways. Modeling and predicting the flow of such systems represents a great scientific and computational challenge, requiring large scale simulations. In collaboration with scientists in NIST's Engineering Laboratory, we are developing an application, called QDPD (Quaternion based Dissipative Particle Dynamics), which is capable of performing large scale simulations of suspensions. QDPD is highly parallel and has been shown to efficiently scale up to at least 16,000 processors when running on a Blue Gene supercomputer at Argonne National Laboratory. Our goal is to advance our understanding of the flow properties of a specific material, fresh concrete, which is a dense suspension composed of cement, water, sand, and rocks.

William L. George
Nicos Martys

Concrete is the most widely used building material, representing a $100B US industry crucial for our nation's physical infrastructure. There is now a strong interest in making concrete a more sustainable material by finding new ways to recycle it, and by changing its ingredients in order to reduce the amount of greenhouse gas from its production (the manufacture of concrete's key ingredient, cement, accounts for 8-10% of global CO_2). As new concrete mixtures are developed to meet these needs, it is important to control rheological properties, i.e., flow properties, to satisfy performance specifications. Failure to control the flow of concrete on a job site can lead to significant cost overruns and delay by having to correct errors.

Yield stress and viscosity, both functions of shear rate, are important quantities for characterizing fluids. Yield stress is the force applied per unit area to initiate the flow. Viscosity is the applied force per unit area needed to maintain a shear rate. Shear rate is the velocity gradient perpendicular to the flow direction.

Many factors control viscosity and yield stress. For example, in building materials like concrete, viscosity and yield stress depend on the ratio of water to cement, the volume of sand or rocks used, as well as their shape and size distribution. There can be great variation among samples depending on their history and where they were obtained. For example, rocks from quarries are usually angular because they are crushed when processed, whereas rocks obtained from river beds are typically rounded due to erosion. Also, the more similar the size of the rocks in a concrete suspension, the harder it is to get it to flow. In this case, the concrete may actually jam when poured through a narrow opening causing construction delays. Clearly, to optimize the flow properties of concrete and other suspensions, one needs to understand the relationship between flow and properties of the fluid's constituents.

High fidelity modeling of the flow of concrete is a great scientific challenge. In particular, accounting for the size and shape variation of the solid components (cement, sand, and rocks) poses many computational difficulties. A representative system may entail keeping track of up to 100,000 particles of varying shape and size. Further, many of the forces between particles depend on the local surface curvature of the aggregate at points close to neighbors, which requires keeping track of the location, orientation and shortest distance between neighboring particles. Clearly, modeling such systems necessitates large-scale simulations. We have adopted and developed some novel approaches that can successfully take into account many of the features of a suspension. Our code, QDPD [1], has been validated by both theory and experiments on idealized systems and has been extended to account for random shaped objects with different inter-particle interactions.

QDPD uses modified versions of the recently developed DPD (Dissipative Particle Dynamics) technique [2] for the simulation of Newtonian fluids, and the Smoothed Particle Hydrodynamics technique (SPH) [3], for the simulation of non-Newtonian fluids, to simulate dense suspensions such as cement paste, mortar, and concrete. In addition to the forces computed using DPD and SPH, other forces are computed to better account for the interaction between inclusions (large particles). These include lubrication forces that help keep the inclusions separated, and van der Waals forces that introduce an attractive interparticle force. Brownian forces are also present in QDPD to maintain system temperature.

We started with the original serial version of QDPD and enhanced it to utilize large parallel machines with 500+ processors, sometimes using 2,000 or more processors, to simulate systems with more than 32,000 inclusions and 1M mesoscopic fluid particles. QDPD remains under constant development improve its parallel performance and to add new capabilities.

During 2010 we had access to the 164,000 processor IBM Blue Gene/P supercomputer Intrepid, having been awarded 2M CPU-hours of compute time as part of DOE's INCITE program. This has enabled us to perform several very large simulations. For example,

we performed a simulation of a relatively sparse suspension (15% volume fraction) sheared at a very low rate, which alone required approximately 360,000 processor hours, for comparison to a physical experiment for validation. We also used some of our 2010 allocation to develop code improvements to QDPD that now enable us to run simulations efficiently on up to 16,000 processors. This new capability will be needed in the next few years as we extend our research into larger systems and the simulation of vane rheometers.

Our latest proposal to DOE resulted in an award of 25M processor hours for 2011, with the possibility of equivalent support for 2012 and 2013. This will allow us to continue this research into areas not previously possible due to intensive computational requirements.

Through numerical modeling and visualization, our work has provided insights into the physical mechanisms associated with the onset of concrete flow. Aspects of yield stress and viscosity can now be linked to spatio-geometric properties of suspensions including the number of neighboring rocks and their relative orientation. Further, by examining very long time scale behavior, we can link the motion of suspended rocks to visco-elastic material properties.

Our recent simulations have shown that the mechanisms that control the onset of flow can be linked to macroscopic properties such as yield stress and viscosity. We developed a novel way of describing the interparticle stress fields and their spatial correlations. Through this, it was discovered that under shearing, although the suspended particles remain in a liquid order, the interparticle stress is strongly anisotropic [4]. In addition, a transition under flow was observed: during a transient regime at low deformation, the stress propagates along the compression direction of the shear, whereas at larger deformations the stress is organized into layers parallel to the flow direction. Further, we found that yield stress is shear rate dependent [5]. The higher the shear rate the greater the yield stress. However, in the limit of zero shear rate, yield was found to go to zero due to of temperature effects.

We have recently modeled cementitious materials composed of cement and fly ash [6]; see Figure 17. We studied the effect on flow of substituting 10% of cement with fly ash. To do this we modeled a system of angular shaped particles (cement) combined with smaller spheres (ultra fine fly ash) and found that there is a decrease in yield stress and viscosity in comparison to the same system without fly ash.

Finally, while our main interest is on predicting the rheological properties of cement based materials, the improved understanding of flow properties of complex suspensions derived from this research should have a broad impact. Understanding mechanisms for the dispersion or agglomeration of such systems remains a challenge in many industries ranging from pharmaceuticals to coatings.

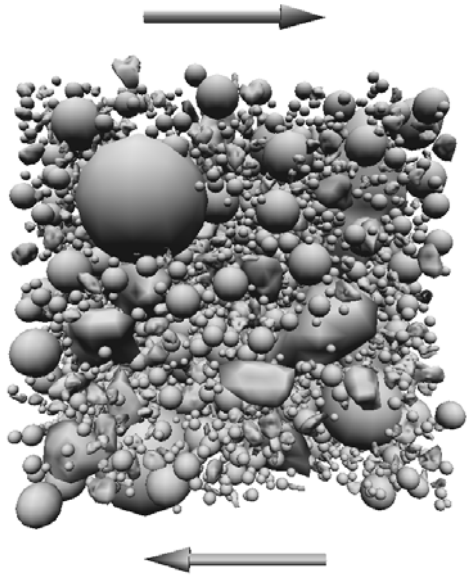

Figure 17. *Snapshot of a flowing cement paste. The cement paste is composed of 33 percent cement particles (angular particles) and 67 percent fly ash (round). This simulation is part of a study to determine the effect of replacing cement particles with fly ash, a by product of burning coal in energy plants. This allows us to identify the optimal size distribution of particles to improve flow.*

References

[1] N. S. Martys, Study of a dissipative particle dynamics based approach for modeling suspensions, *Journal of Rheology* **49**(2) (March/April 2005), pp. 401-424.

[2] P. J. Hoogerbrugge and J. M. V. A. Koelman, Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics, *Europhysics Letters* **19** (1992), pp. 155-160.

[3] J. J. Monaghan, Smoothed particle hydrodynamics. *Reports on Progress Physics* **68** (2005), pp. 1703-1759.

[4] N. S. Martys, D. Lootens, W. George and P. Hebraud, Contact and stress anisotrophies in start-up flow of colloidal suspensions, *Physical Review E* **80** (2009), article 031401.

[5] N. S. Martys, M. Khalil, W. George, D. Lootens, and P. Hebraud, Stress propagation in a concentrated colloidal suspension under shear, submitted.

[6] N. S. Martys, Multiscale modeling of the flow of cement based materials, *Rilem State of the Art Report on Numerical Simulations of Fresh Concrete Flow*, 2010.

Participants

William George, Steve Satterfield, Marc Olano, Judith Terrill; Nicos Martys and Ed Garboczi (EL); Pascal Hebraud (CNRS/ESPCI, France).

http://www.nist.gov/itl/math/hpcvg/dpdhpc.cfm
http://www.nist.gov/itl/math/hpcvg/concretevis.cfm

High Precision Calculations of Properties of Few-electron Atomic and Molecular Systems

NIST has long been involved in supplying critically-evaluated data on atomic and molecular properties such as the atomic properties of the elements contained in the Periodic Table and the vibrational and electronic energy level data for neutral and ionic molecules contained in the NIST Chemistry WebBook. Fundamental to this endeavor is the ability to predict, theoretically, a property more accurately than even the most accurate experiments. It is our goal to be able to do this for few-electron atomic and molecular systems. The quantum chemical wave function methods in current use for most electronic structure computations have accuracy limits arising from their fundamental inability to properly describe electron-electron cusp behavior. Our work is devoted to the development of a rigorous, "explicitly-correlated" method that solves the electron cusp problem and delivers energy levels for small atomic and molecular systems of high precision in parallel computing environments.

James S. Sims

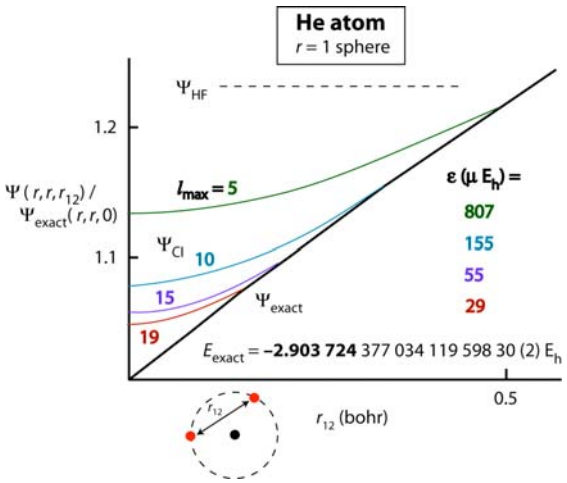

Figure 18. *Failure of conventional CI wave functions to describe the electron cusp in the helium atom. The cusp region of the full Cartesian coordinate space can be envisioned by reflecting the plots about the vertical axis.*

The revolutions in physics in the early decades of the past century provided essentially exact, predictive theories for all chemical properties and processes. However, the mathematical intractability of the Schrödinger equation prevented the computation of accurate numerical solutions for atomic and molecular systems until recently. In the past two decades, there have been breathtaking improvements in computer hardware and innovations in mathematical formulations and algorithms, leading to "virtual experiments" becoming a more and more cost-effective and reliable way to investigate chemical and physical phenomena.

Virtually all *ab initio* methods of quantum chemistry in some way involve the orbital approximation, in which the many-electron wave function (Ψ) is represented as superpositions of antisymmetrized products of one-electron functions. Such configuration interaction (CI) methods have been quite successful in approaching experimental accuracy for relative energies of modestly-sized atoms and molecules. However, orders of magnitude improvements are needed to expand the spectroscopic databases into inaccessible realms, establish its building blocks beyond dispute, and supersede expensive experimental approaches.

The essential flaw in theoretical methods built on the orbital approximation is their inability to correctly describe the mathematical cusp behavior of many-body wave functions in regions of close electron proximity, the so-called electron cusp region of the exact electronic wave function [1-3]. This flaw leads to incomplete accounting of instantaneous, short-range correlation among electrons. We are undertaking theoretical development of our hybrid Hylleraas-CI wave function method to solve the electron cusp problem and bring subchemical accuracy to atomic systems with more than two electrons.

A depiction of the electron-electron cusp in an essentially exact Hy-CI wave function of the helium (He) atom ground state is shown in Figure 18. In the region of the electron coalescence point, the exact wave function is linear in the interelectronic distance (r_{12}). However, conventional quantum chemical CI wave functions effectively incorporate only even powers of r_{12}, do not have sufficient flexibility to fully relax into the conical region of the cusp, and thus poorly account for the short-range electron correlation. In Figure 18, these deficiencies are clearly exhibited by CI wave functions using special analytical and numerical techniques for extremely high angular momentum (l) cutoffs. With an orbital (one-electron) basis saturated through l = 5, CI is too large by 14% at the coalescence point, and the corresponding error in the electronic energy is 807 microhartree (μh). Even after extending the basis set to an unprecedented l = 30, the result of some 70 years of trying [4] is that the best CI treatment for He is accurate to only 5 decimal places, demonstrating that converging absolute energies even to the μh level is impossible in computations with orbital treatments.

In contrast, the early work of Hylleraas [5] showed the superiority of explicitly-correlated methods, which directly incorporate the r_{12} variable into the wave func-

tion. Our hybrid Hylleraas-CI result, shown in Figure 18, achieved better than 20 digits of accuracy in the absolute energy [4], at least 14 orders of magnitude better than the best conventional CI treatments. The challenge for computational scientists is to extend the phenomenal accomplishments on atomic helium to three, four, and more electron states and to molecular systems.

Hylleraas's original method (Hy) has been extended to three electrons [6, 7] resulting in some of the most accurate calculations on lithium (Li) and Li-like systems to date, way beyond spectroscopic accuracy. Like helium, virtual experiments can be done that are more accurate than current experimental capabilities, but not without huge computational costs (the lithium calculations require an estimated 6,000 times more computational power than helium). However, already at the four electron level there are significant unresolved integration problems with the original Hy approach. To get around these problems we have developed a hybrid Hy-CI method that merges the ease of calculation of the CI method with the more rapid achievement of accurate results and offers the hope of breaking the four electron integral barrier (with only a single r_{ij} in any term, the most difficult integrals are the 4-electron integrals present in beryllium), enabling extension to systems with more than four electrons.

Our hybrid Hy-CI method has been employed this past year to explore its utility for both three electron lithium systems and the four electron beryllium atom. In the case of lithium, we have computed four excited states of the lithium atom to two orders of magnitude greater than has been done before [8].

At the four electron level, it is still an open theoretical question whether unlinked terms like $r_{12}^{m}\ r_{34}^{n}$ with m and n odd are really necessary in either Hy or Hy-CI or is it sufficient to use Hy-CI or the formally equivalent Hy with only a single odd power of unlinked r_{ij} factors. In calculations submitted for publication [9], we have demonstrated the ability of Hy-CI calculations to achieve 0.1 μh accuracy for beryllium.

All results reported in the lithium and beryllium calculations were obtained using quadruple precision (30+ digits) floating point subroutines written in Fortran 90, and required removing the bottleneck to highly accurate Hy-CI calculations, the three electron triangle integrals [10], and treating the remaining three-electron kinetic energy and nuclear attraction integrals [11], as well as treating all four-electron integrals [12].

In going from He (two electrons) to Li (three electrons) to Be (four electrons), the situation vis a vis high precision calculations degrades to the point that already at four electrons (Be) there are no calculations of the ground or excited states with an error of less than a nanohartree. Our Be calculations, submitted for publication, are preliminary results and we are currently reworking our four electron integral codes with the goal of achieving nanohartree accuracy for Be. This (unfinished) beryllium calculation will determine whether really accurate calculations on atoms with more than four electrons will become a reality.

References

[1] T. Kato, On the eigenfunctions of many-particle systems in quantum mechanics, *Communications in Pure and Applied Mathematics* **10** (1957), pp. 151-177.

[2] R. T. Pack and W. B. Brown, Cusp conditions for molecular wavefunctions, *Journal of Chemical Physics* **45** (1966), pp. 556-559.

[3] W. Kutzelnigg and J. D. Morgan III, Rates of convergence of the partial-wave expansions of atomic correlation energies, *Journal of Chemical Physics* **96** (1992), pp. 4484-4508.

[4] J. S. Sims and S.A. Hagstrom, High precision Hy-CI variational calculations for the ground state of neutral helium and helium like ions, *International Journal of Quantum Chemistry* **90** (2002), pp. 1600-1609.

[5] E. A. Hylleraas, *Z. Phys.* **54** (1929), pp. 347-366.

[6] Z.-C. Yan, W. Nörtershäuser, and G. W. F. Drake, High Precision Atomic Theory for Li and Be+: QED Shifts and Isotope Shifts, *Physical Review Letters* **100** (2008), article 243002.

[7] M. Puchalski, D. Kedziera and K. Pachucki, Ground state of Li and Be+ using explicitly correlated functions, *Physical Review A* **80** (2009), article 020101.

[8] J. S. Sims and S. A. Hagstrom, Hy-CI Study of the 2 doublet S ground state of neutral Lithium and the first five excited doublet S states, *Physical Review A* **80** (2009), article 052507.

[9] J. S. Sims and S. A. Hagstrom, Hylleraas-configuration interaction study of the singlet S ground state of beryllium, *Physical Review*, to appear.

[10] 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: Atomic, Molecular, and Optical Physics* **37** (2004), pp. 1519-1540.

[11] J. S. Sims and S. A. Hagstrom, Math and computational science issues in high-precision Hy-CI calculations II. Kinetic Energy and electron-nucleus interaction integrals, *Journal of Physics B: Atomic, Molecular, and Optical Physics* **40** (2007), pp. 1575-1587.

[12] J. S. Sims and S. A. Hagstrom, Math and computational science issues in Hy-CI calculations III. 4-electron integrals, in preparation.

Participants

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http://www.nist.gov/itl/math/hpcvg/atomic.cfm

Nano-optics, and How to Squeeze Light Out of Quantum Dots

Research and development of nanotechnology, with applications ranging from smart materials to quantum computation to biolabs on a chip, has the highest national priority. Semiconductor nanoparticles, also known as nanocrystals and quantum dots, are one of the most intensely studied nanotechnology paradigms. Nanoparticles are typically 1 nm to 10 nm in size and contain a thousand to a million atoms. Precise control of particle size, shape and composition allows one to tailor charge distributions and control quantum effects to tailor properties completely different from either the bulk material or small clusters.

As a result of enhanced quantum confinement effects, nanoparticles act as artificial, man-made atoms with discrete electronic spectra that can be exploited as light sources for novel enhanced lasers, discrete components in nanoelectronics, qubits for quantum information processing, and enhanced ultrastable fluorescent labels for biosensors to detect, for example, cancers, malaria or other pathogens, and to do cell biology. We are working with the NIST Physical Measurement Laboratory to develop computationally efficient large scale simulations of such nanostructures. This past year these simulations were used to show that nanomechanical strain can be used to dynamically re-engineer the optics of quantum dots and, conversely, that quantum dots can be used as a local probe or control for nanomechanical strain.

We are also working to develop interactive immersive visualization techniques and tools to enable measurement and analysis of highly complex computational results of this type. Such techniques not only encapsulate the physics but also allow one to easily see features that might be missed by just perusing the voluminous amounts of data coming from supercomputer size computations.

James S. Sims

Quantum dots (QD) have attracted great interest for applications in photonics, sensors, quantum information, and precision measurement. Passive control of QDs is obtained by tailoring dot size, shape, and composition via growth. Dynamical control of exciton energies, polarization, and phase is highly desirable for QD nanophotonics. An imposed nanomechanical strain provides a route to dynamically reengineer QD structural symmetry to control excitations, polarize transitions, tune exchange splitting, induce entanglement, or modify coupling between QDs. These are capabilities needed to use QDs in nanophotonics, quantum information processing, and in optically active devices, such as optomechanical cavities and semiconductor nanotubes. Employing an imposed nanomechanical strain to dynamically reengineer QD devices leads to hybrid nanomechanical-QD devices. Such hybrid systems are becoming increasingly important areas of study, the goal being to connect multiple functionalities from the components into new capabilities of the hybrids.

We are engaged in a joint effort with the NIST Physical Measurement Laboratory to develop computationally efficient large scale simulations, along with visualization and analysis tools to enable the study of such hybrid nanomechanical-QD devices. Highly parallel computational platforms are critical for obtaining the computational speeds required for systematic study.

Our approach utilizes an atomistic tight-binding theory of quantum dots in nanomechanically strained structures, such as a nanomechanical cantilever or bridge. Excitons in mechanically strained dots (mechanoexcitons) are studied in detail in order to focus on the optical response of QDs. Conversely, we also show how the response of the quantum dots could be used as a local probe of the applied strain. Using an atomistic model is critical for an accurate description of nanomechanical-QD hybrids with atomic scale variations in composition and shape, and significant local and imposed strain. Our tight-binding theory for electron and hole states employs an sp^3s^* orbital model, nearest-neighbor coupling, spin-orbit effects, strain from lattice mismatch, and imposed mechanical strain. Relaxation of local and imposed strain is included via atomistic valence force field theory. Exciton states are determined with a configuration-interaction treatment.

To understand how applied stress can be used to actively control dot optical properties, dots buried at different points in a nanobridge oscillator or cantilever are considered. For the simulations, the bridge is 80 nm wide in the lateral directions and 25 nm thick, with 10 million atoms. A bend in a nanomechanical structure acts like a DC electric field, inducing Stark-like level shifts. The strain can mimic either a vertical or a lateral electric field, depending on how the strain is applied. The results are sensitive to bend geometry and dot location. Calculations for different bends, boundary conditions, and dot positions must be done to build a complete picture of nanomechanical strain effects.

As the computational model has been extended to handle more complex and larger systems by including not only the nanostructures but also the substrate and environment around them, parallel processing has become even more of a necessity. Both shared memory OpenMP parallelization and distributed memory MPI are employed. Calculations were carried out on NIST's 394-processor Linux cluster.

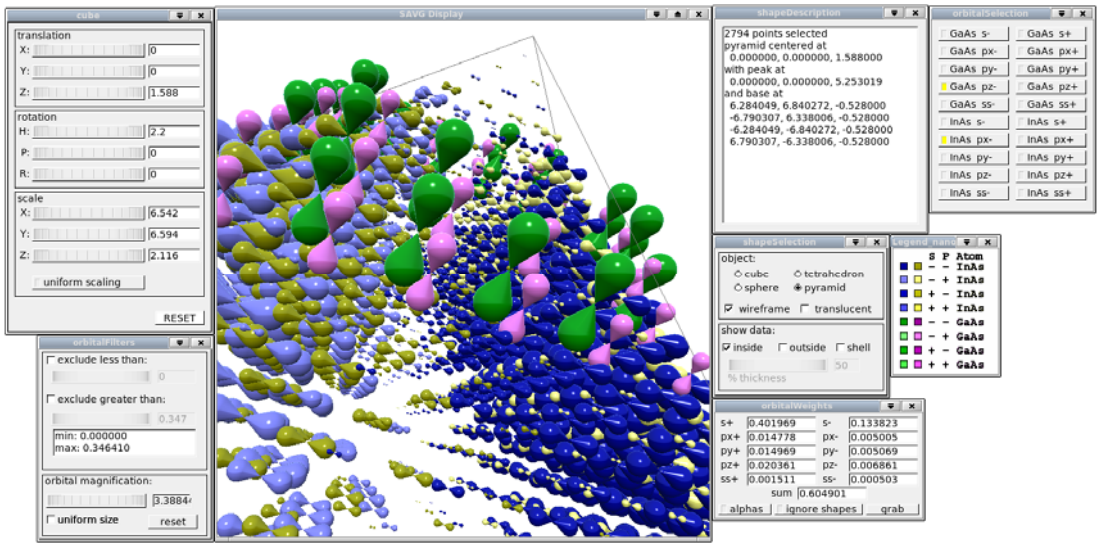

Figure 19. *Using NanoVis, the Nano-Structure Visualization, Measurement, and Analysis tool, to measure the properties of orbitals bounded by a user selected geometric object.*

In a paper published this year [1], we show that nanomechanical strain can be used to reengineer the optics of quantum dots and, conversely, that quantum dots can be used as a local probe or control for nanomechanical strain. Specifically, we show that:

- Electron and hole energies and distributions shift together, or in opposite directions, depending on how strain is applied, giving control to tune optical response. We explain why applied mechanical strain provides such control.
- Strain can be used to transfer carriers between dots. This control provides a tool to move qubits between adjacent dots for quantum information processing.
- Changes in band gap, fine-structure splitting, charge shifts and polarization correlate to applied strain, giving signatures to use QDs as a local strain gauge.
- Internal strain from lattice mismatch, nanomechanical strain, and internal readjustment to undo the applied strain must all be included.
- The applied strain can be used to manipulate the mechanoexciton fine structure and tune the phase of spin mixing and rotate polarization, providing control to modify the inner workings of excitons. Polarization rotation in a variety of contexts has been predicted or measured. These results provide the first clear explanation of how and why this occurs by bringing out the connection between the phase and spin mixing, the polarization, and the orientation of the exciton. Because applied strain can be used to tune the phase of the mixing, this gives a tool to control directly the phase of qubits.

  Usually, this polarization change is thought of as a single-particle dipole matrix element effect. As our results show, that is not the dominant effect. Phase control via the engineering of the phase of the asymmetric exchange coupling is the dominant effect. The results provide a new interpretation of these effects. This is perhaps the most important contribution of our work: that strain can not only be used to control exciton energies and splittings, but also exciton phase, which is a critical new feature.

This year we also released NanoVis, a visualization and analysis tool, which we are using to measure orbital data. See Figure 19. In the coming year, we will use this tool to study the spatial distribution of spin.

References

[1] G. W. Bryant, M. Zieliński, N. Malkova, J. Sims, W. Jaskólski, and J. Aizpurua, Effect of Mechanical Strain on the Optical Properties of Quantum Dots: Controlling Exciton Shape, Orientation, and Phase with a Mechanical Strain, *Physical Review Letters* **105** (2010), article 067404 (4 pages).

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http://www.nist.gov/itl/math/hpcvg/nanovis.cfm

Monte Carlo Methods for Computing Network Reliability

Graphs are embedded in structures that we use daily such as communications networks and the power grid. Ability to measure network properties is essential to maintaining the reliability, safety and, in some cases, the security of these systems. Many aspects of complex systems can be presented as questions about graphs. Examples include determining the reliability of a network and computing the number of linear extensions of a directed acyclic graph. Some of the most important aspects of these graphs are computationally intractable. Obtaining exact solutions is often NP hard. But sometimes the solutions to these hard problems can be approximated using Monte Carlo methods. Methods to compute network reliability as well as insights into how and when they can be used have been developed by the group here at NIST.

Isabel Beichl

A graph is a set of vertices and edges (or links) between the vertices. Graphs can be used to model computer networks and other infrastructure networks such as the power grid. A quick way to estimate the reliability of large-scale networks would have great impact. One measure of reliability is the probability that a graph is connected given the probability that each edge is connected [1].

If p is the probability that an edge is connected, then the *reliability of a graph* with n vertices and m edges, $R(p)$, is defined as

$$R(p) = p^m + C_1(1-p)p^{m-1} + \ldots + C_k(1-p)^k p^{m-k} + \ldots$$

where C_k is the number of connected spanning subgraphs with m-k edges. Determining the C_k and thus $R(p)$ is a counting problem. While there is earlier work on finding point estimates for reliability [3], previously suggested methods for the computation of reliability coefficients are impractical [4].

We have developed two methods for determining approximate values of the C_k. The first is based on sequential importance sampling (SIS). This method operates by removing edges from the graph until a spanning tree is reached [2]. The edges are chosen from the set of edges whose deletion does not disconnect the graph, called "good" edges. Before an edge is deleted at step k, we note the number of possible choices and use this to give an estimate, $g(k)$. This selection of edges produces a tree as in Figure 20, whose size, that is, number of nodes at level k, gives

$$C_k = mean\ (g(1)g(2)\cdots g(k)/k!)$$

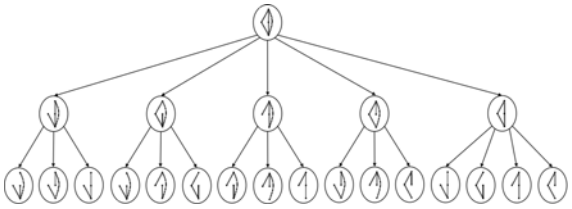

Figure 20. *Approximating the number of connected subgraphs of a given graph is equivalent to counting the leaves of a certain tree. Here the given graph is the root of the tree and selection and deletion of a ``good'' edge leads to selecting a branch of the tree. This figure illustrates all possible selections.*

This SIS method is very fast, but the variance can be bad. Importance sampling, a variance reducing technique, can sometimes help. Instead of sampling uniformly, we sample with a different probability, called the importance of the sample. We get an unbiased sample by dividing the estimate by its importance. But a good importance function is hard to find and, generally, more computation is needed per sample. For reliability, we have an excellent importance function, namely, the number of spanning trees removed by deleting an edge e. When normalized, this quantity can be used as the importance of e. This quantity is not too difficult to compute because it is a certain determinant

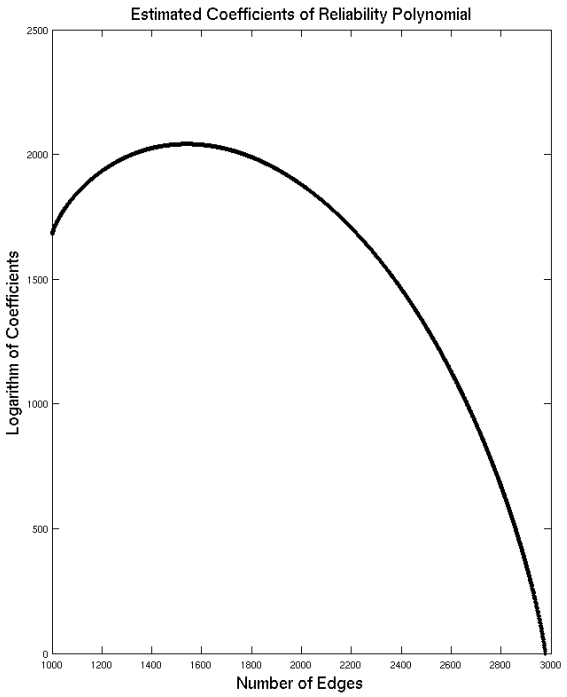

Figure 21. *The approximate coefficients of the reliability polynomial for a 1,000 node, 3,000 edge graph whose degrees were selected from a power-law distribution. Approximation was done with the SIS method.*

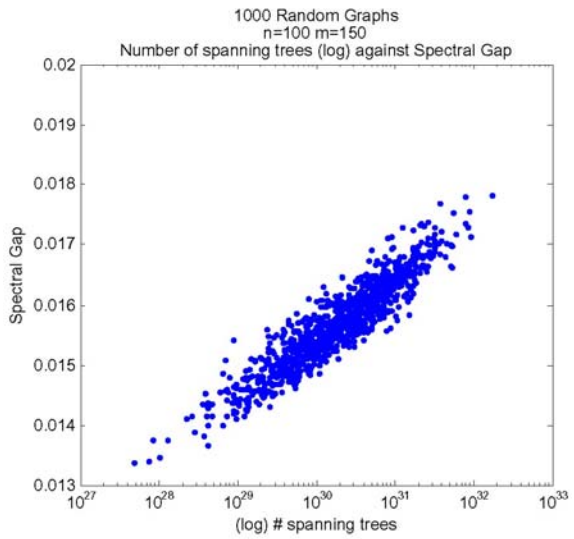

Figure 22. *The spectral gap versus the number of spanning trees for 1,000 random graphs. The spectral gap gives the mixing rate for a given MCMC algorithm. Computation of the spectral gap used our SIS method.*

which can be computed from previous steps by a low rank update. Figure 21 shows the reliability of a 1,000 node power-law graph with more than 3,000 edges computed with our SIS method.

Another way to compute the reliability coefficients is the Monte Carlo Markov Chain method (MCMC). MCMC is a class of algorithms for sampling from a limiting distribution by a series of "steps" from one configuration to the next. In this case, we step from one connected spanning subgraph to another by swaps, deletions, and additions between edges. After a large number of steps determined by the mixing time of the chain, the first sample is taken. The mixing time (or mixing rate) is the number of steps needed to give a sample that is independent of the previous sample. MCMC is slow even in the rapidly mixing case, but the theory of MCMC, and especially the theory of variance, is much better developed than that of SIS. No such parameter exists for predicting the variance of SIS. In MCMC, the first and second eigenvalues of the transition matrix will give the mixing rate, but writing down the transition matrix is impractical and equivalent to, or harder than, the original question. This turns the focus to computing bounds on the eigenvalue.

One method of computing bounds for the eigenvalue is to simplify the Markov chain into aggregated Markov chains where many states are collapsed into one. For reliability, we aggregate by the m-n+1 levels, that is, number of edges that we have removed. The transition matrix for the aggregated chain is much smaller than the transition matrix for the entire Markov chain and thus easier to work with. The aggregated process is also the process that gives the quantities of interest, in this case the coefficients C_k, the number of spanning connected subgraphs of size m-k.

In an effort to make the MCMC method usable, we have used our SIS method to estimate the mixing rate of the Markov chain for a particular graph in question. We do this by using SIS to approximate the aggregated transition matrix and then compute the eigenvalue directly. The spectral gap is the difference between the first and second eigenvalues. The mixing rate is determined by the spectral gap.

We also use the SIS method to estimate optimal fugacities for the MCMC method. Use of fugacity is a MCMC technique that allows us to sample in areas that would not be sampled ordinarily, but does so in a way that does not create bias. The value of the fugacity determines the rate at which proposed Monte Carlo moves are accepted. It is called "fugacity" by analogy with the term used in chemistry related to the rate of reaction. The optimal fugacity is not known, so in practice many fugacities are selected, usually more than are needed. We have used the SIS method to generate optimal fugacities for the reliability MCMC.

References

[1] C. J. Colbourn, The Combinatorics of Network Reliability, Oxford University Press, New York, 1987.

[2] I. Beichl, B. D. Cloteaux, F. Sullivan, An approximation algorithm for the coefficients of the reliability polynomial, *Conrgessus Numerantium* **197** (2009) pp. 143-151.

[3] R. Karger, A randomized fully polynomial time approximation scheme for the all-terminal reliability problem. *SIAM Journal on Computing* **29** (1999), pp. 492-514.

[4] C. J. Colbourn, B. M. Debroni and W. J. Myrvold Estimating the coefficients of the reliability polynomial, *Congressus Numerantium* **62** (1988) pp. 217-223.

Participants

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Up-conversion Single Photon Detectors and their Application in Measurement Science

The development of quantum computer networks requires the efficient and reliable transmission of quantum information over long distances. Photons traveling over optical fiber are a typical transmission media. Photons experience the least lost (and hence longest distance) at typical telecom wavelengths of 1310 or 1550 nm. Unfortunately, cost-effective photon detectors, such as silicon avalanche photon detectors (Si-APDs), are very inefficient at these wavelengths. To alleviate this mismatch, we have developed wavelength conversion technology to upconvert 1310 nm photons to visible or near-visible wavelengths for efficient detection. We have since made performance improvements and developed significant new applications. For example, we developed an upconversion spectrometer that can measure spectra of single photons in the near infrared, the sensitivity of which is three orders of magnitude higher than that of existing commercial optical spectra analyzers. Using these detectors we demonstrated, for the first time, that the converted single photons preserve their original quantum properties. This technology is being transferred to US industry through the NIST SBIR Program.

Xiao Tang

Light in the telecom wavelengths in the near infrared (NIR) range, most commonly in the 1310 nm and 1550 nm bands, can be transmitted in optical fiber for long distances since the optical attenuation and/or dispersion in fiber are lowest at the wavelengths. When light intensity is reduced to the single photon level, detection of photons at the telecom wavelengths becomes very challenging. InGaAs-based detectors are effective at these wavelengths, but their performance needs improvement. Superconducting-based detectors work well but they need to be cooled to liquid helium temperature. On the other hand, commercially available silicon-based single photon detectors (Si-APDs) perform extremely well for visible and near visible photons, but do not work at the telecom wavelengths. For some time researchers have sought methods for converting telecom photons to visible or near visible wavelengths with high conversion efficiency for detection by Si-APDs with low dark count rates.

In 2007 we developed upconversion detectors for our quantum key distribution (QKD) system operating at 1310 nm for longer distance secure communication. The upconversion detectors reached a high overall conversion efficiency of 32%, and dark count rates as low as 2,000 c/s, 25 times lower than that reported by other groups. Due to the excellent performance of these detectors, our 10-km fiber-based 1310 nm QKD system generated sifted keys at a rate of 1 Mb/s, enough to demonstrate one-time pad encryption and decryption of streaming video signals in real time [1].

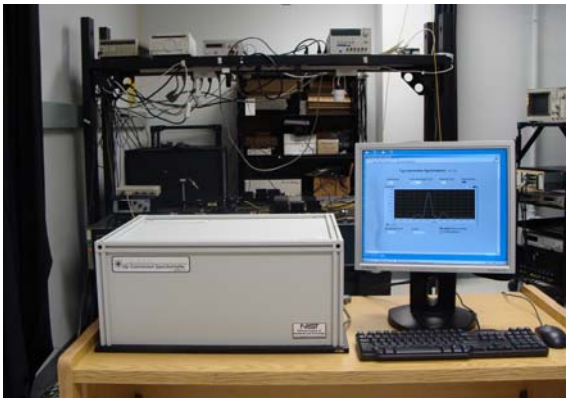

Figure 23. *The ITL upconversion single photon detector.*

The wavelength conversion is based on sum frequency generation in a nonlinear optical crystal, such as a periodically poled lithium niobate (PPLN) waveguide. A signal photon at the telecom wavelength can be converted to a visible wavelength by a strong pump beam under the so called quasi-phase matching (QPM) condition, which requires energy and momentum conservation for the pump, signal and idler photons. These conditions make the device a tool with unique properties of interest in many applications.

One important extension has been to develop the upconversion detector into an upconversion spectrometer. Due to the requirement of energy conservation, if we tune the pump photon wavelength, the signal photon wavelength must be tuned accordingly, generating an output photon at a fixed wavelength. Here, the tuning of the pump photon wavelength is equivalent to the tuning of a grating or a prism in a traditional spectrometer for input wavelength selection. Based on this principle, an upconversion single photon detector can be modified into an upconversion spectrometer with high detection sensitivity and low noise. In August 2009, we demonstrated such a spectrometer for signals at single photon levels in the near infrared region [2]. The overall single photon detection efficiency of the up-conversion spectrometer is about 32%. The spectrometer also demonstrates ultra high sensitivity, measuring spectra for signals at a power level as low as -126 dBm, three orders of magnitude better than that of commercial optical spectra analyzers. This development opens up new research opportunities in

measurement science, providing a powerful tool for practical applications in many areas.

The upconversion spectrometer is sensitive to the polarization of input signal photons due to the QMP requirement in the conversion process. This could be a useful feature if one wants to measure spectra of signal photons at a certain polarization orientation. But it could also be a drawback if the polarization of the input photons is in arbitrary directions. To overcome this problem, we further developed a polarization independent upconversion spectrometer [3]. This improvement retains all advantages in the original, but desensitizes polarization for input signal photons.

More recently we further improved the performance of our upconversion detectors, reducing the dark count rate and increasing the data transmission rate. In particular, by using a holographic grating to filter out residual noise around the signal, the dark count rate of the upconversion detector was further reduced by another order of magnitude, from 2,000 c/s to 100 c/s [4]. In a conventional quantum communication system the data transmission rate is limited by the jitter of the Si-APDs. We proposed and experimentally demonstrated a multi-wavelength pumping technique that increased the system data rate beyond the jitter limitation [5].

The difficulty of detecting single photons in NIR/IR had been a barrier to much scientific research. Our wavelength conversion technique overcomes this, enabling new research in quantum measurement and quantum information. Recently we conducted a joint experiment in collaboration with colleagues in the NIST Center for Nanoscale Science and Technology. Our upconversion detectors were used to detect single photons from a semiconductor quantum dot. Exciton lifetimes were measured using both a commercial InGaAs IR single photon detector and our upconversion detector. The dynamic range of the data measured by the upconversion detector was 25 times better than that of the InGaAs-based detector. Because of this the exciton lifetime can be determined with a much higher accuracy. It has been well known that photons emitted from a quantum dot possess their special quantum characteristic, known as antibunching. Because of the high sensitivity and low dark count rate, our upconversion detector was able to measure the second order intensity correlation function for the photons from the quantum dot. This measurement demonstrated for the first time that the converted photons preserve the quantum antibunching characteristic. This important conclusion was reported in *Nature Photonics* [6].

Through the NIST Small Business Innovative Research (SBIR) Program, the technology of our upconversion detectors is being adapted for commercialization by two US companies, AdvR Inc. and Lepton Technologies Inc. Phase 1 of this work has been completed and Phase 2 is at an advanced stage.

We plan further study to enable full utilization of the unique features of wavelength conversion devices. The first task is to expand the detection wavelength from 1.3 μm to 1.5 and 0.98 μm. Upconversion devices at 1.5 μm is being developed in collaboration with researchers at Stanford University. A device at 0.98 μm will be produced by AdvR Inc. The second and most important task will be to develop quantum interfaces based on wavelength conversion devices. In order to connect two independent quantum systems to form a quantum network, photons from two independent systems must be made to interfere with each other. However, this requires that the two photons have exactly same wavelength and polarization, and arrive at an exactly same time. A quantum interface can be used to adjust the wavelength of the two photons, and a quantum memory can be used to adjust their arrival time so that better interference can take place. These are necessary steps towards our final goal, the development of a quantum repeater.

References

[1] H. Xu, L. Ma, A. Mink, B. Hershman, and X. Tang, 1310-nm quantum key distribution system with up-conversion pump wavelength at 1550 nm, *Optics Express* **15** (2007), article 7247.

[2] L. Ma, O. Slattery, and X. Tang, Experimental study of high sensitivity infrared spectrometer with waveguide-based up-conversion detector, *Optics Express* **17** (2009), article 14395.

[3] L. Ma, O. Slattery and X. Tang, Single Photon Level Spectrum Measurement at Fiber Communication Band Using Frequency Up-conversion Technology, *Laser Physics* **20** (7) (May 27, 2010), pp. 1612-1617.

[4] X. Tang, L. Ma and O. Slattery, Ultra Low Dark-count-rate Up conversion Single Photon Detector, 2010 IEEE Photonics Society Annual Meeting, Denver, CO, November 7-11, 2010, IEEE catalog: CFP10LEO-CDR.

[5] L. Ma, J. C. Bienfang, O. Slattery and X. Tang, Up-conversion single-photon detector using multi-wavelength sampling techniques, submitted.

[6] M. T. Rakher, L. Ma, O. Slattery, X. Tang and K. Srinivasan, Quantum transduction of telecommunications-band single photons from a quantum dot by frequency upconversion, *Nature Photonics* **4** (2010), pp. 786-791.

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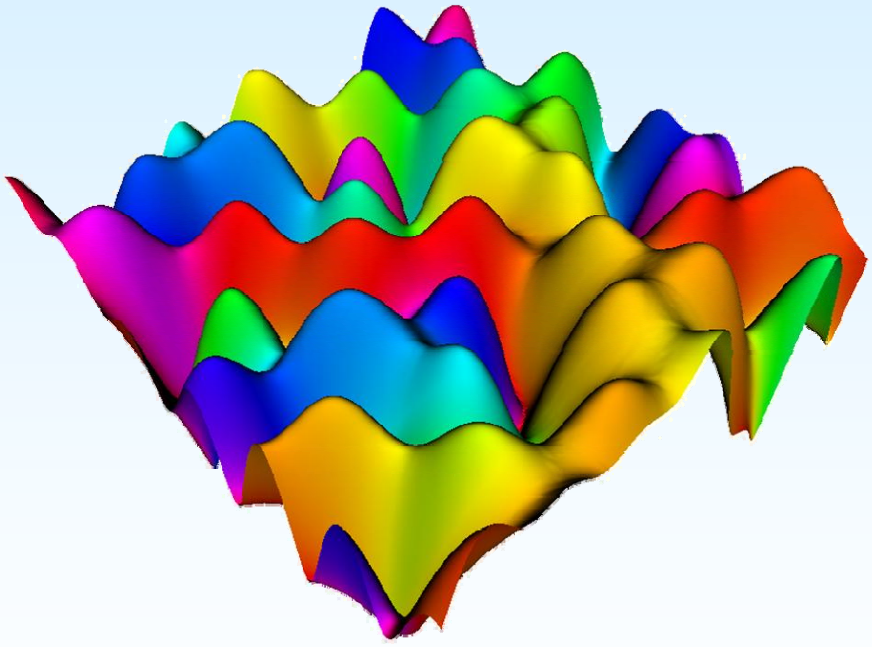
Part III

Project Summaries



Mathematics of Metrology

Mathematics plays an important role in the science of metrology. Mathematical models are needed to understand how to design effective measurement systems, and to analyze the results they produce. Mathematical techniques are used to develop and analyze idealized models of physical phenomena to be measured, and mathematical algorithms are necessary to find optimal system parameters. Finally, mathematical and statistical techniques are needed to transform the resulting data into useful information. Our goal is to develop fundamental mathematical methods and analytical tools necessary for NIST to continue as a world-class metrology institute, and to apply them critical measurement science applications.

Linnik Densities, Logarithmic Diffusion Equations, and Blind Deconvolution of Hubble Space Telescope Imagery

Alfred Carasso

See feature article, page 29.

ITL Program: *Enabling Scientific Discovery*

Modeling Reactive Wetting

Geoffrey B. McFadden
William J. Boettinger
James A. Warren (NIST MML)
W. Villanueva (Royal Inst. of Technology, Sweden)

See feature article, page 31.

ITL Program: *Enabling Scientific Discovery*

Denoising of Helium Ion Microscope Nanoscale Imagery

Alfred Carasso
András Vládar (NIST PML)

ACMD mathematical technology involving fractional diffusion equations, used successfully in NIST image deblurring work, has now found an unexpected, but highly significant, new application: denoising state-of-the-art nanoscale imagery. Surprisingly, this method can outperform computationally more sophisticated denoising techniques based on *curvelet transform* thresholding, or on minimizing image *total variation*.

Helium ion microscopes (HIM) are an exciting new tool in nanoscale imaging, producing images that are particularly rich in morphological surface detail. Such imagery is very much needed in current research and development, as well as production. The important nano-structures are usually very small, and only the sharpest focused beams can resolve them. Such beams involve a few hundred to a few thousand atoms, and do not generate a lot of signal. This necessarily produces very noisy images. Any technique that can reduce this noise is very much needed, and would result in otherwise unavailable acquisition speed and/or information. However, preserving the fidelity of the essential sample-related fine details is of paramount interest.

A denoising technique that has been applied successfully in medical computed tomography is based on appropriately thresholding the image curvelet transform. A MATLAB implementation of that approach has been developed by its authors. Another well-known method is based on minimizing the image total variation (TV) norm $\int |\nabla f(x,y)|\, dxdy$. The split Bregman iterative procedure is an efficient method for solving the TV minimization problem, and a MATLAB implementation of the TV Bregman procedure has likewise been developed.

The *fractional diffusion method* uses the given noisy image $f(x,y)$ as initial data in the well-posed problem $w_t = -(-\Delta)^{\beta} w$, $t > 0$, with fixed β, $0 < \beta \ll 1$. The denoised image is the solution at some positive time, determined interactively by the user. Fast Fourier Transform algorithms are used to generate the forward evolution. When $\beta \approx 0.2$, smoothing is very gentle as t increases, and small-scale features in the initial data $f(x,y)$ tend to persist for small positive t, while the noise is considerably reduced. This is not the case with Gaussian or heat equation smoothing ($\beta = 1$), which leads to aggressive smoothing out of edges and small-scale information, in addition to eliminating noise.

Both the curvelet and TV methods are especially useful when the ideal sharp image is piecewise smooth, and consists of isolated smooth objects with well-defined edges. Such images belong to the class $BV(R^2)$ of functions of *bounded variation*. However, HIM images are not in $BV(R^2)$. Rather, they are examples of images where texture and detailed surface morphology are of prime interest, and for which TV or curvelet denoising may not be appropriate. This expectation is

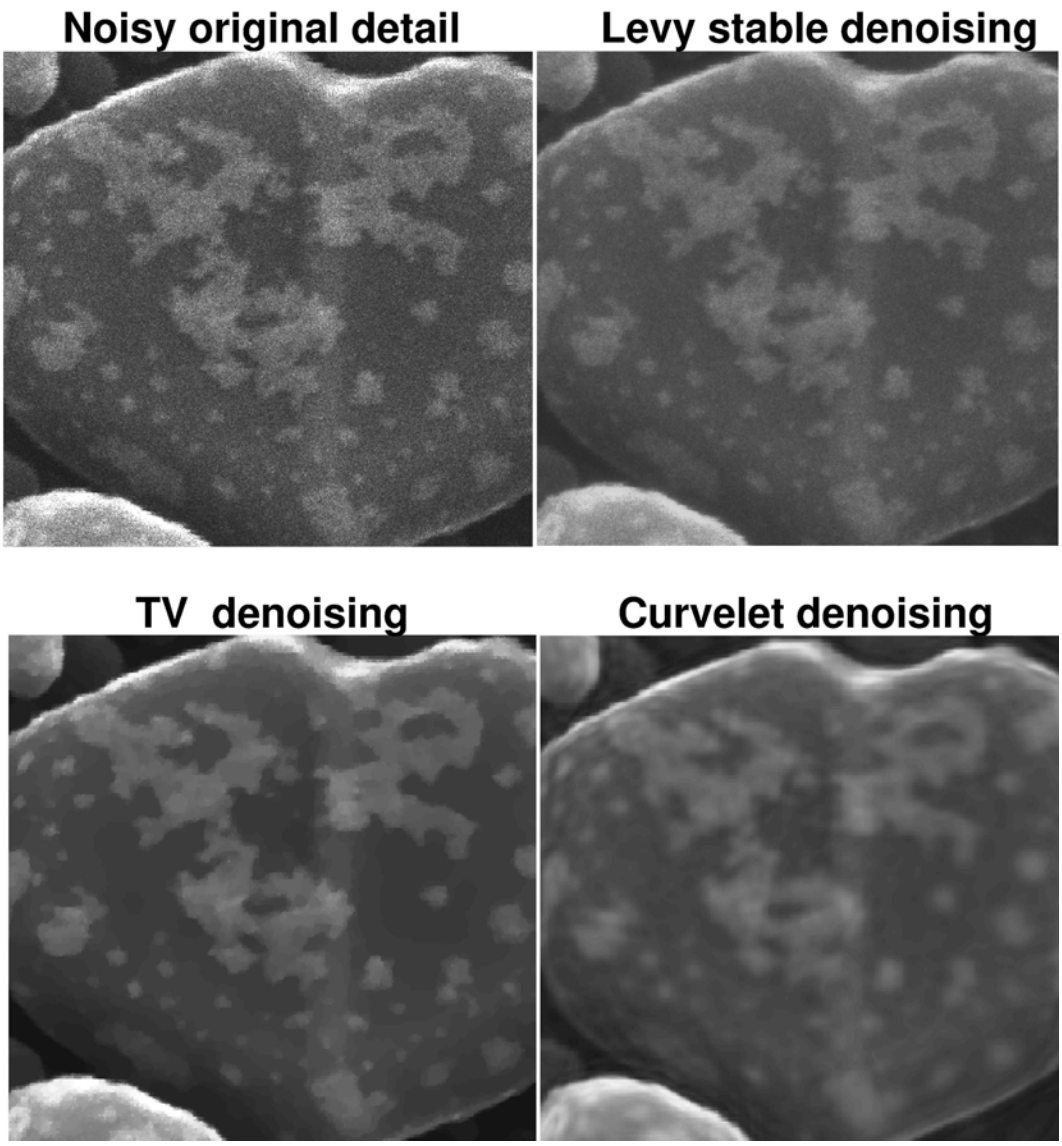


Figure 24. *Poor recovery of surface morphology in TV and Curvelet denoising, as compared with Lévy stable processing, in Au-decorated gold on carbon sample. Field of view is 300 nm. Relative performance in the three denoising methods is quantified in Table below.*

Table. *Behavior of* $\| f \|_1$, $\| f \|_2$, $\| \nabla f \|_1$ *and Lipschitz* α *in above denoising experiment. Note severe* $\| \nabla f \|_1$ *reduction in curvelet and TV denoising.*

Image $f(x,y)$	$\| f \|_1$	$\| f \|_2$	$\| \nabla f \|_1$	Lip α
Noisy original (600 nm)	88	99	25000	0.236
Lévy stable ($\beta = 0.2$, $t^{\dagger} = 0.1$)	88	94	8500	0.462
Split Bregman TV ($\omega = 0.025$)	74	89	3400	0.778
Curvelet thresholding ($\sigma_n = 30$)	81	91	2700	0.845

borne out in practice. When TV or curvelet denoising is applied to the two noisy HIM images below, fidelity to the original surface morphology cannot be maintained. The image L^1 norm is not conserved, while $\| \nabla f \|_1$ is reduced by factors of five to nine, and the image Lipschitz exponent is sometimes tripled. In contrast, with fractional diffusion or Lévy stable smoothing, a considerable portion of the noise is removed, while conserving most of the original surface texture, including jagged edges. In addition, the image L^1 norm is maintained, $\| \nabla f \|_1$ is moderately reduced, while the image Lipschitz exponent is not even doubled.

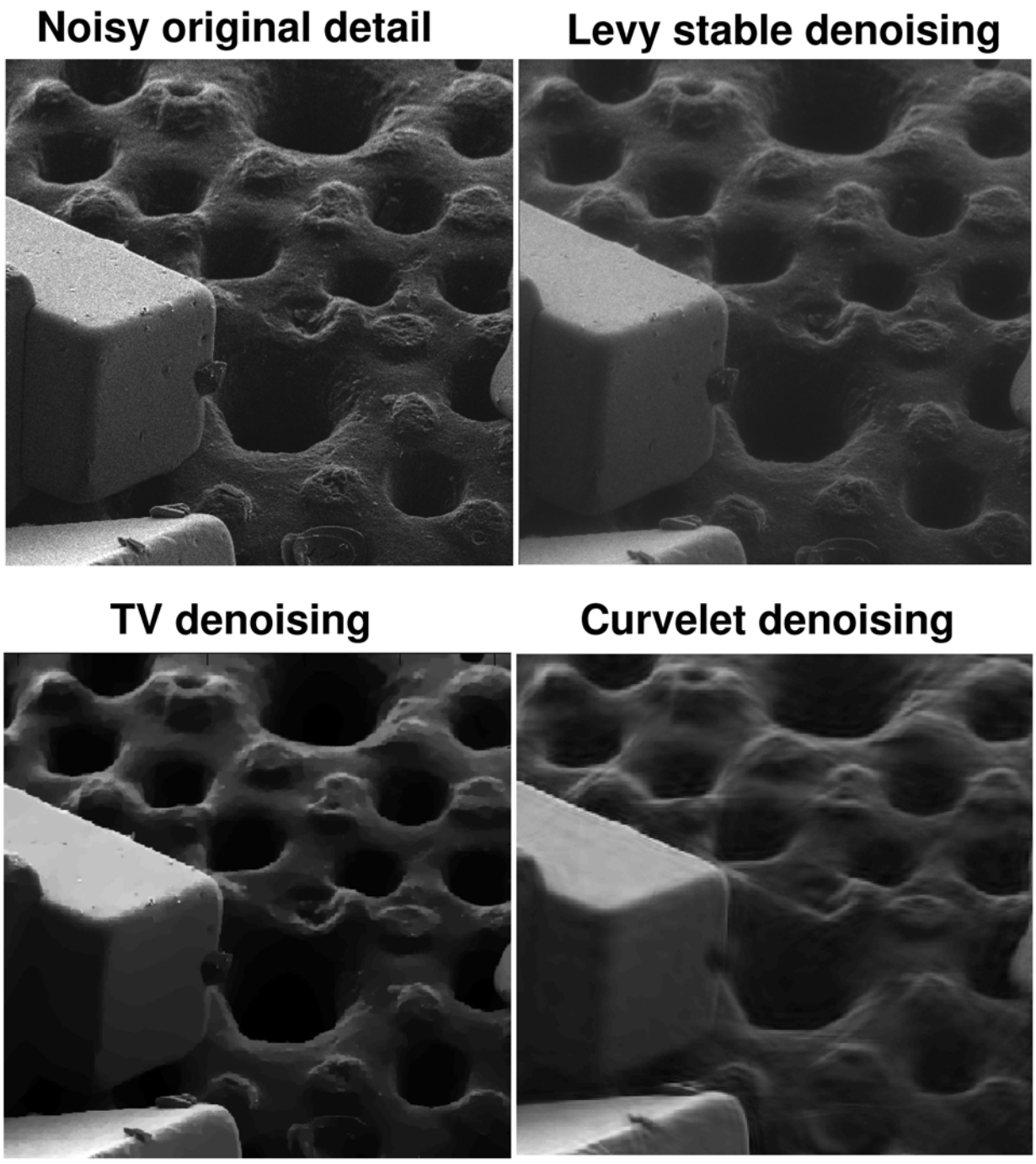


Figure 25. *Examination of parts of the salt crystals in above radiolaria sample under magnification, reveals significant erosion of surface morphology in TV and curvelet images, as compared with Lévy stable image. Field of view is 45 μm. Relative performance in the three denoising methods is quantified in the Table below.*

Table. *Behavior of* $\| f \|_1$, $\| f \|_2$, $\| \nabla f \|_1$ *and Lipschitz* α *in above denoising experiment. Note severe* $\| \nabla f \|_1$ *reduction in curvelet and TV denoising.*

Image $f(x,y)$	$\| f \|_1$	$\| f \|_2$	$\| \nabla f \|_1$	Lip α
Noisy original (90 μm)	54	65	14000	0.288
Lévy stable ($\beta = 0.2$, $t^{\dagger} = 0.1$)	54	61	4900	0.492
Split Bregman TV ($\omega = 0.025$)	37	57	3000	0.666
Curvelet thresholding ($\sigma_n = 30$)	46	56	2600	0.674

Sparse Representations in High Dimensional Geometry

Bradley Alpert
Yu Chen (New York University)

Laboratory and clinical diagnostic systems often produce images that lack quantitative information or comparability across imaging systems, which can lead to difficulties in diagnosis and long-term management of disease that requires patient monitoring. Elaborate measurements are taken, digitally processed, then reported in essentially qualitative form. For MRI, functional MRI, and other processes, formation of the images relies on filtering and Fourier transformation.

Although the computational recovery of functions from their Fourier representations is considered routine, aside from possible efficiency concerns arising from non-grid data, standard approaches assume that the functions are smooth and can be recovered with the discrete Fourier transform (computed via the FFT). When this assumption fails, as is evident from Fourier data that are not small at the highest frequencies measured, some sort of attenuation, or belling, scheme is typically used. This procedure tends to blur sharp features and, being more art than science, can lead to different functions (images) in different systems. Although this problem, and the Gibbs phenomenon, has received considerable attention, recently developed methods tend to work well only in an asymptotic sense; they do not exploit available data efficiently.

Despite inherent limits on resolution that can be obtained from truncated Fourier data, a change of assumptions from *smooth* to *piecewise smooth* can lead to significantly improvement. Procedures implementing this idea are not completely established even for functions (signals) in one dimension; they are yet more challenging in two and three dimensions, where discontinuities may be expected to occur along mostly smooth curves or surfaces. This constraint, which magnifies the advantage of the piecewise smoothness assumption, must be appropriately reflected in the methods used. Alpert and Yu Chen are conducting numerical experiments to understand this environment and to develop reliable procedures for these problems.

In recent months, understanding is developing of how to generate, test, and refine hypotheses regarding locations of discontinuities. This approach uses a spatial (i.e., physical domain) divide-and-conquer strategy enabled by use of prolate spheroidal wave functions in a statistical estimation procedure. These tools are used to cope with the non-convexity of the problem. As estimates are increasingly aggregated spatially, less-supported hypotheses are eliminated and more-supported ones are refined. Once the discontinuity locations are known, recovery of the discontinuous function is a generally well-conditioned procedure consisting of solving a linear system of equations.

A related, yet more general, challenge is parsimonious, or sparse, representation and recovery of functions under assumptions appropriate to an application. Although there is considerable current interest in the mathematical community in these problems (L^1-norm minimization, compressive sensing, sparse representation in high-dimensional geometry), and much recent progress (initiated in pivotal work by Candes, Romberg, and Tao) most of the methods being explored are limited to linear spaces. While linearity is a natural starting point, strong evidence suggests that image recovery cannot be done this way yet nevertheless is within reach. It is the goal of this project to develop procedures for robust recovery of piecewise smooth, or otherwise constrained, functions from Fourier data.

ITL Program: *Enabling Scientific Discovery*

A Standard Candle for Extragalactic Metrology

Bert W. Rust
Dianne P. O'Leary
Katharine M. Mullen (NIST MML)

Type Ia supernovae are often more luminous at maximum brightness than are their parent galaxies, and their light curves are so regular and uniform that they make good "standard candles" for estimating extragalactic distances. An empirically established correlation between peak absolute magnitudes and the rates of decline of the light curves provides a means of estimating the peak absolute magnitude of a distant supernova from its observed decline rate. The estimate thus obtained can then be combined with a measurement of its peak apparent magnitude to give an estimate of its distance. We have developed mathematical model for the luminosity which, using seven adjustable parameters, gives superior fits to measured light curves and should prove useful in calibrating the correlation described above. Such fits are given in Figure 26 and Figure 27 where the model explains 99.91% of the variance in the record.

It is widely believed that, beginning a few days after maximum luminosity, the light curve is powered by the radioactive decay chain Ni → Co → Fe, even though observed luminosity decline rates do not match the terrestrial decay rates of Ni and Co. In 1976 Rust, Leventhal and McCall [*Nature* **262**, pp. 118-120] presented evidence that those decay rates are accelerated because the decays occur in the extremely high density interior of a carbon-oxygen white dwarf.

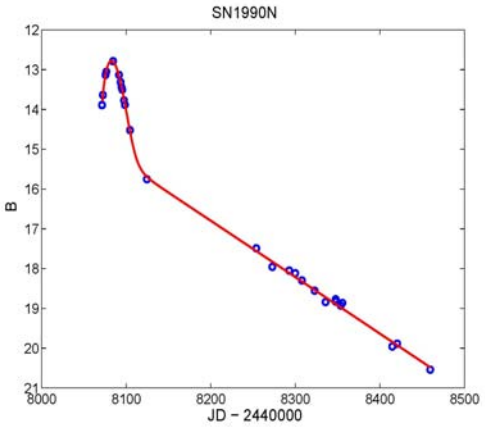


Figure 26. *The B-magnitude light curve for the supernova SN1990N. The time variable is measured in Julian Day units. The discrete data points are the observed B-magnitudes and the smooth curve is the model fit.*

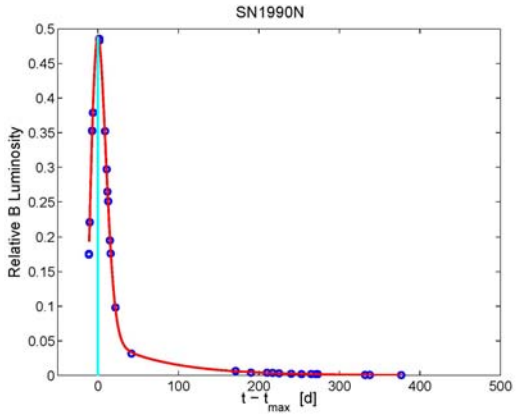


Figure 27. *The light curve of SN1990N in relative luminosity units. The time scale has been shifted to have t = 0 at maximum luminosity.*

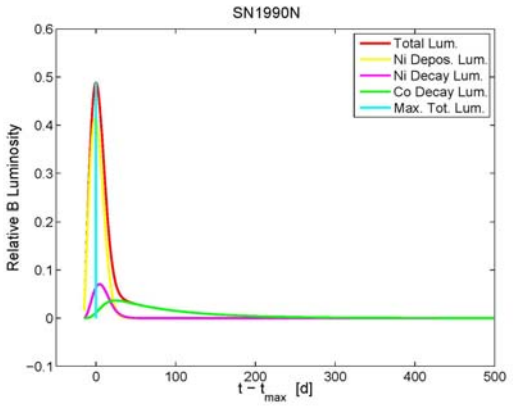


Figure 28. *The three components of luminosity for SN1990N. The time scale here is the same as in Figure 27.*

Our current model [1] is a sum of three terms corresponding to luminosity generated by (1) the fusion reactions that deposit the Ni, (2) the radioactive decay of the Ni to Co, and (3) the radioactive decay of the Co to Fe. We use a three-parameter Weibull probability distribution function to model the pulse of Ni deposition and three coupled linear ordinary differential equations to model the radioactive decays. The three luminosity components for SN1990N are plotted in Figure 28. The strong similarity of the pulse locations and shapes for the Ni deposition and the Ni decay pulses make the seven-parameter fitting problem impossibly ill conditioned, but assuming that the total energies emitted by the two decays (the areas under the two decay pulse curves) have the same ratio as the known energies emitted by the decay of a single atom of each isotope makes it possible to reduce the number of free parameters to six, thus making the estimation problem tractable.

Fits of our model imply an acceleration of radioactive decay rates as compared to the terrestrial values, in accordance with the results of Rust, Leventhal and McCall. This acceleration and the prolonged presence of the fusion pulse indicate that the star remains intact after the initial explosion for durations of a month or more, challenging previous light curve interpretations.

[1] B. W. Rust, D. P. O'Leary, and K. M. Mullen, "Modelling Type Ia Supernova Light Curves," in *Exponential Data Fitting and its Applications*, (Victor Pereyra and Godela Scherer, eds.), Bentham Electronic Books, 2010, pp. 145-164.

Modeling Equilibrium, Stability and Transport during Magnetic Fusion

Geoffrey B. McFadden
Paul R. Garabedian (New York University)

A hot plasma of hydrogen isotopes can be confined in a strong magnetic field with toroidal geometry so the ions fuse to form helium and release energetic neutrons. Models of such magnetic fusion devices developed in computational science have been implemented previously by P. Garabedian and his students and colleagues at New York University as codes that comprise an effective numerical simulation of the most essential features of modern tokamak and stellarator experiments. This has led to the discovery of advanced concepts that make fusion reactors a future prospect for a commercial source of energy. In recent work [1] we have applied computer codes to issues of equilibrium, stability and transport that provide an example of the theory. The codes have been used to evaluate possible stellarator designs as candidates for follow-up ("DEMO") experiments that may eventually be performed after the completion of the planned international experiments ("ITER") that are based on tokamak configurations. Tokamaks have axisymmetric

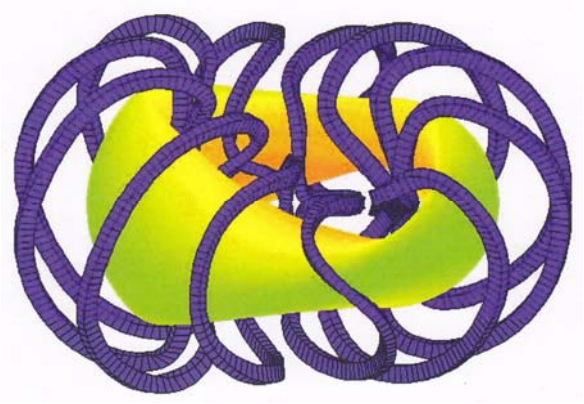


Figure 29. *Magnetic fusion of hydrogen forms helium and emits energetic neutrons from a torus of plasma shaped to optimize confinement. Modular coils generate a field keeping the ions from hitting walls.*

symmetry, which is an advantage for purposes of particle confinement, but they rely on strong toroidal currents in the plasma to generate the magnetic fields that can lead to stability issues. The magnetic fields for stellarators are generated by external coils which can alleviate many of the stability problems of tokamaks, but generally lack the high symmetry of tokamaks associated with enhanced confinement. The stellarator designs reported recently [1] offer the advantages of a type of quasi-axisymmetry (see Figure 29) that combines the best features of each, with the possibility of both good stability and transport properties.

Professor Garabedian passed away in May, 2010. G. McFadden contributed an obituary to *SIAM News* [2], and served as co-organizer of a memorial conference held in his honor at the NYU Courant Institute in December 2010.

[1] P. R. Garabedian and G. B. McFadden, The DEMO quasiaxisymmetric stellarator, *Energies* **3** (2010) pp. 277-284.

[2] *SIAM News* **43**, No. 7 (September 2010), pp. 2-3.

A Structural Optimization Approach to Multihazard Design

Florian Potra
Emil Simiu (NIST EL)

Multihazard design is a branch of structural engineering aimed at developing design practices that achieve superior performance by accounting holistically for all the hazards to which a structure is exposed. For some types of hazard no more than one hazard may be expected to occur at any one time. This is true, for example, of strong winds and earthquakes. In current practice structures that may be subjected to wind loads and seismic loads are typically not designed by using a multihazard approach. Rather, they are designed separately for each of the two loads; for each structural member the controlling design then corresponds to the more demanding of the two loads.

It is desirable to achieve design synergies, that is, when performing the design for one of the two hazards it is desirable to take advantage of features inherent in the design for the other hazard, and conversely. This can in principle be accomplished in some cases through ad-hoc, practical engineering judgment. However ingenious and useful ad-hoc design solutions may be, there is a need for fundamental, science-based approaches to multihazard design.

The purpose of this study is to propose such approaches which bring to bear on the multihazard structural design problem the powerful mathematical apparatus of modern optimization theory. Instead of designing a structure so that it performs satisfactorily, or optimally, given that it is subjected to seismic loads, and then repeating the design process independently for wind loads, we propose that the structure be designed so that it performs optimally given that it is subjected to either seismic or wind loads [1].

We have developed such an optimization-based approach to multihazard design. Here the design variables are member sizes, the constraints pertain to structural strength and serviceability (e.g., keeping the load-induced stresses and deflections below specified thresholds), and the objective function is the structure cost or weight. In a multihazard context, the design variables are subjected to the constraints imposed by all the hazards to which the structure is exposed.

In [2] we describe this methodology and illustrate it by identifying the optimal design for supporting steel columns with hollow elliptical cross sections with constant thickness subject to wind and seismic forces. The numerical experiments show that interior point methods are significantly more efficient in solving the resulting nonlinear programming problem than classical numerical optimization methods. Although the structure considered in the numerical experiments is relatively simple, we argue that our methodology has the potential for being used, more generally, under a wide variety of hazards, types of structure, and structural engineering constraints.

[1] F. Potra and E. Simiu, Optimization and Multihazard Structural Design, *Journal of Engineering Mechanics* **135** (2009), pp. 1472-1475.

[2] F. Potra and E. Simiu, Multi-hazard Design: A Structural Approach, *Journal of Optimization Theory and Applications* **144** (2010), pp. 120-136.

Analysis of Diffusion and Stress in Binary Alloys

Geoffrey B McFadden
William J. Boettinger (NIST MML)

The *Kirkendall effect* refers to the motion of lattice planes in a crystalline binary alloy that is caused by a difference in the rates of diffusion of the two species. The difference in diffusion rates leads to a stress-free stain in the sample, and the process is an example of the coupling between diffusion and elasticity during phase transformations. Current interest in stress generation in thin films due to diffusion processes has stimulated new interest in this classical problem. The effect can lead to measurable shape changes perpendicular to the direction of diffusion. It is often detected by a shift of inert markers parallel to the diffusion direction; that is, deformation with pure axial displacement.

In recent work [1] we analyzed the time-dependent bending of a bimetallic strip due to interdiffusion in a binary alloy. In this case the deformation is due to diffusion across the short dimension of the strip, making deformation and diffusion co-linear. The results, which use a Fourier method, couple beam theory and diffusion, and are in agreement with experiments.

Current work includes the development of models for grain boundary motion coupled to the Kirkendall effect, including the effect of stress on vacancy concentration at the interface. Idealized one-dimensional models with a sharp interface are being studied, and compared with alternate phase-field (diffuse interface) models that allow computation of more complicated geometries such as whisker growth. Here, long, thin single crystals are extruded from individual grains that are under high stress in thin films. These whiskers can bridge the gaps that separate individual components in electronic devices, causing electrical failure in some cases. Understanding the mechanisms behind whicker growth is important for the prediction of the lifetimes and performance of small-scale electronic components.

[1] W. J. Boettinger and G. B. McFadden, Bending of a bimetallic beam due to the Kirkendall effect, *Journal of Phase Equilibria and Diffusion* **31** (2010) 6-14.

ITL Program: *Enabling Scientific Discovery*

Modeling Fluid Flow in Materials Processing

Geoffrey B. McFadden
P. Aaron Lott
Sam R. Coriell (NIST MML)
Daniel Anderson (George Mason University)
Bruce Murray (SUNY Binghamton)

The study of the stability of a fluid-fluid interface is important in a number of scientific and technological applications. In this project we consider two fluid layers separated by a horizontal planar interface subject to a vertical temperature gradient. The effects of various driving forces on the stability of the system can be taken into account, including buoyancy (known as Rayleigh-Benard convection), the effects of bulk density differences (known as Rayleigh-Taylor instabilities), and the effects of surface tension gradients along the interface (known as Marangoni instabilities). If the two layers represent different phases of the same material the stability results for a two-phase bi-layer system are quantitatively and even qualitatively different than for those of an immiscible system. To estimate the relative importance of these types of instabilities for a two-phase system, we have considered a bi-layer geometry in which a horizontal fluid-fluid interface separates two semi-infinite layers of a binary (two-component) fluid [1,2]. We have performed linear stability calculations for horizontal fluid bi-layers that can undergo a phase transformation, taking into account both buoyancy effects and thermocapillary effects. We find that the phase transformation gives rise to an instability that is independent of buoyancy and thermocapillary effects, and can occur for either heating from above or from below. The instability can give rise to traveling waves, and can occur in the limit of large wavelength perturbations. These large-wavelength instabilities can be studied analytically by employing a lubrication approximation to obtain a simplified set of governing equations. We have been able obtain both numerical and analytical solutions which help explain the physical mechanism of the instability.

In a related study, the effect of buoyant convection on the stability of a mushy zone in a ternary alloy has been considered. The mushy zone is an idealized model of a two-phase region where liquid and solid co-mingle. With a three component system we show that instabilities can occur that are driven by the difference in the rates of diffusion of heat and solute ("double diffusive convection"), even when the density in the system is stably stratified, with heavy fluid underlying light fluid. This work was published in an issue of the *Journal of Fluid Mechanics* (Cambridge University Press) that was dedicated to Professor S. H. Davis of Northwestern University on his 70th birthday; the guest

editors of the volume were G. B. McFadden and P. H. Steen from Cornell University.

[1] G. B. McFadden, S. R. Coriell, and P. A. Lott, Onset of convection in two layers of a binary liquid, *Journal of Fluid Mechanics* **647** (2010) 105-124.

[2] G. B. McFadden, S. R. Coriell, and P. A. Lott, Onset of Morphological Instability in Two Binary Liquid Layers, submitted.

[3] D. M. Anderson, G. B. McFadden, S. R. Coriell, and B. T. Murray, Convective instabilities during the solidification of an ideal ternary alloy in a mushy layer, *Journal of Fluid Mechanics* **647** (2010) 309-333.

ITL Program: *Enabling Scientific Discovery*

Modeling of Self-similar Grain Size Distributions

Geoffrey B. McFadden
C.S. Pande (Naval Research Laboratory)

Polycrystalline solids typically consist of a large number of grains that differ in the orientation of their crystallographic axes. These grains have a distribution of sizes, and are separated by curved grain boundaries that in turn meet at grain boundary junctions. Driven by combinations of elasticity, diffusion, or capillary forces the grain boundaries migrate in time, and the distribution of grain sizes consequently evolves dynamically.

A statistical description of the process is given by a grain size distribution function, which is assumed to depend on a mean grain radius and time. Grain growth under usual circumstances is known to approach a quasi-stationary distribution of grain sizes after a transient period. The quasi-stationary state in a wide variety of materials exhibits a scaling property, such that the grain size distribution has an invariant form when expressed in terms of the grain size scaled by its mean value. An accurate description of the spatial and temporal evolution of a polycrystal from an initial stage, through the transient period, and finally to the quasi-stationary state is still only poorly understood.

In this work, a size-based continuum stochastic formulation is presented based on topological considerations. This analysis leads to a Fokker-Planck equation for the size distribution which admits a similarity solution that describes the long time behavior of the grain growth [1]. The resulting grain size distributions are shown to be in agreement with those obtained from computer simulations, indicating the validity of the stochastic approach.

[1] C. S. Pande and G. B. McFadden, Self-similar grain size distribution in three dimensions: A stochastic treatment, *Acta Materialia* **58** (2010) 1037-1044.

ITL Program: *Enabling Scientific Discovery*

Materials Data and Metrology for Application to Materials Processes

Timothy Burns
Steven Mates (NIST MML)
Richard Rhorer (NIST EL)
Eric Whitenton (NIST EL)
Debasis Basak (Orbital Sciences Corporation)

Prediction of the best machining parameters for a particular process and work material continues to be a challenge in manufacturing. The fundamental problem that needs to be modeled is chip formation. Here, the workpiece interacts with a cutting tool under extreme pressure and temperature, and large plastic deformation takes place at a very high strain rate, both in the thin primary shear zone, and in the secondary shear zone along the tool/work interface, as the newly cut material slides up the rake face of the tool (see Figure 30). In some materials, the temperature during high-speed cutting can rise to a significant percentage of the melting temperature. Even though great strides have been made in modeling and simulation capabilities in the last few decades, due in large part to the development of user friendly finite-element software packages, there continues to be a need for higher precision and reliability in the modeling and simulation of machining processes. One of the major challenges to improved

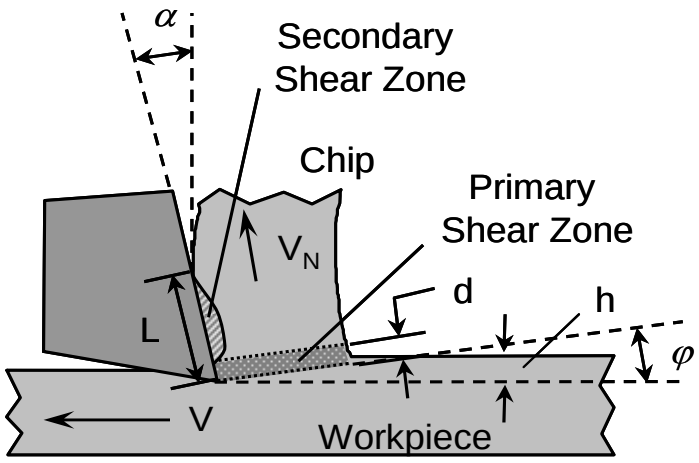


Figure 30. *Schematic illustration of orthogonal cutting.*

modeling and simulation is the determination of an appropriate material description, i.e., constitutive response model, for the flow stress in the workpiece.

Over the past several years, our research program in the NIST Pulse-Heated Kolsky Bar Laboratory has been directed towards obtaining improved constitutive response data under conditions of rapid heating for application to machining studies, as well as for other applications. This year, new experimental data on AISI 1075 carbon steel have been published [1], [2]. The material AISI 1075 is known as a spring steel, and it is not frequently formed in high-speed machining operations. This specific steel was chosen for our study because it begins to undergo a phase transformation to a weaker crystalline form, i.e., austenite, at approximately the lowest temperature among the carbon steels; see Figure 31. The material has been shown to exhibit a stiffer response to compressive loading when it has been preheated using pulse-heating than it does when it has been preheated more slowly to a testing temperature that is below the eutectoid temperature (723 ºC). Furthermore, when the material is pulse-heated to a temperature that exceeds the eutectoid temperature prior to compressive loading on the Kolsky Bar, it has been shown to exhibit a significant (~50 %) loss of strength. As a result, fixed-parameter constitutive models, such as the well-known Johnson-Cook model, cannot be used to describe this flow stress behavior.

Because the lower-carbon steel AISI 1045 is used in the manufacture of automobile parts, and is often shaped by high-speed machining processes, we are designing new pulse-heated Kolsky bar experiments to investigate whether this material has constitutive response behavior similar to that of AISI 1075. Some preliminary results indicate that this is indeed so [3]

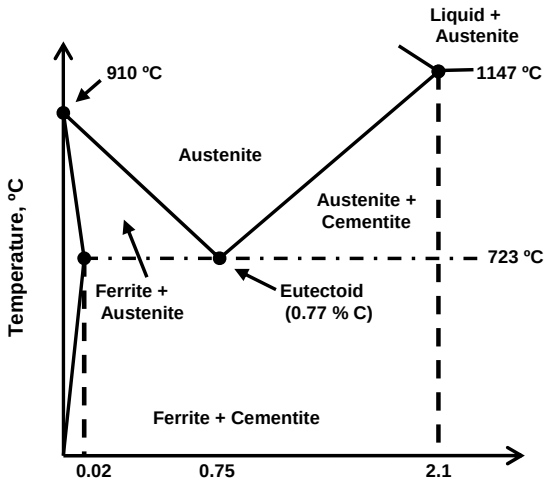


Figure 31. *Schematic drawing of equilibrium iron-carbon phase diagram for carbon percentages and temperatures of interest in this study. Dotted vertical line at 0.75 % carbon is close to the eutectoid composition at 0.77 % carbon.*

[1] T. J. Burns, S. P. Mates, R. L. Rhorer, E. P. Whitenton, and D. Basak, Dynamic Properties for Modeling and Simulation of Machining: Effect of Pearlite to Austenite Phase Transition on Flow Stress in AISI 1075 Steel *Machining Science and Technology*, to appear.

[2] T. J. Burns, S. P. Mates, R. L. Rhorer, E. P. Whitenton, D. Basak, and R. H. McFadden, Modeling of the Temperature Field in the Chip and in the Tool in High-Speed Machining of a Carbon Steel: Effect of Pearlite to Austenite Phase Transition in AISI 1075, *International Journal of Material Forming* **3** (2010), Supplement 1, pp. 491-494.

[3] T. J. Burns, S. P. Mates, R. L. Rhorer, E. P. Whitenton, and D. Basak On Modeling the Peak Temperature on the Tool-Chip Interface During High-Speed Machining of AISI 1045 Steel, in *Proceedings of the Eighth International Conference on High-Speed Machining*, Metz, France, December 8-10, 2010.

ITL Program: *Enabling Scientific Discovery*

Optimization for Inverse Problems in Mechanics

Peter M. Ketcham
Steven P. Mates (NIST MML)

We are collaborating on the development of optimization tools suitable for deducing parameters for viscoplastic constitutive models of metals by inverse methods. The project involves full-field displacement history data and force history data combined with finite element models of dynamic materials tests performed in a Kolsky bar. Optimization is used to minimize cost functions representing differences between the simulations and the data with constitutive constants and friction as the primary unknown variables. Particular attention is paid to the uniqueness and stability of the optimized parameter set in order to assess the usefulness of the discovered parameters in modeling a variety of viscoplastic problems.

This year we investigated optimization approaches, identified relevant mathematical resources, and established foundations for the associated software tools. Future work will include the development of prototype optimization tools with Mathematica and the evaluation of finite element analysis packages with respect to models of dynamic materials tests.

Molecular Movies: Imaging Femtosecond Motion during Electrochemical Transitions

Bradley Alpert
Joel Ullom et al. (NIST PML)
Christopher Cromer et al. (NIST PML)
Ralph Jimenez et al. (NIST PML/JILA)
Henry Kapteyn et al. (University of Colorado/JILA)

Vital to the development of next-generation nanomaterials, including photovoltaics and industrial catalysts, is an understanding gained through measurement of electron generation, transport, and transfer in engineered nanostructures. This project, recently chosen for an Innovations in Measurement Science (IMS) award, proposes a revolutionary, table-top x-ray imaging system to capture the motion of electrons, atoms, and molecules on femtosecond time scales and with picometer spatial resolution.

The combination of table-top x-ray lasers, a dramatic recent breakthrough developed at JILA, with transition-edge sensor (TES) microcalorimeter spectroscopy, intensively developed and refined in NIST's Quantum Electrical Metrology Division, promises to enable these new measurement capabilities. The integration of these components, accompanied by significant increase in detector array sizes, to achieve large increases in temporal and spatial resolution while maintaining extraordinary TES energy resolution, requires new data modeling and processing techniques. These techniques will overcome current limitations by

- Resolving temporal overlap in photon detection while achieving energy resolution of temporally isolated arrivals,
- Improving efficiency in elimination of low-frequency background noise, and
- Extending multiplexing and reducing cross talk in extracting the signals from below 1 degree kelvin to room temperatures.

Wiener filtering, long used among astronomers for estimating amplitudes of pulses of known shape contaminated with noise of known spectral (frequency) content, is suitable for measuring isolated pulses. Novel processing approaches are being developed and characterized that rely on this knowledge but are suitable for overlapping pulses.

Another processing issue concerns sensor nonlinearities at higher frequencies. As the new systems are built and characterized, other sources of uncertainty will undoubtedly arise and need to be understood, and this broad collaboration has been assembled for this purpose.

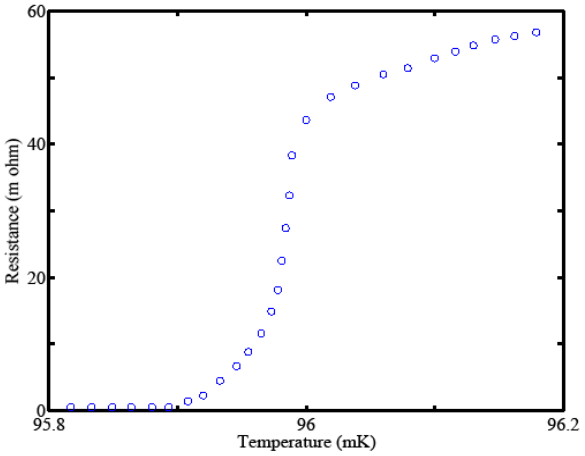


Figure 32. *The steep transition of superconducting film (a Mo/Cu proximity bilayer), provides temperature sensitivity that enables its use for photon spectroscopy. Note the narrow temperature range of approximate linearity.*

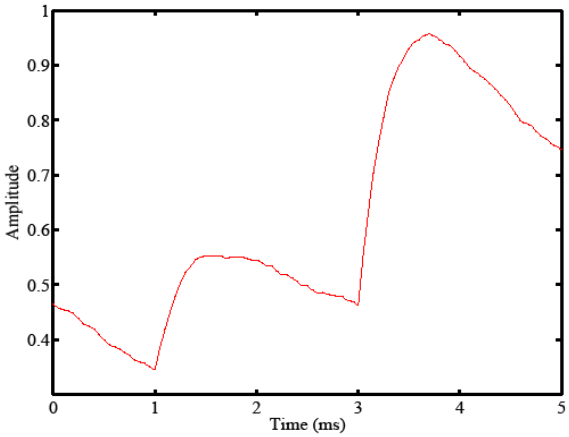


Figure 33. *For overlapping responses due to multiple photons poorly separated in time, accurate amplitude determination requires good elimination of low-frequency background noise.*

Accelerating Monte Carlo Simulation for Modeling Thermodynamic Properties

Bradley Alpert
Andrei Kazakov (NIST MML)
Kenneth Kroenlein (NIST MML)

To provide critically-evaluated data essential to industrial processes, the NIST Thermodynamics Research Center (TRC) develops and applies to published laboratory measurements several modeling technologies to evaluate, extend, and establish uncertainties for reported quantities.

Metropolis Monte Carlo simulation, despite having been developed more than a half century ago, widely known, and extensively studied, has not been an important tool in this arsenal due to its extraordinarily high computational cost for all but the simplest compounds. Nevertheless, steadily improving computational power, continuing advances in Monte Carlo methods, and increasing demands for properties data beyond what can be feasibly obtained in labs, continue to shift the balance in favor of these computations.

In addition, a major refrigerant properties characterization effort previously undertaken at NIST for the transition away from hydrochlorofluorocarbon refrigerants (such as Freon), successful in characterizing substitutes, now is no longer sufficient to enable compliance with new European environmental laws. The TRC intends to perform Monte Carlo simulations to obtain, for some currently poorly-characterized refrigerants, property data including critical parameters, saturated densities, saturated pressures, liquid densities, and vaporization enthalpies. These computations are barely feasible currently and therefore TRC has considerable interest in accelerating the code, MCCCS Towhee, used for the simulations.

Alpert's initial involvement in the effort arose from the potential to accelerate the many-body Coulomb interaction energy computations through use of the fast multipole method (FMM). To do so requires development of an incremental FMM in which energy changes due to position changes of a small number of atoms are computed efficiently. This algorithm work is underway. In addition, the Towhee random number generator has been replaced, for improved efficiency, and other code changes under consideration will improve the ease of incorporating additional algorithm changes, such as Hamiltonian Monte Carlo.

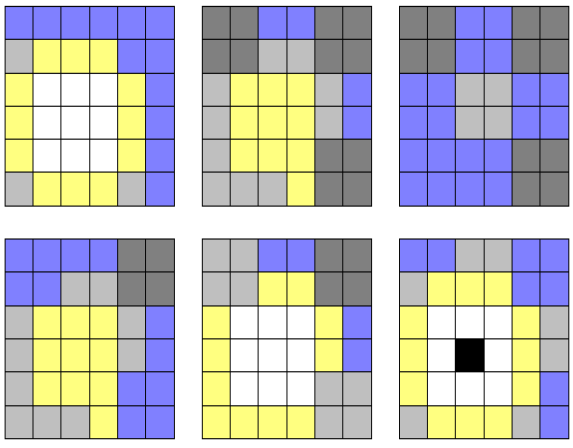


Figure 34. *The fast multipole method divides space into cubes hierarchically, with communications based on 6 x 6 x 6 aggregations (left to right, bottom then top). In the incremental update algorithm for Coulomb energy, additional efficiency gains are achieved by revised aggregations, involving 2 x 2 x 2 blocks (dark gray), 2 x 2 x 1 blocks (blue), 2 x 1 x 1 blocks (gray), and 1 x 1 x 1 blocks (yellow). The white cubes are nearest neighbors to the source cube (black).*

Uncertainty in Virtual Measurements from Quantum Chemistry Models

Raghu Kacker
Ruediger Kessel
Karl K. Irikura (NIST MML)
Russell D. Johnson III (NIST MML)

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

Predictions from computational quantum chemistry models seldom agree with the corresponding high-quality physical measurements. The differences are not random but systematic. Therefore, a common practice is to apply an empirical scaling factor to computational predictions to bring them closer to the true quantity values. The empirical scaling factor carries uncertainty. We have developed a methodology to quantify the uncertainty associated with a scaling factor. This approach is based on the Guide to the Expression of Uncertainty in Measurement, which is an international standard. The uncertainties for scaling factors lead to the corresponding uncertainties for virtual predictions. We reported in 2005 uncertainties in the scaling factors for ab initio vibrational frequencies

from 40 models (combinations of theory and basis sets) intended for predicting fundamental frequencies from computed harmonic frequencies [1]. The uncertainties were larger than generally acknowledged. This paper has received 121 citations.

Subsequently in 2006-2007, we determined a new reference data set of 60 diatomic and 15 polyatomic experimental vibrational zero-point energies (ZPEs) that includes estimated uncertainties. In 2008 we refined the methodology for calculating uncertainties and reported uncertainties for 32 models intended for predicting vibrational ZPEs form computed harmonic frequencies. Our paper on this appeared in 2009 [2].

This year we considered anharmonic scaling factors and their associated uncertainties for six theory-basis set pairs [3]. Recent comments on our papers indicate that scientific community has started paying attention to uncertainties in computational models.

In FY 2011 we will investigate the benefit of computing anharmonic frequencies which are much more expensive but do not avoid need of scaling.

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

[2] K. K. Irikura, R. D. Johnson III, R. N. Kacker, and R. Kessel, Uncertainties in Scaling Factors for ab Initio Vibrational Zero-Point Energies, *Journal of Chemical Physics* **130** (2009), article 114102 (11 pages).

[3] R. D. Johnson III, K. K. Irikura, R. Kacker, and R. Kessel, Scaling Factors and Uncertainties for ab-initio Anharmonic Vibrational Frequencies, *Journal of Chemical Theory and Computation* **6** (9) (2010), pp. 2822-2828.

ITL Program: *Virtual Measurement Systems*

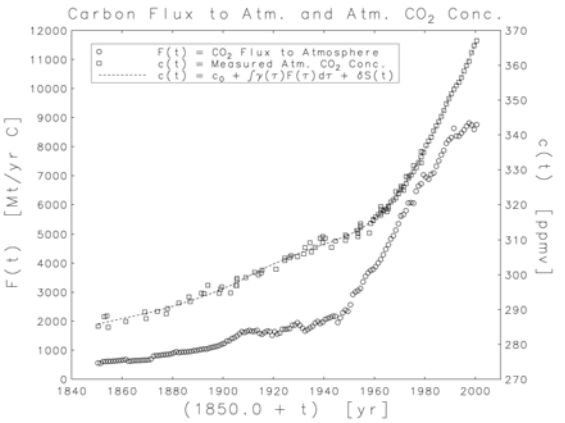


Figure 35. *The lower plot gives yearly total CO_2 emissions F(t), measured in megatons of carbon per year [Mt/yr C]. The upper plot gives the atmospheric CO_2 concentration c(t), measured in parts per million by volume [ppmv]. The c(t) measurements after 1959 are highly accurate averages of weekly air samples over the South Pole, but earlier measurements were obtained from Antarctic ice cores, which are less accurate, with many missing years.*

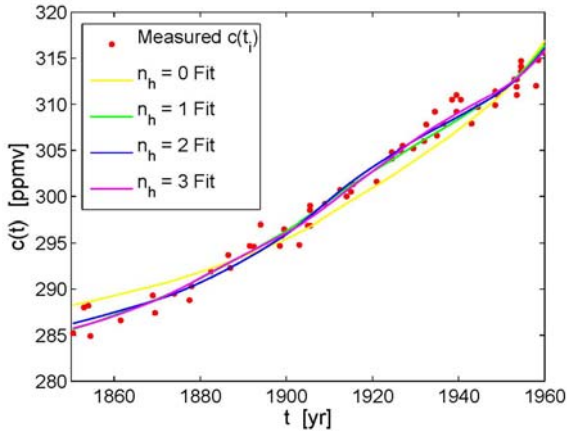


Figure 36. *Harmonic approximation fits to c(t). After 1960 the highly precise South Pole measurements dominate, causing all of the fits to merge very closely.*

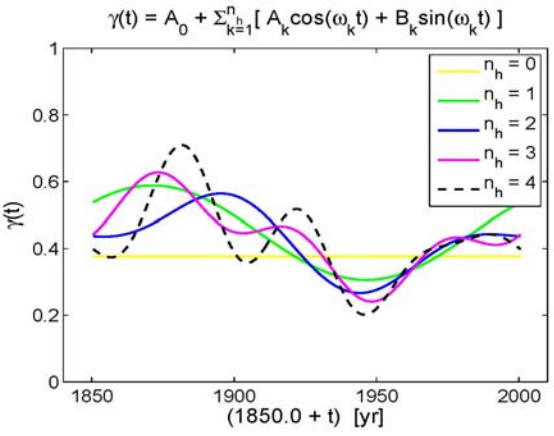


Figure 37. *Estimates of the fraction of CO_2 emissions remaining in the atmosphere.*

Atmospheric Retention of Man-made CO_2 Emissions

Bert W. Rust

Most scientists agree that the observed warming of the Earth is chiefly caused by increases in atmospheric CO_2 concentration $c(t)$, which are driven by man-made CO_2 emissions $F(t)$. Figure 35 shows that these emissions have increased quasi-exponentially since 1850. If $\gamma(t)$ is the fraction of the emissions in year t which remains in the atmosphere, then $c(t)$ can be related to $F(t)$ by the first kind integral equation

$$c(t) = c_{1850} + \int_{1850}^{t} \gamma(\tau) F(\tau)\, d\tau, \quad 0 \le \gamma(t) \le 1.$$

Discretizing by quadrature gives an 83 x 151 linear system which, even with the constraints on $\gamma(t)$, yields highly unstable estimates of $\gamma(t)$.

Assuming a harmonic expansion for $\gamma(t)$ on the interval $1850 \le t \le 2000$, i.e.,

$$\gamma(t) = A_0 + \sum_{k=1}^{n_h}\left[A_k \cos\left(\frac{2\pi kt}{150}\right) + B_k \sin\left(\frac{2\pi kt}{150}\right)\right]$$

allows the parameters A_0, A_k, B_k to be estimated by least squares, so long as $2n_h < 83$. The fits for $n_h = 0$, 1, 2, 3 are shown in Figure 36. Each successive fit in the sequence estimated 2 more free parameters than did the preceding one, so the standard F-test provides a criterion for terminating the sequence. *A new harmonic should be included only if the two additional parameters produce a statistically significant reduction in the SSR*. In the present case, the $n_h = 4$ fit failed to produce such a reduction. The $\gamma(t)$ estimates corresponding to the fits are plotted in Figure 37 which also gives the $n_h = 4$ estimate for comparison. It is clearly more wiggly than the preceding estimates, and if n_h is pushed to even higher values, the corresponding estimates become wildly oscillating and violate the $0 \le \gamma(t) \le 1$ constraint, so $n_h = 3$ is clearly the optimal choice.

[1] B. W. Rust, Atmospheric Retention of Man-made CO_2 Emissions, *Mathematics and Computers in Simulation*, to appear.

Modeling the Fluid Dynamics of Tear Films on the Cornea

Geoffrey B. McFadden
Richard J. Braun (University of Delaware)
Toby A. Driscoll (University of Delaware)
L. P. Cook (University of Delaware)
R. Usha (Indian Institute of Technology)
P. E. King-Smith (Ohio State University)

Dry eye disorders refer to eye problems associated with insufficient amounts of fluids coating the surface of the cornea. They can be caused by reduced production of aqueous tears, and/or increased evaporation due to a deficient lipid layer in the fluid. In both of these conditions, tear film breakup is more rapid than normal. Breakup can be observed either as dark spots in fluorescein-stained tear films, or, noninvasively, by distortions in the reflected image of a grid.

In order to better understand the dynamics of the spreading of tear films on the human eye we have studied two hydrodynamic models based on lubrication theory [1]. The eye is modeled by an ellipsoid of revolution, using a prolate spheroidal coordinate system. One model is a self-consistent leading-order hyperbolic PDE for relatively large substrate curvatures; the other retains another order resulting in a fourth order parabolic partial differential equation (PDE) for the film dynamics. We consider both Newtonian viscous flow models and non-Newtonian models that take into account shear-thinning of the tear fluid. We explore a wide parameter range of shear thinning and find a significant effect on finite-time singularities present in the model, representing discontinuous solutions allowed by the underlying hyperbolic PDE. Approximate results illustrating the nature of the flows are obtained both numerically and analytically.

We are able to use this approach to evaluate the influence of the cornea's shape in providing a driving force for fluid motion through the Laplace-Young boundary condition that relates pressure and interface curvature, an effect neglected in previous studies.

[1] R. J. Braun, R. Usha, G. B. McFadden, T. A. Driscoll, L. P. Cook, and P. E. King-Smith, Thin Film Dynamics on a Prolate Ellipsoid with Application to the Cornea, in review.

Simulation of Bioregulatory Networks Involved in Cell Cycle Control

Geoffrey B. McFadden
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G. McFadden is a co-advisor to Sohyoung Kim, a postdoctoral fellow, and Augustin Luna, a graduate student from Boston University, who are both doing research at the Laboratory of Molecular Pharmacology in the National Cancer Institute at NIH; their co-advisors are NIH researchers M. Aladjem and K. Kohn. The team is developing models of bioregulatory networks that are involved in cell cycle control. The models consist of systems of nonlinear ordinary differential equations or delay differential equations that typically exhibit switching behavior, limit cycles, and other types of bifurcations.

Proper cell growth depends on a network of interacting molecules that monitors cellular metabolism and environmental signals. This network ensures that cells halt their growth in response to unfavorable conditions such as the absence of sufficient nutrients or the presence of potentially damaging agents. When cells escape these controls, the results are developmental abnormalities, genomic instability, and cancer.

Much current work focuses on a protein known as p53, a tumor suppressor that causes cell cycle arrest or programmed cell death in response to stress signals such as DNA damage. Regulating the appropriate levels of p53 is essential for cell survival. Two associated proteins, Mdm2 and Mdmx, are known regulators of

p53. Mdm2 can facilitate degradation of p53, whereas the mechanism of the regulatory interaction of Mdmx with p53 is not clear. It is also not obvious how those three molecules will operate together under various conditions.

To address those questions a mathematical model has been developed [1] to investigate the interactions of these three partner molecules by numerical simulations. An interesting feature of this system is the experimental observation of time-periodic behavior of the measured amounts of p53 and Mdm2 in the system under certain conditions. These results show the stabilizing effect that Mdmx has on the system at long times: for large enough amounts of Mdmx in the system the entire branch of steady state solutions is found to be linearly stable.

This modeling work is intended to guide experimental investigations of the role of Mdmx in the cell cycle that are being performed by Dr. Kim. Augustin Luna has recently joined the team to conduct his Ph.D. research, which includes the development of models of the role played by a protein, SirT1, in regulating cellular response to DNA damage. Resveratol, naturally found in red wine and linked with extended lifespans in rodents, stimulates the gene that produces SirT1. G. McFadden is serving on his Ph.D. committee at Boston University.

[1] S. Kim, M.I. Aladjem, G.B. McFadden, and K.W. Kohn, Predicted functions of MdmX in fine-tuning the response of p53 to DNA damage, PLoS Computational Biology 6 (2010), article e1000665 (18 pages).

Automated Biological Cell Feature Identification

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Biological cells are composed of many subsystems and organelles. The subsystem called the cytoskeleton is composed of long rod-shaped filaments. They give the cell form and help attach the cell to the substrate and neighbors. One of the filaments is called actin.

In studying cells, biologists use microscopes that can be focused at different levels and can be automated to take multiple images. Stain treatments are used to bring out cell characteristics. In this study a computational method is implemented that automatically isolates the actin structures in cell imagery.

Figure 38(a) shows a cell with the actin fiber cytoskeleton structure. This is one isolated cell in a group of thousands of cells. Cell biologists are interested in automatically identifying and sometimes measuring the groupings of fibers. The computer program developed for this project uses imaging techniques coupled with a data structure, called a graph, to identify and isolate groupings of actin fibers.

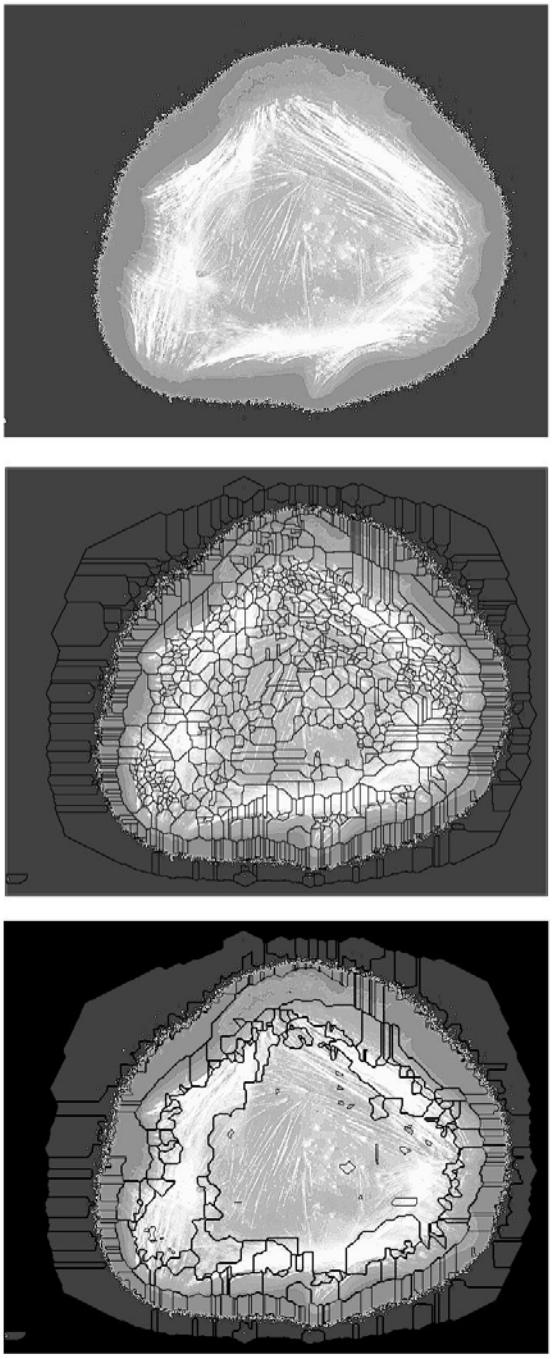

Figure 38. *(a) Top: Cell image showing the actin fiber structure. (b) Middle: Oversegmented image of the cell in top image. (c) Final feature isolation for the cell in the top image.*

The program begins by using an image processing method called watershed image segmentation. This method decomposes the image into regions with similar properties by outlining the boundaries of areas with valleys. However, due to image noise and the large

number of minima, this technique has a tendency to break the image into too many small segments. This is referred to as oversegmentation. An oversegmentation of the cell in Figure 38(a) is shown in Figure 38(b). It is clear from the figure that this segmentation does not create regions that isolate groups of fibers, for example. The objective of the program was to group the segments into more meaningful regions or features.

The approach was to develop a measure of similarity or closeness of regions. In the current program the average image intensity of the regions was used as the defining characteristic of a region. A distance function to differentiate between regions was then created based on the average intensity differences. A tolerance was established that isolated nearest neighbor regions and an adjacency graph (or adjacency matrix) was created that established links between regions and their nearest neighbors. Regions that are neighbors are not necessarily nearest neighbors. It would depend on whether the distance function between them fell below the tolerance. Each region would have an associated list of nearest neighbors. All of these nearest neighbors themselves have linked nearest neighbors, thus forming a chain of connected regions. This allowed the use of an efficient search algorithm to link all regions with nearest neighbors within the tolerance into connected components. These connected components were taken as the desired features. Figure 38(c) shows the result of applying the algorithm to the image in Figure 38(a).

Although this image has areas with more segments than necessary, the program successfully identifies the major groupings of actin fibers. Further work is underway to develop an iterative approach to feature identification. Initial experiments on an iterative approach using the same average intensity measure did not produce fewer feature groupings. Different measures of region nearness have to be developed for the second and subsequent iterations. The initial algorithm and program are documented in [1].

[1] D. E. Gilsinn, K. Bhadriraju, J. T. Elliott, Biological Cell Feature Identification by a Modified Watershed-Merging Algorithm, NISTIR 7750, November 2010, (47 pages).

ITL Program: *Information Discovery, Use and Sharing*

Estimating Volumes of Simulated Lung Cancer Nodules

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Bruce R. Borchardt (NIST PML)
Amelia Tebbe (St. Mary's College)

Lung cancer is a disease of uncontrolled cell growth in tissues of the lung. It is the most common cause of cancer related deaths in men and second most in women and is responsible for an estimated 560,000 deaths in the US in 2007. Lung cancer lesions may be seen in computed tomography (CT) images. Modern computer tomography is a medical imaging method that uses tomography but also employs digital image processing techniques to generate three dimensional images built from a sequence of two-dimensional X-ray images made around a single axis.

The Food and Drug Administration (FDA) is developing reference cancer lesions, called phantoms, to test CTs and their software. Two samples were loaned to NIST to estimate volumes. The material of which the phantoms are composed simulates lung cancer material. The FDA can insert these into a simulated body torso for testing CT scanning and image recognition. The two phantoms are shown in Figure 39. Although they seem spherical they are slightly non-spherical. The phantom on the right in Figure 39 is referred to as Green and the one on the left is referred to as Pink.

The approach chosen for this study is based on a fundamental theorem in calculus, called the Divergence Theorem, in which a volume integral is shown to be equal to a particular surface integral. In order to develop a surface model of the phantoms, surface data was measured by a coordinate measuring machine (CMM) at NIST; see Figure 40. This machine produced a set of precisely measured (x, y, z) points on the surface of each phantom. As a reference, surface data was obtained on a well calibrated metal sphere in order to test the surface modeling process. In each case, two sets of data points were measured, which we referred to as coarse (121 points) and dense (181 points).

The measured data were transformed to spherical coordinates and modeled using a set of basis functions, called B-splines. The initial best fit, in the sense of

Figure 39. *Simulated Lung Cancer Nodules.*

least squares, of linear combinations of bivariate forms of the B-splines exhibited undesirable oscillations. To mitigate these effects, the least squares objective function was modified to include smoothing terms. This process, called regularization, produced very satisfactory extrapolation values at triangle vertices on the phantom surfaces. The surface triangulation was then used to compute the necessary surface integrals and finally the volumes using the Divergence Theorem.

To test the B-spline modeling process two approaches were taken with surface data from the calibrated metallic sphere. A spherical model was fit by least squares parameter fitting and the B-spline model was fit using the regularized objective function. The predicted volumes differed by approximately 0.01%. This confirmed that the B-spline modeling process, using regularization, was a valid process and volume estimates of the phantoms would be acceptable

As a check on the potential non-spherical shape of the phantoms, a spherical model was fit to each. These produced volume estimates for the coarse and dense data from the Green phantom of 4331.3 mm^3 and 4296.5 mm^3 respectively. The expanded uncertainties for the center point and radius were estimated as order 10^{-1} and 10^{-2} respectively. For the Pink phantom the volumes were estimated as 3892.1 mm^3 for the coarse data and 3912.5 mm^3 for the dense data. The expanded uncertainties for the center point and radius were of the order 1 and 10^{-1} respectively. This suggested a spherical shape for the Green phantom and a slight non-spherical shape for the Pink.

Figure 40. *Coordinate Measuring Machine*

When volumes were estimated using the B-spline model, the values for the Green phantom were computed as 4331.8 mm^3 and 4296.8 mm^3 for the coarse and dense data respectively, Notice the closeness to the spherical model results. The expanded uncertainties for the volumes were estimated as approximately 12 mm^3 for the coarse data and 8 mm^3 for the dense data. For the Pink phantom the volume results were 3854.7 mm^3 and 3906.5 mm^3 with expanded uncertainties of approximately 28 mm^3 and 18 mm^3. These differed slightly from the spherical model fit, again indicating a potential non-spherical form for the Pink phantom. A preliminary [1] and final report [2] have been published.

[1] D. E. Gilsinn, B. R. Borchardt, and A. Tebbe, Estimating Volumes of Simulated Lung Cancer Nodules, NISTIR 7571, July 2009.

[2] D. E. Gilsinn, B. R. Borchardt, and A. Tebbe, Estimating Volumes of Near-Spherical Artifacts, *Journal of Research of the National Institute Standard Technology* **115** (2010), pp. 149-177.

ITL Program: *Information Discovery, Use and Sharing*

Computing Geodesics for Shape Analysis

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Michael Halter (NIST MML)

The recognition and classification of objects in observed images is an important goal in image analysis. For this purpose the analysis of shapes of objects in images has become an important tool. Accordingly biomedical image analysis is a major application of shape analysis. In particular biomedical images that show cells responding to stimuli are good candidates for shape analysis. This is because change in shape is a known response of a cell to stimuli.

Shape space can be formalized with the Riemannian metric. In a space with this metric, a line between two points is generalized to a geodesic path between two shapes. The shapes of two cells can then be compared by computing the Riemannian length of the geodesic path between the two cells.

In this work numerical routines for computing geodesics for shape analysis will be implemented. Implementation will be used for understanding changes in shape of biological cells as a response to stimuli.

ITL Program: *Information Discovery, Use and Sharing*

Neural Networks

Javier Bernal

As part of the Computational Biology project, a back-propagation algorithm is being implemented for training neural networks. It is hoped that the neural network approach will be useful for the identification of subcellular features in cell images relevant to cell biologists. Approaches exist for recognizing objects or pattern classes associated with an image based on the use of sample patterns (training patterns) to estimate statistical parameters of each pattern class. However the statistical properties of the pattern classes might not be known or might be difficult to estimate. Therefore a method such as the neural network approach that produces the required decision functions based solely on training without assumptions about probability density functions associated with the pattern classes may be more successful at handling the problem.

A neural network is a computational model that consists of computing elements called "neurons" organized as a network reminiscent of the way in which neurons are believed to be interconnected in the brain. It is an adaptive system that changes its structure based on information that flows through the network during a training phase. It is mostly used for modeling relationships between input and output data and for partitioning data into classes.

During the training with the backpropagation algorithm the average squared error between the networks output and a target value is minimized for each point or pattern (in d-dimensional space) in the training set using gradient descent. Via training, coefficients of decision functions are obtained and associated with neurons in the network. Once the training is done other data points or patterns are put through the network and assigned to a class according to the output obtained. For our purposes the resulting implementation will be used for identifying pattern classes in d-dimensional space as each pixel in an image is associated with a d-dimensional pattern, the coordinates of the pattern corresponding to d distinct attributes associated with the pixel.

ITL Program: *Information Discovery, Use and Sharing*

High Performance Computing and Visualization

Computational capability is advancing rapidly. This means that modeling and simulation can be done with greatly increased fidelity (e.g. higher resolution, more complex physics). However, developing large-scale parallel applications remains highly challenging, requiring expertise that application scientists rarely have. In addition, the hardware landscape is changing rapidly so new algorithmic techniques must constantly be developed. We are developing and applying facilities and expertise of this type for application to NIST problems. Large scale computations and laboratory experiments invariably produce large volumes of scientific data, which cannot be readily comprehended without some form of visual analysis. We are developing the infrastructure necessary for advanced visualization of scientific data, including the use of 3D immersive environments and applying this to NIST problems. One of our goals is to develop the 3D immersive environment into a true interactive measurement laboratory.

Large-scale Simulation of Suspensions

William George
Steve Satterfield
Marc Olano
Judith Terrill
Nicos Martys (NIST EL)
Edward Garboczi (NIST EL)
Pascal Hebraud (CNRS/ESPCI, France)

See feature article, page 31.

ITL Program: *Enabling Scientific Discovery*

High Precision Calculations of Properties of Few-electron Atomic and Molecular Systems

James S. Sims
Stanley A. Hagstrom (Indiana University)

See feature article, page 36.

ITL Program: *Virtual Measurement Systems*

Nano-optics, and How to Squeeze Light out of Quantum Dots

James S. Sims
John Kelso
Marc Olano
Garnett Bryant (NIST PML)
Natalia Malkova (NIST PML)

See feature article, page 38.

ITL Program: *Enabling Scientific Discovery*

Modeling and Visualization of Cement Paste Hydration and Microstructure Development

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Steven Satterfield
Judith Terrill
Jeffrey Bullard (NIST EL)
Edith Enjolras (NIST EL)
Clarissa Ferraris (NIST EL)
Edward Garboczi (NIST EL)
Nicos S. Martys (NIST EL)
Paul E. Stutzman (NIST EL)

http://www.nist.gov/itl/math/hpcvg/hydrationhpc.cfm
http://www.nist.gov/itl/math/hpcvg/hydrationvis.cfm

When cement powder is mixed with water, the process that transforms the paste from a fluid suspension into a solid (hydration) involves complex chemical and microstructure changes. Understanding and predicting the change rates is a longstanding but extremely challenging technological goal. Fundamental computational modeling of the hydration of cement is difficult because it involves a large number of coupled nonlinear rate equations that must be solved in an irregular three-dimensional spatial domain.

To address these challenges, we are applying a new computational model called HydratiCA, which has several advantages over previous attempts to model cement paste hydration. HydratiCA is based on the principles of mass action and detailed balances and uses stochastic cellular automaton algorithms to simultaneously model 3-D reaction and transport phenomena. This allows us to track the detailed kinetics and equilibria that occur in a diverse range of cementitious systems. At the length scales required to finely resolve the reaction mechanisms and microstructure changes in cement paste, HydratiCA must take small time steps (approximately 10^5 per second) to remain numerically stable. In other words, tens of millions of time steps are required to simulate the behavior

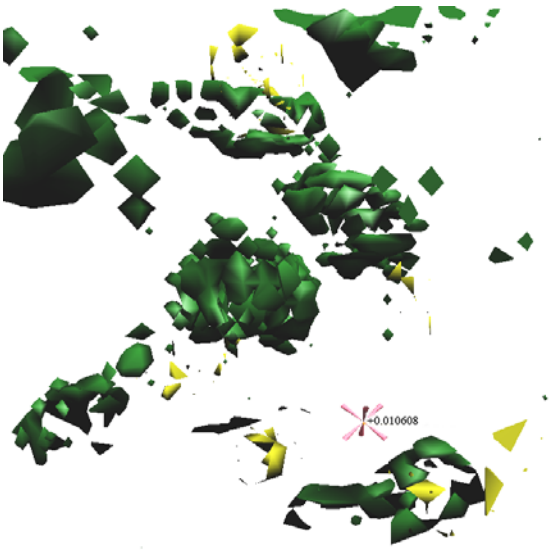

Figure 41. *A snapshot from an interactive visualization of a hydration run at a very early stage of the hydration process. Only the calcium sulfate and calcium aluminate phases are shown. Using a virtual interactive tool, the sulfate ion concentration in solution is measured at a spot in the pore space.*

of cement paste for just one hour. Therefore, parallelization of the model is important so that we can simulate systems that are large enough to be realistic, avoiding finite size effects, and still be able to complete the simulations in a reasonable amount of time.

Visualization of the output of this model is important both for validation and to understand the distribution of phases in 3D; see. Figure 41 The output is a 3D volume of data with percentage values for each of multiple material phases at each lattice site. Over the course of the simulation time, a series of data volumes is produced at the time values of interest. This year we completed a simulation of a large-scale alite system on Columbia, the NASA/NAS SGI Altix machine. This simulation required approximately 100,000 CPU-hours, running on 448 CPUs for over 240 hours.

We will be using HydratiCA to help resolve two prominent hypotheses for reduced alite dissolution rates during the induction period.

[1] J. W. Bullard, E. Enjolras, W. L. George, S. G. Satterfield, and J. E. Terrill, Validating a Scalable Parallel Computer Model of Cement Hydration and Microstructure Development, Modeling and Simulation, *Materials Science and Engineering* **18**(2) (March 2010), article 025007 (16 pages).

[2] E. Garboczi, J. Bullard, N. Martys, and J. Terrill, The Virtual Cement and Concrete Testing Laboratory: Performance Prediction, Sustainability, and the CSHub, in *Proceedings of the NRMCA Concrete Sustainability Conference*, Tempe, AZ, April 13-15, 2010.

[3] J. W. Bullard, E. J. Garboczi, W. L. George, N. S. Martys, S. G. Satterfield, and J. E. Terrill, in *Advancing the Materials Science of Concrete with Supercomputers*, to appear.

[4] J.W. Bullard, C.F. Ferraris, E.J. Garboczi, N.S. Martys, P.E. Stutzman, and J.E. Terrill, Virtual Cement and Concrete, *Innovations in Portland Cement Manufacturing*, in press.

ITL Program: *Enabling Scientific Discovery*

Modeling Clinical Tumors to Create Reference Data for Tumor Volume Measurement

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Alden Dima (NIST ITL)

http://www.nist.gov/itl/math/hpcvg/bioimgvis.cfm

The change in pulmonary nodules over time is an extremely important indicator of tumor malignancy and rate of growth. Physicians base both diagnoses and treatment on perceived changes in size, so accurate and precise measurement of such changes can have significant implications for the patient. Many techniques exist for calculating tumor volumes and/or the change in tumor size between two sets of data on the same tumor. To compare volumetric techniques, we need reference data with a variety of known tumor volumes with different levels of background noise, and no ground truth data is available is a realistic environment. Current phantom data do not replicate the complications of calculating volume change where tumors are embedded in the lung wall and attached to blood vessels. In this work, we create reference data sets to test volumetric change measurement in realistic lung environments.

We are able to recreate clinical tumor shapes using combinations of spheres, ellipsoids, cones, and cylinders, which can be assembled at arbitrary sizes and angles with respect to one another. During assembly, partial voxel volumes are calculated by subdividing each voxel and testing for the appearance of each geometric object in the subsections. Using this technique, we are able to get an accurate estimate of the final volume for the combined set of objects. We first approximate the pixel intensity distribution of a clinical tumor in the same data set, using a normal distribution and the mean and standard deviation of the clinical tumor's pixel distribution. Any grid point completely inside of the synthetic tumor is then assigned a random value from this normal distribution. Pixel intensities for the partially filled voxels are computed based on parameters that we derive from the clinical tumor data, which define the upper and lower boundaries for pixel intensities at the tumor surface. We find the lower boundary for surface pixel intensity from the magnitude of the gradient of the pixel intensities at the tumor surface. K2, the lower boundary for surface pixel intensity, is the intensity with the maximum average

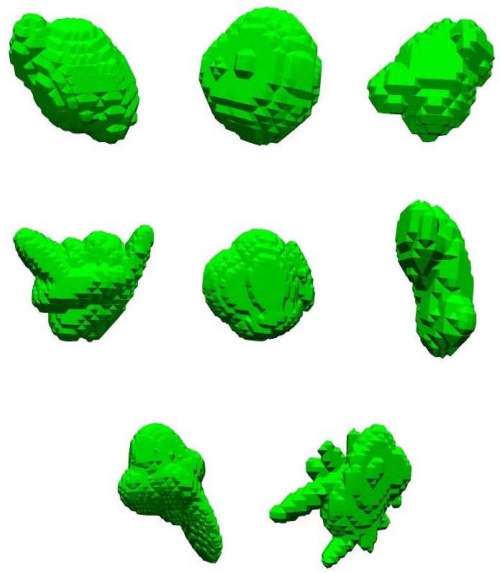

Figure 42. *The eight geometric objects that were inserted into clinical data at the initial time of the test.*

gradient magnitude at the tumor edge. The upper limit for edge pixels, K1, is determined from a ratio based on our previous work [1]. Figure 42 shows the 8 geometric objects that were inserted into the clinical data. Figure 43 shows a few example slices, where both the clinical tumors and modeled synthetic tumors can be seen. Future work includes a further study of lung tumor shapes and growth patterns.

[1] A, Peskin , K. Kafadar, A. Dima , J. Bernal, and D. Gilsinn, Synthetic Lung Tumor Data Sets for Comparison of Volumetric Algorithms, in *The 2009 International Conference on Image Processing, Computer Vision, and Pattern Recognition*, Las Vegas, NV, July 13-16, 2009.

[2] A. Peskin and A. Dima, Modeling Clinical Tumors to Create Reference Data for Tumor Volume Measurement, in *The 6th International Symposium on Visual Computing 2010*, Las Vegas, NV, November 22-December 1, 2010.

ITL Program: *Information Discovery, Use and Sharing*

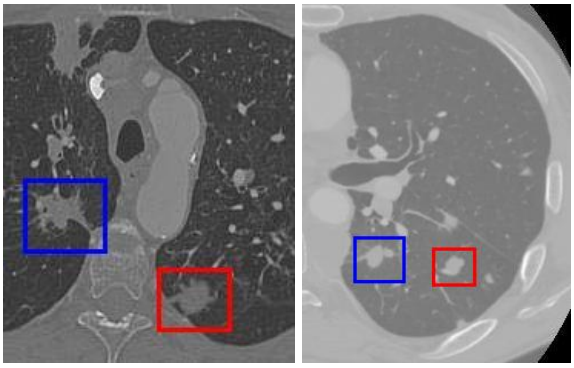

Figure 43. *Clinical tumors in blue boxes; synthetic tumors in red; One slice from each of 2 of the data sets produced for this study.*

Predicting Segmentation Accuracy for Biological Cell Images

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Alden Dima (NIST ITL)
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John Elliott (NIST MML)

http://www.nist.gov/itl/math/hpcvg/bioimgvis.cfm

Cell microscopy is used extensively to monitor cellular behavior under experimental settings. One of the most common image analysis procedures for cellular images is segmentation of an image object from the remainder of the image, which provides information on cell characteristics and comparisons of experimental conditions. In this project we provide a method to estimate segmentation error based on the clarity of the image and the geometry of the image objects. We developed a new concept called the extended edge neighborhood to quantify the accuracy that can be expected from data used in cellular analysis [1].

Many software packages are available for segmentation of cellular objects in biological images. Our NIST collaborators were in need of methods to help evaluate which methods to use and how to use them most effectively. It became clear that quantitative methods were needed to evaluate how to use the image data they were creating. To study this problem, a range of cellular image data was created that varied in cell geometry and imaging conditions. A10 rat smooth vascular muscle cells and 3T3 mouse fibroblasts were stained with Texas Red cell body stain and compared under five sets of imaging conditions: combinations of low, medium, and high illumination, and an optimal and non-optimal filter, to span a wide range of image qualities [2]. Figure 44 provides a visual rendition of the five conditions.

In an initial study of a large number of segmentation methods tested over all of our imaging conditions, it became apparent that information about the image clarity and cell characteristics could be used to determine how segmentation methods performed. We were able to quantify these factors into a single concept that can be used to predict how segmentation methods will work and the accuracy that be expected when using them. The apparent cell edges vary widely in clarity and sharpness across the five different images of the same cells. Cell edge quality can be measured in terms of the number of pixel lengths (distance between pixels) needed to represent the thickness of the edge regions, which we have previously quantified as the cell edge quality index (QI) [3]. In a paper in which we compare manual segmentation masks on a set of 16 of the images used here, we find that our manual segmentation sets differ from one another, and that the extent of misalignment from one set to another depends upon

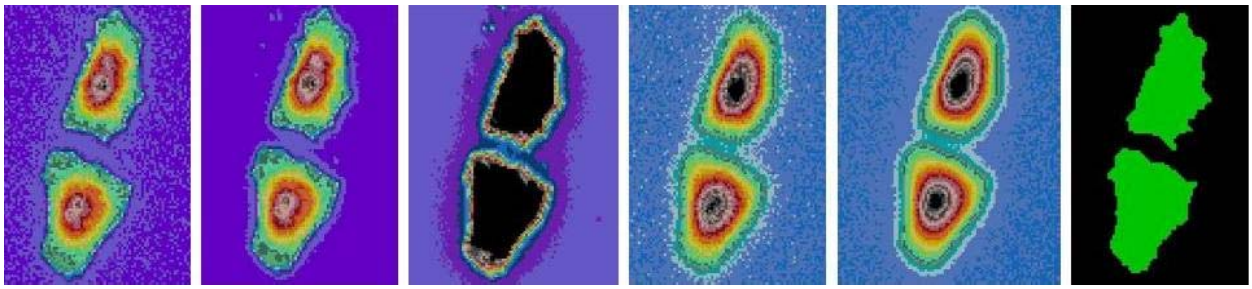

Figure 44. *Individual pixel intensities are color-coded over the range in each image, to show differences in edge sharpness. The ground truth mask is shown for comparison.*

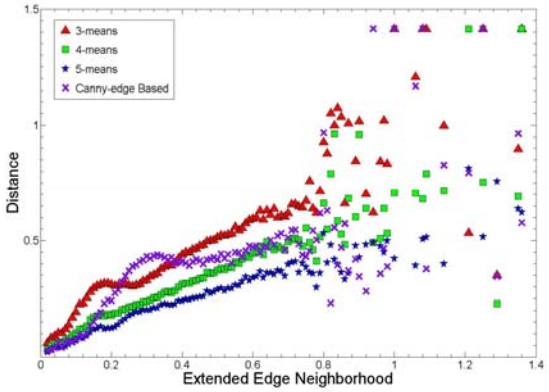

Figure 45. *Average segmentation distance as a function of extended edge neighborhood for 3-means clustering (red), 4-means clustering (green), 5-means clustering (blue), and Canny edge (purple).*

the cell geometry [4]. We combine these concepts into a single quantity that can be calculated quickly for each cell. The metric represents the size of the extended edge neighborhood of pixels and is a fraction derived from the ratio of pixels at risk to the total cell area. The pixels at risk are determined by multiplying the cell perimeter by a factor determined from the QI representing the physical thickness (Th) of the cell edge.

40,000 cell images from the two cell lines and five imaging conditions were tested. In order to scale up our study to this size, we created reference data for segmentation comparisons automatically, using a new technique also created this year in our group [6]. We then segment each of the cell images using four different segmentation techniques. We compare the reference pixel set T, with a segmentation mask, pixel set E, with a pair of indices designed to distinguish between under- and over-segmentation. A single overall score for an individual segmentation can measured as a function of these bivariate indices.

Segmentation analysis was performed on all 40,000 images using four techniques, chosen from a previous study as the most consistent techniques that do not require large quantities of computational time: 5-means, 4-means, and 3-means clustering, and a Canny edge segmentation [4]. Figure 45 shows the combined results from all the cell images as a function of extended edge neighborhood. 5-means clustering gives the best results for all but very low extended edge neighborhoods, where Canny edge segmentation does a better job for images with very high edge quality.

To see the direct relationship between extended edge neighborhood and segmentation accuracy, we looked only at those results for which we had the most data: for each cell line, we chose the region of the extended edge neighborhood curve where 90% of our results appeared. These regions include 0.05-0.2 for the A10 cells, and 0.2-0.5 for the NIH 3T3 cells. Cell counts plotted along with 5-means clustering results for these two regions are shown in Figure 46. In Figure 47, we graph the A10 cells in the extended edge region

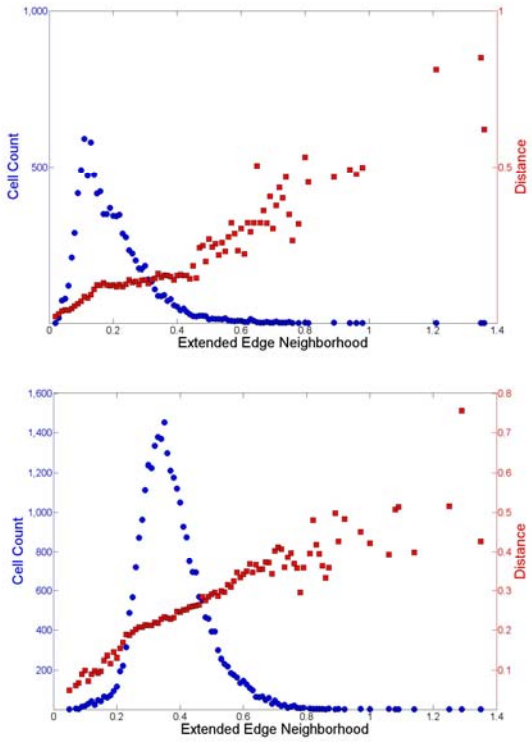

Figure 46. *Averaged segmentation distance (red) for the A10 cells (top) and 3T3 cells (bottom) along with a plot of cell numbers as a function of extended edge neighborhood (blue).*

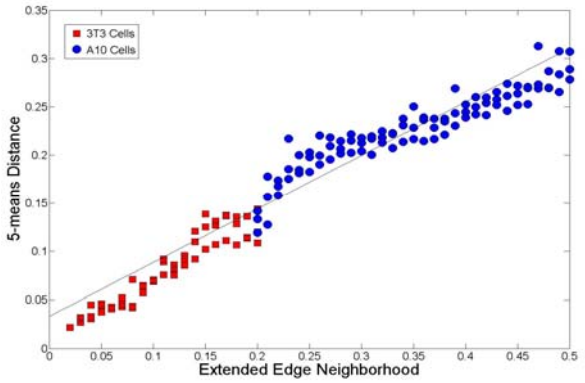

Figure 47. *Results from the A10 cells (red) and NIH3T3 cells (blue) fit to a straight line.*

from 0.02 to 0.2, and the NIH3T3 results in the extended edge region 0.2 to 0.5, where 90% of the cells from each cell line occur. Both of these data sets are fitted with a linear model, which is also plotted in Figure 47: predicted distance = 0.051 + EEN × 0.477, with a correlation coefficient of 0.9815.

From this large scale test, we define a method to pre-process images and determine their vulnerability to segmentation error. The accuracy possible from any segmentation technique is directly proportional to the extended edge neighborhood of each cell in an image. Future work will include tests on a wider variety of methods, as well as using the extended edge neighborhood concept to choose appropriate segmentation methods during large scale screening tests.

[1] A. Peskin, A. Dima, J. Chalfoun, and J. Elliot, Predicting Segmentation Accuracy for Biological Cell Images, in *The 6th International Symposium on Visual Computing 2010*, Las Vegas, NV, Nov. 22 - Dec. 1, 2010.

[2] A. L. Plant, J. T. Elliott, A. Tona, D. McDaniel, and K. J. Langenbach, Tools for Quantitative and Validated Measurements of Cells, *High Content Screening: A Powerful Approach to Systems Cell Biology and Drug Discovery. Humana Press*, (L. Taylor, K. Giuliano, and J. Haskins, eds.), Totowa (2006).

[3] A. Peskin, K. Kafadar, and A. Dima, A Quality Pre-Processor for Biological Cell Images in *Computational Bioimaging 2009, 5th International Symposium on Visual Computing*, Las Vegas, NV, Nov. 30 – Dec. 2, 2009.

[4] J. Chalfoun, A. Dima, A. Peskin , J. Elliot and J. Filliben, A Human Inspired Local Ratio-Based Algorithm for Edge Detection in Fluorescent Cell Images, in *The 6th International Symposium on Visual Computing 2010*, Las Vegas, NV, Nov. 22 – Dec. 1, 2010.

[5] A. Dima, J. Elliott, J. Filliben, M. Halter, A. Peskin, J. Bernal, B. Stottrup, M. Kociolek, M. Brady, H. Tang, A. Plant, Comparison of Segmentation Algorithms for Fluorescence Microscopy Images of Cells, submitted.

ITL Program: *Information Discovery, Use and Sharing*

Visualizing Fire and the Resulting Deformation of Structures

Pradeep Gaddam
Marc Olano
Judith Terrill
Dilip Banerjee (NIST EL)
John Gross (NIST EL)

http://www.nist.gov/itl/math/hpcvg/firedeformvis.cfm

We are collaborating with researchers in the NIST Engineering Laboratory (EL) to study the effects of fire on building structures to improve structural engineering and building safety. We are using a sequential process in which the EL Fire Dynamics Simulator (FDS) is used to simulate the start and propagation of fire in a room, after which a second code (heat transfer analysis) calculates how gas temperatures computed by FDS diffuses into the structural members. A third program takes the output of the second code and computes how the structure deforms over time due to combined effects of thermal and mechanical loads. We use a test case with a single beam in a room. We link the fire, thermal, and structural data with a separate real-time visualization capability that can be run on the desktop and in the NIST 3D immersive environment. This enables interactive analysis of the resulting data.

This year we integrated the data output from the three simulations into the analysis tools and performed validation on the results. We developed tools to interactively examine and visualize the scalars, vectors, and tensors output from the simulations. We created utilities to make fracture patterns in windows (see Figure 48), and calculate the dynamics of the glass shards blowing out using the Bullet Physics Engine.

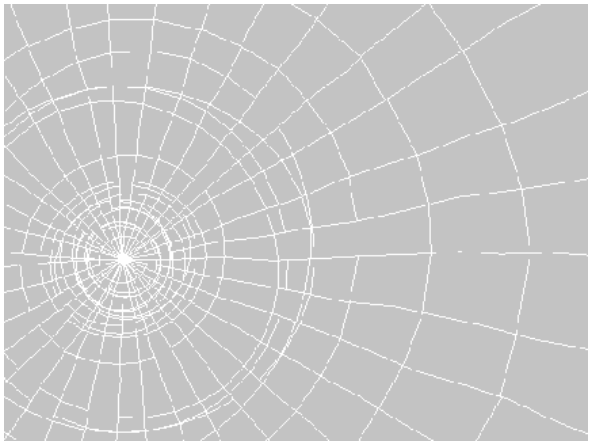

Figure 48. *Random fracture pattern in a glass window.*

In the coming year, we will be expanding the interface and adding additional visualization and analysis techniques.

[1] D. Banerjee, J. Gross, P. Reddy Gaddam, M. Olano, W. Hess, J. Terrill, T. Griffin, J. Hagedorn, J. Kelso, and S. Satterfield, "An Integrated Interactive Visualization and Analysis Environment to Study the Impact of Fire on Building Structures," in *Proceedings of SIGGRAPH'10*, ACM SIGGRAPH 2010 Posters, Los Angeles, CA, July 25-29, 2010, article 149 (1 page).

Measuring Errors in Polygonal Representations of Surfaces

John Hagedorn
Marc Olano
Judith Terrill

http://www.nist.gov/itl/math/hpcvg/psurferr.cfm

Surfaces are important in diverse scientific disciplines and the depiction of surfaces and interactions with them are important tasks in scientific visualization. In this context, we typically work with surface models that are approximations of the true surfaces that they represent. When surface representations are used to make decisions or to make quantitative assessments of properties of the underlying surfaces, it is critical to understand the errors inherent in the representations. The most common way of approximating surfaces is with sets of polygons. We have developed metrics for assessing how well these polygonal representations portray the underlying surfaces.

We look at three types of errors in polygonized surfaces: distance, surface area, and volume. For distance errors, we start by looking at a point on the polygonal representation and seeing how far away from the true surface that point lies. We can then assess the error over the entire surface by integrating over the surface. Surface area and volume errors are much simpler to assess. For surface area, we sum the areas of the polygons in the polygonal representation and compare with the true surface area of the underlying surface. Similarly, for closed polygonal representations, we can easily calculate the enclosed volume, which can be compared with the analytically determined volume.

We have implemented these error metrics in software and tested them on a variety of quadric surfaces. We polygonized each surface in several ways, either directly from the analytic definition of the surface or by creating a gridded data set and generating a polygonal isosurface. The isosurface polygonizations are intended (in some ways) to emulate an experimental situation, and in that vein we added various levels of noise to the gridded data sets. These methods can be applied to any surface type and any polygonization.

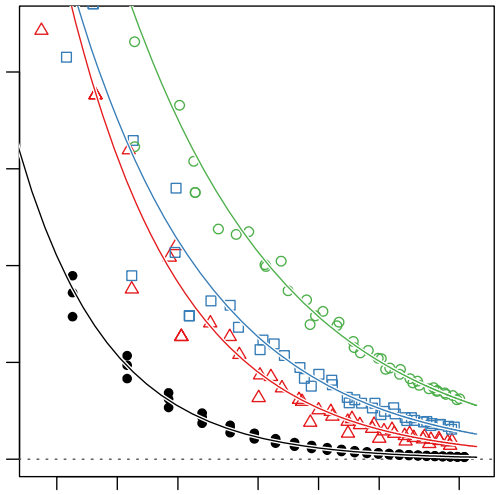

Figure 49. *Scatterplot of normalized mean distance error versus number of triangles for all polygonizations of the elliptic paraboloids. Data for each of the four polygonization schemes has been fitted and the resulting lines plotted.*

For each surface and each scheme, we tested polygonizations at progressively finer scales. The finer polygonizations have more polygons and are expected to more closely approximate the surfaces. The results of our tests enable us to quantify the errors of these polygonal representations relative to the underlying true surfaces. Furthermore, we see clear relationships between the measured errors and the number of triangles in a given approximation. These relationships can be modeled with simple formulas. Figure 49 shows a scatterplot of our normalized mean distance error metric versus the number of triangles for each of four polygonization schemes for elliptic paraboloids. This plot also shows the curves fit to the data.

Unlike the other statistics, the surface area error metric does not appear to tend to zero as the number of triangles increase in the presence of noise. By analyzing the marching cubes isosurface polygonization algorithm we were able to explain this limit behavior. The limits predicted by our analysis correspond closely to those calculated by fitting the error data.

Qualitatively our results are entirely expected; for example, coarser polygonizations have greater error. But these methods enable us to quantify this qualitative understanding. This quantitative understanding of error is critical as we apply other quantitative methods to these polygonal approximations of surfaces.

[1] J. Hagedorn, M. Olano, and J. Terrill, Measuring Errors in Polygonal Representations of Surfaces, in preparation.

ITL Program: *Virtual Measurement Systems*

Scientific Software

Modern science and engineering in general, and modern measurement science in particular require a wide variety of software tools for scientific discovery, exploration, and analysis. As scientific inquiry becomes deeper and more specialized, so must the supporting software tools. The goal of this work is to develop critical software tools that support measurement science at NIST, as well as computational science and engineering at large.

Micromagnetic Modeling

Michael Donahue
Donald Porter
Robert McMichael (NIST CNST)
June Lau (NIST MSEL)

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 CNST, MML, and PML, to improve the state-of-the-art in micromagnetic modeling.

Michael Donahue and Donald Porter in ACMD 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 has a modular structure that allows independent developers to contribute extensions that add to the basic functionality of OOMMF. OOMMF also provides a fully functional micromagnetic modeling system, handling both two and three-dimensional problems, with sophisticated extensible input and output mechanisms.

In FY 2010 alone, the software was downloaded more than 4,500 times, and use of OOMMF was acknowledged in more than 120 peer-reviewed journal articles. This year OOMMF also passed the milestone of more than 1,000 citations. OOMMF has become an invaluable tool in the magnetics research community.

Key recent developments in OOMMF include

- Focused development on measurement, analysis, and improvement of the performance of the new modules providing multi-threaded computation on multi-processor, multi-core computers, while maintaining the cross-platform nature of the code.
- Development of new techniques to compute the elements of the demagnetization tensor. Prior methods produced a loss of accuracy of six decimal digits per decade in the far field. New algebraic and asymptotic methods preserve at least ten decimal digits of accuracy at all distances.

Ongoing work includes extending parallelization to tens of processor cores on non-uniform memory access (NUMA) architectures, and evaluating various methods for modeling finite temperature effects, such as the Landau-Lifshitz-Bloch equation which adjusts the local effective saturation magnetization as a function of temperature and magnetic configuration.

OOMMF is part of a larger activity, the Micromagnetic Modeling Activity Group (μMAG), formed to address fundamental issues in micromagnetic modeling through two activities: the development of public domain reference software, and the definition and dissemination of standard problems for testing modeling software. MCSD staff members are involved in development of the standard problem suite as well. There are currently four standard problems in the suite, testing both static and dynamic magnetization properties. A new standard problem proposed jointly by several authors [1] aims at validation of simulations of spin momentum transfer in the "current parallel to plane" geometry. While testing the proposed problem, we discovered errors in the treatment of boundaries in the OOMMF module for computing spin momentum transfer. This discovery also highlighted the need to have a set of boundary condition assumptions specified in the problem itself. Work continues to develop additional standard problems to address the spin momentum transfer phenomenon in other geometries.

In addition to the continuing development of OOMMF, the project also does collaborative research using OOMMF. The project plays an instrumental role in the 2007 NIST Innovation in Measurement Science project (with CNST, MML and PML), "Magnetic nanostructures for post-CMOS electronics." We also provide modeling and simulation consultation for work in PML on spin momentum transfer. In collaboration with the University of Konstanz we have used OOMMF to study magnetic structures in nanowires. The ACMD micromagnetic project produced three

journal papers [2-4] and two conference presentations this past year.

[1] M. Najafi, et al., Proposal for a Standard Problem for Micromagnetic Simulations Including Spin-transfer Torque, *Journal of Applied Physics* **105** (2009), pp. 113914-113921.

[2] M. J. Donahue, Parallelizing a Micromagnetic Program for Use on Multi-processor Shared Memory Computers, *IEEE Transactions on Magnetics* **45** (2009), pp. 3923-3925.

[3] K. M. Lebecki and M. J. Donahue, Comment on 'Frustrated Magnetization in Co Nanowires: Competition between Crystal Anisotropy and Demagnetization Energy,' *Physical Review B* **82** (2010), article 096401 (4 pages).

[4] H. Min, R. D. McMichael, M. J. Donahue, J. Miltat, M. D. Stiles, Effects of Disorder and Internal Dynamics on Vortex Wall Propagation, *Physical Review Letters* **104** (2010), article 217201 (4 pages).

ITL Program: *Enabling Scientific Discovery*
ITL Program: *Virtual Measurement Systems*

OOF: Finite Element Analysis of Material Microstructures

Stephen A. Langer
Andrew C. E. Reid
Valerie R. Coffman
Gunay Dogan
Lingda Tang

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

The OOF Project, a collaboration between ACMD and MML, 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 or simulated 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.

OOF is currently being used in research at industrial, academic, and government laboratories and as a teaching tool in universities. Including all available versions, OOF2 was downloaded 1,683 times this year, a 40% increase from last year. The on-line version, available at Purdue's nanohub site for computational materials science, was run by 143 users.

During FY10 the OOF team concentrated on improving the nonlinear and time dependent solvers in the 2D program, OOF2, and on developing the 3D version, OOF3D. Issues addressed in the 2D code included: simultaneous solutions of static and time dependent equations; nonlinear versions of time stepping algorithms; time dependent boundary conditions; new user interfaces for time dependent problems; better status reporting; finite-element based image segmentation algorithms; new programming interfaces for material physics, with examples for users writing OOF extensions; nonlinear large strain elasticity; surface and interface physics; plasticity models; and new code governing multi-threaded execution and progress bars. All of these improvements will carry over into the 3D code. In addition, this year large portions of the 3D code were rewritten to improve speed and memory use, enabling OOF3D to create meshes on a scale suitable for research on realistic problems. Figure 50 shows a meshed sample of a 3D bone micrograph.

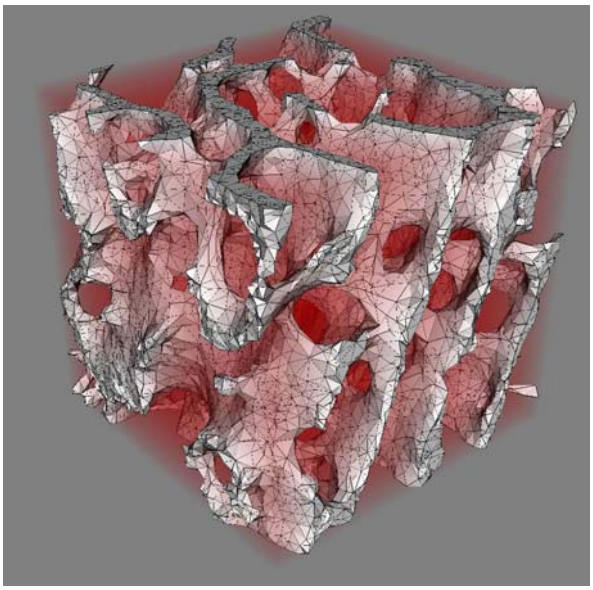

Figure 50. *A element finite element mesh created by OOF3D from a micrograph of trabecular bone. The micrograph consisted of 8,000,000 voxels, and the mesh contains 50,000 elements.*

OOF contains extensive test suites for both its internal workings and its graphical user interface. Maintaining compatibility with tests while adding features and fixing bugs helps to guarantee a quality product and avoid development delays.

Plans for FY 2011 include releasing OOF2 version 2.1 and a beta version of OOF3D, including work on parallelization, 3D image segmentation, plasticity, and merging the 2D and 3D code bases.

[1] V. R. Coffman, A. C. E Reid, S. A. Langer, and G. Dogan, OOF3D: An Image-based Finite-element Solver for Materials Science, in review.

ITL Program: *Enabling Scientific Discovery*

Parallel Adaptive Refinement and Multigrid Finite Element Methods

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Marjorie A. McClain
Eite Tiesinga (NIST PML)
Thomas Hanna (NIST PML)

http://math.nist.gov/phaml

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

This year the effort was focused on three areas. The first is a numerical experiment to study the effectiveness of several competing strategies for *hp*-adaptive refinement. This involves implementing these methods in PHAML, defining a set of test problems, and performing the computations. The second is the application of PHAML to solve the time-dependent Schrödinger Equation for eigenvalues and eigenstates relevant to optical traps for neutral atoms, in collaboration with the Quantum Processes Group of NIST's Atomic Physics Division. Understanding the interactions of adjacent atoms corresponding to qubits of a quantum gate involves computing multiple eigenvalues in the middle of the spectrum, with eigenstates that have sharp gradients, which is a very challenging computation. The third is the extension of PHAML to a different parallel paradigm, that of multicore computers, using OpenMP. This implementation can also be used in a hybrid MPI/OpenMP parallel paradigm on clusters of multicore computers.

The major accomplishments for FY 2010 are:

- Completion of the implementation of *hp*-adaptive strategies in PHAML.
- Performed computations and summary reports for 19 of the 23 test problems of the numerical experiment.
- Began implementation of a time-dependent model of two dipolar molecules held in a cylindrically symmetric trap.
- Modified PHAML to solve Schrödinger's equation with complex potentials.
- Began adding OpenMP directives to PHAML.

Future work will continue to enhance PHAML with additional capabilities and robustness, complete the experiment to compare the effectiveness of *hp*-adaptive strategies, used lessons learned from the experiment to design a more effective *hp*-adaptive strategy, complete the addition of OpenMP directives in PHAML, apply PHAML to a time-dependent model of two dipolar molecules held in a cylindrically symmetric trap, and perform further physics experiments using the code.

[1] W. F. Mitchell, The *hp*-Multigrid Method Applied to *hp*-Adaptive Refinement of Triangular Grids, *Numerical Linear Algebra with Applications* **17** (2010), pp. 211-228.

[2] W. F. Mitchell and M. A. McClain, A Survey of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations, *Annals of the European Academy of Sciences*, to appear.

[3] W. F. Mitchell, A Collection of 2D Elliptic Problems for Testing Adaptive Algorithms, NISTIR 7668 (2010).

[4] W. F. Mitchell, Some Computational Results with *hp*-Adaptive Refinement, SIAM Conference on Parallel Processing for Scientific Computing, February 2010.

[5] W. F. Mitchell, A Summary of *hp*-Adaptive Finite Element Strategies, Workshop on Adaptive Finite Elements and Domain Decomposition Methods, June, 2010 (invited talk).

[6] W. F. Mitchell, A Summary of *hp*-Adaptive Finite Element Strategies, 2nd European Seminar on Coupled Problems, June 2010 (plenary lecture).

ITL Program: *Enabling Scientific Discovery*

Variable Projection for Nonlinear Least Squares Problems

Dianne P. O'Leary
Bert W. Rust

Fitting a model to measured data is essential for discovering patterns and causality. Yet data fitting problems are often numerically challenging. In fitting exponential models, for example, small changes in the data can make large changes in parameter estimates. And data fitting problems are most often nonconvex, so a set of parameter estimates can be locally optimal without being globally optimal, and software can be fooled into accepting a suboptimal estimate.

We focus on fitting nonlinear models in a (weighted) least-squares sense. Most such models have some parameters that appear linearly. For example, in fitting a sum of two exponentials, the model for the data observations $y(t_1), \ldots, y(t_m)$ might be

$$y(t) \approx c_1 e^{\alpha_1 t} + c_2 e^{\alpha_2 t} \equiv \eta(\boldsymbol{\alpha}, \mathbf{c}, t).$$

The parameters $\mathbf{c} = [c_1, c_2]$ appear linearly, so for every choice of nonlinear parameters $\boldsymbol{\alpha} = [\alpha_1, \alpha_2]$, optimal estimates for $\mathbf{c}$ can be found by solving a *linear least-squares problem*. Consider the (full) nonlinear least-squares problem

$$\min_{\boldsymbol{\alpha},\mathbf{c}} \left\| y - \boldsymbol{\eta}(\boldsymbol{\alpha}, \mathbf{c}) \right\|_2^2 ,$$

where y_i is the observed value $y(t_i)$, and η_i is the model prediction at t_i. Then the solution to the full problem is the same as the solution to the reduced problem

$$\min_{\boldsymbol{\alpha}} \left\| y - \boldsymbol{\eta}(\boldsymbol{\alpha}, \mathbf{c}(\boldsymbol{\alpha})) \right\|_2^2 ,$$

where $\boldsymbol{\eta}(\boldsymbol{\alpha},\mathbf{c}(\boldsymbol{\alpha}))$ denotes the model predictions when, given $\boldsymbol{\alpha}$, we determine the parameters $\mathbf{c}$ optimally.

In 1973 Gene Golub and Victor Pereyra presented a *variable projection algorithm* based on the reduced problem, and this was subsequently used by John Bolstad in a Fortran program VARPRO. VARPRO also used some ideas of Linda Kaufman to speed up the computation of derivatives. The beauty of variable projection is that it reduces the number of parameters, thus improving efficiency, and possibly reducing the number of local minimizers. Convergence to the globally optimal solution is therefore more likely. But implementation of the idea is complicated because the derivative matrix for the reduced problem must be derived from that for the full problem.

The present work provides a 21st century sample implementation of the variable projection method that allows a more general problem formulation (i.e., with constraints on the parameters), more clearly identifies its key ingredients so that improvements can be made, and makes future implementations in other languages easy. This implementation, in Matlab, contains more than 400 lines of comments for fewer than 160 lines of code. We have used a high-quality (constrained) nonlinear least-squares algorithm to solve the reduced problem and a high-quality linear least-squares algorithm to determine the linear parameters. We have derived the derivative matrix for the reduced problem from sparse information for the full problem and shown that foregoing the Kaufman idea leads to better performance. Finally, our program computes statistical diagnostics for the estimate in order to help the user validate the computed parameters.

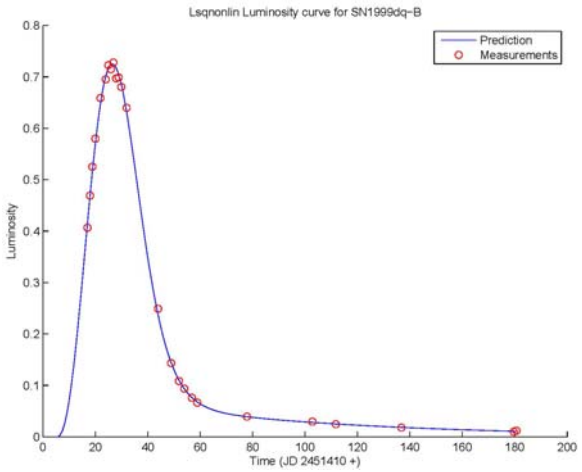

Figure 51. *The data fit for a supernova light curve.*

We validated our implementation on many test problems, comparing the results with those obtained from the Fortran version and from other standard software, and demonstrating enhanced robustness. One resulting fit to supernova light curve data is shown in Figure 51.

[1] B. W. Rust, D. P. O'Leary, and K. M. Mullen, "Modelling Type Ia Supernova Light Curves," in *Exponential Data Fitting and its Applications*, Victor Pereyra and Godela Scherer, eds., Bentham Electronic Books, 2010, pp. 145-164.

Digital Library of Mathematical Functions

The special functions of applied mathematics are fundamental tools enabling modeling and analysis in all areas of science and engineering. To make effective use of such functions, practitioners must have ready access to a reliable source of information on their properties. The goal of this work is the development and dissemination of definitive reference data on the special functions of applied mathematics. The centerpiece of this effort is the DLMF, a freely available interactive and richly linked online resource.

A Special Functions Handbook for the Digital Age

Frank Olver
Daniel Lozier
Charles Clark (NIST PML)
Ronald Boisvert
Bruce Miller
Bonita Saunders
Abdou Youssef
Marjorie McClain
Qiming Wang
Brian Antonishek (NIST ITL)

http://dlmf.nist.gov/

See feature article page 25.

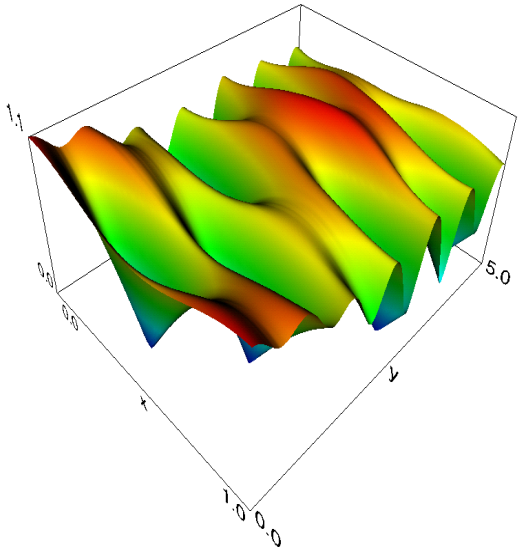

Figure 52. *Scaled Riemann theta function* $\hat{\theta}(x+iy,0\,|\,\Omega)$ *where* Ω *is a specially defined matrix.*

Visualization of Complex Functions Data

Bonita Saunders
Brian Antonishek (NIST ITL)
Qiming Wang
Sandy Ressler
Daniel Lozier
Frank Olver

A mathematical or physical scientist can gain useful information about the behavior of a complex function from the visualization of its data, but providing that visualization to a wide audience on the web presents many challenges. One must ensure the accuracy of both the data and plot, choose software to create the web visualization, find appropriate software for users to view the visualizations on various platforms, and monitor the performance of the software when operating systems or internet browsers are updated. Over the past few years we have tackled all of these problems and successfully created over 200 3D visualizations for the NIST Digital Library of Mathematical Functions (DLMF). Since the release of the DLMF this past May, we have concentrated on the update and maintenance of the visualizations.

Currently the visualizations are rendered using two common technologies for 3D graphics on the web: Virtual Reality Modeling Language (VRML) and X3D. Users may view the visualizations by downloading a free plugin. Numerous choices are available for Windows and Mac platforms, but fewer for Linux. We are making the changes needed to view our graphics files in the most widely used Linux operating systems. We are also attacking the portability problem from another direction by determining file modifications needed to view our files in a WebGL environment. HTML5 will contain WebGL attributes that allow users to view our visualizations inside a web page without the need of a special plugin. We have already successfully displayed simplified versions of our files in experimental HTML5 browsers.

We continue to make improvements to the features of the visualizations. Testing of new cutting plane software is in progress. The modifications will produce smoother cutting plane movement and more accurate cutting plane intersection curves for most visualizations. Improvements are also being made to the underlying grids on which the functions are computed to improve the surface color maps and further improve cutting plane accuracy.

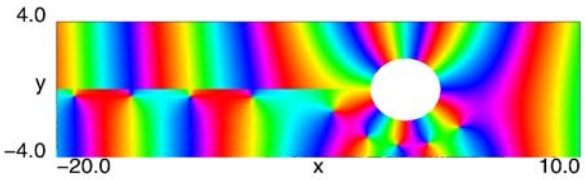

Figure 53. *Phase density plot of Hankel function* $H_5^{(1)}(x+iy)$.

Regular maintenance and testing of the visualizations is important not only because of problems that can arise from operating system and internet browser updates, but also because of VRML/X3D plugin updates. Hopefully this will become a fairly minor effort once we complete the changes needed for WebGL and stable HTML5 compatible browsers are released.

[1] B. Saunders and Q. Wang, "Tensor Product B-Spline Mesh Generation for Accurate Surface Visualization in the NIST Digital Library of Mathematical Functions", in *Mathematical Methods for Curves and Surfaces,* (M. Dæhlen, et al., eds.), Lecture Notes in Computer Science **5862** (2010), pp. 385-393..

[2] B. Saunders, Q. Wang, Tensor Product Grid Generation for Complex Surface Visualizations in a Digital Library of Mathematical Functions, in *Proceedings of the 11th International Society for Grid Generation (ISGG) Conference*, *Montreal Canada*, May 25-28, 2009, p. SV.3.

[3] Q. Wang , B. Saunders, and S. Ressler, Dissemination of 3D Visualizations of Complex Function Data for the NIST Digital Library of Mathematical Functions, *CODATA Data Science Journal* **6** (2007) pp. S146- S154.

[4] B. Saunders, Q. Wang, From B-Spline Mesh Generation to Effective Visualizations for the NIST Digital Library of Mathematical Functions, in *Curve and Surface Design: Avignon 2006,* Sixth International Conference on Curves and Surfaces, Avignon, France, Nashboro Press, 2007, pp. 235-243.

Mathematical Knowledge Management

Bruce Miller
Abdou Youssef (George Washington University)
Michael Kohlhase (Jacobs University, Germany)
Heinrich Stamerjohanns (Jacobs University, Germany)

Although the World Wide Web was originally created to distribute scientific documents, its rapid adoption for entertainment and commerce almost left the scientific community behind. While the web and electronic books are blossoming, assuring that scientific literature benefits from advanced communications technologies requires attention.

Knowledge management deals with the practices used to create, represent, distribute and find "knowledge"; *mathematical knowledge management* deals with the special aspects of *mathematical* knowledge. The special symbols and notations of mathematics create unique difficulties for authoring and delivery. In addition, the disconnect between the familiar notations ("presentation") and the underlying meaning ("semantics") inhibit reuse and accessibility. Each effect creates difficulties for both indexing and querying, making it hard to locate mathematical material.

In 1998 the Math Working Group[7] of the World Wide Web Consortium released Version 1 of the Mathematical Markup Language (MathML) specification. MathML provides a means for describing mathematics as a basis for machine to machine communication. In particular, it provides a foundation for the inclusion of mathematical expressions in Web pages. The adoption of MathML has been slow but steady. This last year has been a good one, however, with increased interest amongst browser developers, and more material appearing on the web — not least, of which is our own Digital Library of Mathematical Functions[8] (DLMF) which was released in May.

The working group released Version 3 of the MathML specification this last fall. Increased usage of MathML by publishers for educational materials demanded better coverage of elementary mathematical constructs such as long division and multiplication. Likewise, increased interest around the world called for support for use of mathematics in right-to-left languages such as Hebrew and Arabic, as well as for mathematics itself written right-to-left, as is done in some parts of the Arabic speaking world. Within the more theoretical communities, such as automated theorem proving, it was important to consolidate efforts towards representing the deeper semantics of mathematical material. Complete alignment of Content MathML, that subset specific to semantics, with the OpenMath standard[9] achieved this goal, as well as providing MathML with fully extensible semantics. These enhancements, along with many additional clarifications and corrections, were incorporated into the updated specification.

Developing the DLMF, forced us to face both authoring and publishing difficulties. The only feasible way to collect the material from the world's special functions experts was to accept it in LaTeX format. And yet, this material must be not only printed, but converted to XML and MathML for use on the web — a non-trivial task, given the complex and powerful nature of TeX. We thus developed LaTeXML as a tool to enable such conversions.

With such a system, a strategy for enriching the semantics of documents, as well as standardizing nota-

[7] http://www.w3.org/Math/
[8] http://dlmf.nist.gov/
[9] http://www.openmath.org/

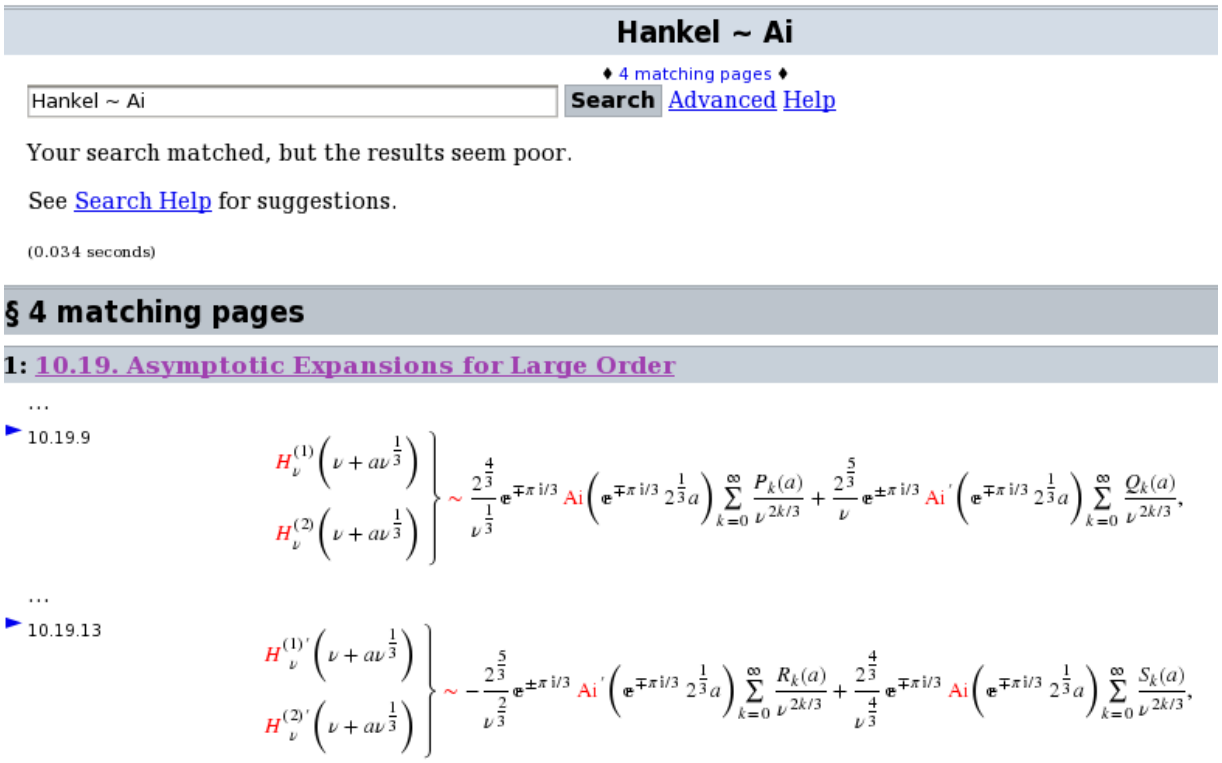

Figure 54. *A search result for a query with both semantic ("Hankel") and presentational ("Ai") terms. The result shows how query relaxation adjusts the query to match the material, as needed. Term highlighting is aided by indexing semantics in parallel to the presentation*

tions, was to develop and use semantic-oriented markup. In particular, to use markup that reflects the meaning of each function or operator, rather than just its appearance. Among other benefits, this technique generates a richer index from which mathematical searches can be carried out. A technique for conversion of mathematical structure and symbols into a flattened textual form allowed us to leverage a powerful text search engine to support mathematical search [1]. Figure 54 shows several such search features.

While LaTeXML was initially focused on the needs of the DLMF project, it was clear that such a tool had broader application. A research group at Jacobs University in Bremen, Germany, sought a large body of scientific literature in electronic format with which to carry out a variety of document processing experiments. They established a project to convert as much of the arXiv[10] as possible to MathML, and LaTeXML was used for this purpose. The arXiv is a large preprint collection hosted at Cornell University, where the documents are publicly available and almost all are written using LaTeX. A large number of LaTeX document styles and format files were prepared and a cluster of workstations was used to carry out document conversion [2]. Currently, over 500,000 documents have been processed with the conversion of 67% being of good quality.

Current and future work on LaTeXML aims to continue to increase its coverage of mathematics, but also to leverage the XML to various other uses, such as ePub, used in electronic books, or Daisy, an accessible document format. Improving the mathematics grammar along with inferring and enhancing the semantic content of documents is also a continuing goal.

[1] B. Miller and A. Youssef, Technical Aspects of the Digital Library of Mathematical Functions, *Annals of Mathematics and Artificial Intelligence* **38** (2003), pp. 121 -136.

[2] H. Stamerjohanns, M. Kohlhase, D. Ginev, C. David, and B. Miller, Transforming Large Collections of Scientific Publications to XML, *Mathematics in Computer Science* **3** (2010), pp. 299-307.

ITL Program: *Information Discovery, Use and Sharing*

[10] http://arxiv.org/

Math Table Generation Service

Daniel Lozier
Bruce Miller
Marjorie McClain
Bonita Saunders
Chris Schanzle
Annie Cuyt (University of Antwerp)
Stefan Becuwe (University of Antwerp)

Old-fashioned published tables have long been used to supply numerical values of elementary and selected special functions. In recent years these have been employed in numerical exploration, software validation, program debugging, algorithm construction, and graphics production. For example, it is known that the special function procedures in Mathematica were validated by comparison with the 1964 NBS Handbook of Mathematical Functions. More recently, in August 2010, a communication was received from Microsoft, which is developing a numerical library and needs assistance with validation of math functions in the library.

The purpose of our project, which we call the Live Tables Project (LTP), is to develop a website at NIST that provides 21st century tools to escape the severe limitations the old published tables: low precision, sparsity of arguments and parameters, lack of coverage of complex variables, and inability to accommodate definitional variations. It will allow users to specify (within reasonable limits) these attributes, and it will return values with an accuracy certification.

The LTP was initiated after the public release in May 2010 of the Digital Library of Mathematical Functions (DLMF). The first step was to identify sources of reliable software, that is, software that establishes an error bound, preferably a priori, together with each function value. A group at the University of Antwerp has developed just such a software package, using continued fractions as the main tool. This package covers a substantial subset of the functions in the DLMF. Prof. Dr. Cuyt and Dr. Becuwe visited NIST in October for intensive discussions, which resulted in an agreement to collaborate and an action plan for FY 2011. The plan calls for a prototype design for the user interface, web software, and computational engine to be completed by midyear, and for a prototype web service to be operational at the end of the year.

ITL Program: *Virtual Measurement Systems*

Quantum Information

An emerging discipline at the intersection of physics and computer science, quantum information science (QIS) is likely to revolutionize science and technology in the same way that lasers, electronics, and computers did in the 20th century. By encoding information into quantum states of matter, one can, in theory, exploit the seemingly strange and counter-intuitive behavior of quantum systems to enable phenomenal increases in information storage and processing capability, as well as communication channels with extremely high levels of security. Although many of the necessary physical manipulations of quantum states have been demonstrated experimentally, scaling these up to enable fully capable quantum computers remains a grand challenge. We are engaged in (a) theoretical studies to understand the true power of quantum computing, (b) collaborative efforts with the multi-laboratory experimental quantum science program at NIST to characterize and benchmark specific physical implementations of quantum information processing, and (c) the development and assessment of technologies for quantum communication.

Up-conversion Single Photon Detectors and their Application in Measurement Science

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See feature article, page 42.

ITL Program: *Quantum Information*

Quantum Computing Theory

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Our work on quantum computing theory aims to make quantum computers more robust given realistic resources, improve the efficiency of algorithms that take advantage of quantum physics, and obtain rigorous tests of the basic principles of quantum mechanics.

In previous years, we contributed several very efficient techniques for realizing quantum computations insensitive to unavoidable noise in the underlying quantum devices. One of these involved general strategies for obtaining high-quality encoded states by purification. We are now revisiting an instance of these purification strategies and applying it to the problem of preparing so-called magic states, which are states enabling universal quantum computing for information encoded in quantum error-correcting codes.

One proposal for optical quantum computation requires encoding the information of a two dimensional quantum bit into the continuous state space of an optical field. The proposal is attractive, because the encoded qubits can be manipulated fault-tolerantly and logic operations can be performed with only linear devices, squeezing, homodyne detection, and special input states. Unfortunately, we lack a practical method to prepare the encoded qubit states. In 2010 we developed a method to prepare these states by a scheme that uses optical Schrodinger cat states (such as those described in the "Quantum State Estimation Theory and Applications" project), homodyne measurements, and feed-forward. A description of this scheme was published in *Optics Letters*.

Some of the potentially most important applications of quantum computers are to search, optimization and physics simulation problems. Many quantum strategies for solving these problems are based on preparing special states. For example, many physics and optimization problems can be solved by making measurements of ground states for different physical systems. A powerful strategy for preparing the desired states is to start with a simple-to-prepare eigenstate of an operator and then "walk" it toward the desired state by following eigenstates of a path of operators. We have developed efficient strategies for walking along such paths [4]. One strategy can be applied even if little control is available, such as in proposed "analog"

quantum simulators. A more efficient strategy was designed for the case where universal quantum computing is possible. Both strategies are better and more reliable than conventional adiabatic strategies.

Quantum strategies can also be used to improve measurement accuracy beyond the so-called classical limit. In particular, it may be possible to improve the accuracy of the quantum logic clocks under development in the ion storage group by taking advantage of quantum correlations among two or more ions. We are investigating the application of semidefinite programming techniques originally developed for optimizing quantum query algorithms. These techniques can determine the optimal strategy for measuring the frequency of a clock transition in ion qubits. Unlike previous work, we are taking into consideration the fact that the frequency is already known within a narrow range, and that phase noise in the classical oscillator driving the clock contributes to frequency noise. The goal is to determine how much improvement is possible with the use of two correlated versus two independent ions in the quantum logic clocks.

A goal of the quantum optics community is to realize a "loop-hole free" test for the absence of a locally-realistic explanation of quantum mechanical measurements. The biggest hurdle at present is the absence of sufficiently low-loss optical elements. Additional problems are that experiments so far rarely account for drifts and dependencies. Furthermore, the results of a test are usually reported in the form of "number of standard deviations of violation" of a Bell inequality. We have found that this leads to over-optimistic estimates of the confidence of rejecting local realism. We have developed a prediction based ratio test that works even in the presence of experimental drifts and dependencies while being asymptotically optimal for ideal experiments. The test reports a provable significance level for rejecting local realism and can be used for on-line monitoring of experimental progress. We are planning on releasing code implementing the test.

[1] E. Knill, News and Views Q&A: Quantum Computing, *Nature* **463** (Jan. 2010), pp. 441-443.

[2] H. M. Vasconcelos, L. Sanz, and S. Glancy, All-optical Generation of States for Encoding a Qubit in an Oscillator, *Optics Lett*ers **35** 2010, pp. 3261-3263.

[3] Y. Zhang, E. Knill, and S. Glancy, Statistical Strength of Experiments to Reject Local Realism with Photon Pairs and Inefficient Detectors, *Physical Review A* **81** (March 2010), 032117.

[4] S. Boixo, E. Knill, and R. Somma, Fast Quantum Algorithms for Traversing Paths of Eigenstates, submitted.

ITL Program: *Quantum Information*

Quantum Computing Benchmarks

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Dietrich Leibfried (NIST PML)
David Wineland (NIST PML)

Today, researchers claim to be able to quantum computing with two or more qubits with ions, atoms, superconducting circuits, impurities in diamond, nuclear spins and photons. But how can we compare experimental results from such a diverse collection of physical systems? Which ones have demonstrated the most accurate computations? Can we quantify the "amount" of computation performed? The quantum computing benchmark project aims to answer these questions and to establish standardized sets of experiments to quantify the answers in a device independent way. We collaborate with experimental groups to implement the proposed experiments.

Our most successful benchmark so far is a randomized benchmarking strategy for determining the effective error probability per gate (EPG) for physical qubits. Previously, we have standardized the strategy for one qubit and implemented it with ion qubits, demonstrating a good EPG of about 0.005. The benchmark has now been implemented by others with nuclear spin, superconducting and atomic qubits. We are in the process of demonstrating better EPGs with other ion qubits being developed in the ion storage group. We are collaborating with the quantum dot group at Stanford to implement the benchmark with their very fast one-qubit gates. Although the basic benchmarking strategy is the same, we have greatly improved the toolkit used for generating and analyzing the benchmark. It is easily adaptable to a wide variety of qubits.

Although the randomized benchmark is a very effective way to determine EPGs, as originally conceived, it was not a good diagnostic tool. We are improving the analysis of data from such benchmarks to back out more information about the individual gate errors. Eventually such information might be useful for optimizing strategies for error correction.

Another important ongoing research track is to establish straightforward and equally device independent benchmarking strategies for multiple qubits. The difficulty is that for more than one qubit the number of possible ways in which gates can be randomized increases greatly, making standardization and comparison less obvious. We are pursuing several strategies for comparing experiments using different randomization strategies based on a small number of quantitative measures.

ITL Program: *Quantum Information*

Quantum State Estimation Theory and Applications

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Gene Hilton (NIST PML)
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Adriana Lita (NIST PML)
Alan Migdall (NIST PML)
Richard Mirin (NIST PML)
Sae Woo Nam (NIST PML)
Leila Vale (NIST PML)
Manuel A. Castellanos-Beltran (Yale University)
Tracy Clement (University of Colorado)
Hsiang S. Ku (University of Colorado)
Francois Mallet (University of Colorado)
Aaron Miller (Albion College)

Many emerging technologies will exploit quantum mechanical effects to enhance metrology, computation, and communication. Developing these technologies requires improved methods to measure the state of quantum systems. Quantum state estimation is a statistical problem of estimating an underlying quantum state using a collection of measurements made on independently prepared copies of the state. Accurate quantum state estimation allows experimentalists to answer the questions "What quantum state does my device prepare?" and "How confident am I that it has prepared that state?" In the last year we have made a few small improvements to the algorithms used to answer these questions. We implemented a new strategy for choosing the step size of the iterative algorithm used to infer the quantum state. We also explored a new method to associate confidence intervals to the results of quantum state estimation based on the ability of the estimate to predict the results of an independent set of measurements.

We have been applying quantum state estimation in two experiments. The first of these is an experiment to prepare Schrödinger cat states of light, which is part of the NIST Innovations in Measurement Science project "Quantum Optical Metrology with N-Photons". This experiment uses high efficiency transition edge sensors to subtract three photons from a pulse of squeezed vacuum light. The photon subtraction prepares the Schrodinger cat state, which is measured by homodyne detection. Our quantum state estimation software is used to reconstruct the state from the measurements. Our state estimation algorithm corrects for the photon loss and electronic noise of the homodyne detector to infer the originally created state. The state created in the laboratory has a fidelity of 59^{+4}_{-14} % with an ideal Schrodinger cat state and had a mean of $2.75^{+0.06}_{-0.24}$ photons. This work was published in *Physical Review A* and received some attention in the popular press.

The second experiment where we have been applying quantum state estimation is the DARPA funded collaboration with JILA titled "Analog Quantum Integrated Circuits". The goal of this project is to create entangled states in superconducting microwave circuits and to use that entanglement for quantum teleportation. In 2010 we successfully prepared a squeezed state of quantum microwaves and verified the squeezing with full quantum state tomography, which has never been done before in a microwave system. Our analysis shows that the squeezed state's noise is reduced to 48^{+45}_{-19}% of the noise present in the vacuum. In the next phase of this project we will use two squeezed states to create entanglement between two microwave modes.

[1] T. Gerrits, S. Glancy, T. Clement, B. Calkins, A. Lita, A. Miller, A. Migdall, S.W. Nam, and R. Mirin, Generation of Optical Coherent-state Superpositions by Number-resolved Photon Subtraction from the Squeezed Vacuum, *Physical Review A* **82** (2010), 031802(R).

[2] Research Highlights: Quantum Information Coherent-state Superposition, *Nature Photonics* **4** (2010), pp. 804–805.

[3] F. Mallet, M. A. Castellanos-Beltran, H. S. Ku, S. Glancy, E. Knill, K. D. Irwin, G. C. Hilton, L. R. Vale, and K. W. Lehnert, Quantum State Tomography of an Itinerant Squeezed Microwave Field, arXiv:1012.0007v1 [quant-ph], in review.

ITL Program: *Quantum Information*

Quantum Communication

Alan Mink
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Joshua Bienfang (NIST PML)

We negotiated an agreement for NIST to partner with Telcordia that allows NIST to participate in the development of QKD standards that are currently being managed through the European Telecommunications Standards Institute (ETSI). Normally NIST is not able to participate in groups such as ETSI, because they are governed under European law. But by partnering with an existing ETSI member, Telcordia (a U.S. based company), NIST is able to participate without obligation to European law. Although ETSI normally focuses on European standards, the expertise in this area is too small to support multiple standards groups. So the ETSI QKD group is now a worldwide effort with rep-

resentatives from North America and Asia as well and interest from Africa (South Africa).

NIST has attended the three ETSI/QKD meetings in Europe during 2010 and reviewed all draft documents. NIST was instrumental in drafting the QKD "Application Interface" document, which specifies the interface between security applications and a QKD system and is based on the NIST QKD approach. This document has been recently approved as an ETSI standard. This standard neatly dovetails with a pending IETF RFC for the IPsec security protocol using QKD keys. NIST has become a principal contributor to this ETSI QKD group.

For the high-speed data handling part of our quantum communications project, we have developed and tested an entangled photon pair measurement system and an associated signal interface to our entangled photon generation system. This repurposing of our high-speed instrumentation will allow continuous measurement of our correlated and entangled photon generation experiments. We have also redesigned our newer high-speed instrumentation for 2.5 GHz operations on our current hardware, twice the previous speed. That design is now running in our lab. This design incorporates the complete QKD protocol in hardware, entirely freeing CPU cycles for supporting applications rather than running the error correction and privacy amplification portions of the QKD protocol – a set of very CPU cycle demanding algorithms. We will be using this higher speed hardware in a pending experiment with the NIST Physical Measurement Lab for a free-space QKD system. We continue to investigate some alternative photon measurement techniques, that will achieve 100 ps time-bin resolution and possibly as low as 25 ps.

[1] Mink, L. Ma, B. Hershman and X. Tang, An Application of Quantum Networks for Secure Video Surveillance, in *Video Surveillance* I-TECH Education and Publishing, Vienna, Austria, to appear.

ITL Program: *Quantum Information*

Foundations of Measurement Science for Information Systems

Modern information systems are astounding in their complexity. Software applications are built from thousands of interacting components. Computer networks interconnect millions of independently operating nodes. Large-scale networked applications provide the basis for services of national scope, such as financial transactions and electrical power distribution. In spite of our increasing reliance on such systems, our ability to build far outpaces our ability to secure. Protocols controlling the behavior of individual nodes lead to unexpected macroscopic behavior. Local power anomalies propagate in unexpected ways leading to large-scale outages. Computer system vulnerabilities are exploited in viral attacks resulting in widespread loss of data and system availability. The long term stability of our critical infrastructure is simply unknown. Measurement science has long provided a basis for the understanding and control of physical systems. Similar types of deep understanding and insight are lacking for complex information systems. We seek to develop the mathematical foundations needed for the emergence of a true measurement science for complex networked information systems.

Monte Carlo Methods for Computing Network Reliability

Isabel Beichl
Brian Cloteaux
Francis Sullivan (IDA Center for Computing Sciences)

See feature article, page 40.

ITL Program: *Complex Systems*

Modeling Affiliations in Networks

Brian D. Cloteaux

Many networks can be naturally represented as relationships between entities and the groups (or *affiliations*) to which the entities belong. An affiliation network is a bipartite graph which links the set of entities in a network to the set of groups. An example of a network and its associated affiliation network is shown in Figure 55.

We are currently researching new methods to extract and analyze affiliations in arbitrary networks. One purpose of this research is to be able to better classify network structure and to understand how a network's affiliations affects its characteristics, such as reliability and security. Understanding affiliations also has applications to national security.

Currently, we have developed new methods to mine the affiliations associated with a network, and, in particular, when there are missing links in the network. Links can be missing because of measurement error or purposeful obfuscation; but in either case, incomplete information can dramatically alter the structure of the affiliations. In a recent result, we have implemented a new method for finding affiliations associated with a network even when there are some missing links. In our method, we collect the possible affiliations using a relaxed definition for the network. Then we process those collected affiliations to minimize the size of the set while still being consistent with the information in the original network. We have tested our method on a number of synthetic networks, and are now extending our research to analyze real networks.

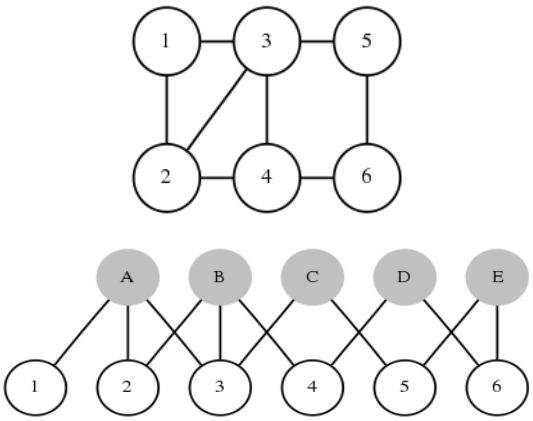

Figure 55. *A example network (top) and an associated affiliation network (bottom).*

ITL Program: *Complex Systems*

Community and Cluster Detection in Network Graphs

Roldan Pozo
Clement Rey

Detecting meaningful community structure in large graphs is one of the fundamental challenges in network science. This line of research can be critical in revealing the underlying structure of complex graphs. A

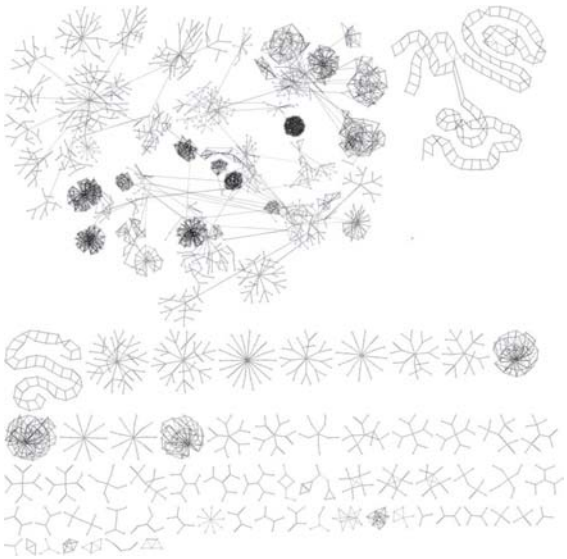

Figure 57. *Isolation profiles of the math.nist.gov webgraph.*

community is loosely defined as a subset of nodes which are highly connected to each other, but less connected to nodes in the remaining graph. Identifying such node groups is important in understanding graph evolution, synchronization, and the dynamics of networks. In various application contexts community detection can classify customers with similar purchasing habits, model the spreading of infectious diseases, help identify crime cells, and determine graph layouts for visualization.

Extracting such structure reliably from large-scale networks, however, is a difficult problem. First, one must devise a metric for what constitutes a graph community; secondly, an algorithm for finding such communities must be prescribed (some such problems are NP-complete); lastly, there must be some method of verifying that the computed groups are indeed meaningful. Various metrics have been proposed and several corresponding algorithms have been introduced in the literature.

The underlying question remains: how well do these approaches work in practice? So far, there has been little work in verifying and validating the results on a wide array of application domains. We aim to do this. As part of this study, we are currently investigating eigenvalue-based methods and fast greedy algorithm approaches which run in $O(n \log^2 n)$ for sparse graphs, and studying their behavior on specific data sets for which we have detailed community information available. The results show that current state-of-the-art algorithms work well in some situations, such as when vertices clearly belong to one (and only one) community. But the real world is not so ideal. More complicated approaches allow for overlapping communities, but fundamental problems remain. For example, one issue with modularity-based approaches is the difficulty of correctly identifying small clusters. (This is referred to as the "resolution limit" in the literature, and is an artifact of using a random graph with similar degree distribution as the null model.)

As an alternative approach, we have been investigating a different notion of "community" which does not fit previous methodologies but nonetheless provides interesting insights. Rather than being based on conventional graph cuts, this approach builds "cells" or "clusters" from the ground up by isolating low-degree nodes into a separate subgraph and analyzing the connectedness of the resulting network. That is, given a degree threshold, we create a subgraph consisting of only nodes with that degree value or less. This subgraph is largely fragmented into disconnected components, which can be useful in finding small, isolated fringe groups amidst the noise of large-degree hubs.

Figure 57, for example, shows the fragments of a web network (math.nist.gov) obtained by restricting it to a subgraph of nodes with degree 30 or less. It reveals various components: e.g. DNA-like ladders, as well as star and cluster patterns representing tightly coupled web pages. These form the nucleus of graph communities, and by varying the degree parameter we can direct the size and granularity of communities revealed. This information can be used to augment a conventional algorithm to better identify small communities.

We are expanding this line of investigation by asking the question of what happens as one varies the degree parameter in this experiment. At a low degree threshold (near 1) we get a small fragmented graph of either isolated nodes, or individual pairs of nodes. (These usually represent terminal nodes.) As we increase this value, we include more nodes in the subgraph, increasing the number of communities, but some of these communities increase in size and merge with others, thus effecting a contraction. As the threshold is increased to the maximum degree, we are left with a single community: the whole graph. Thus, as

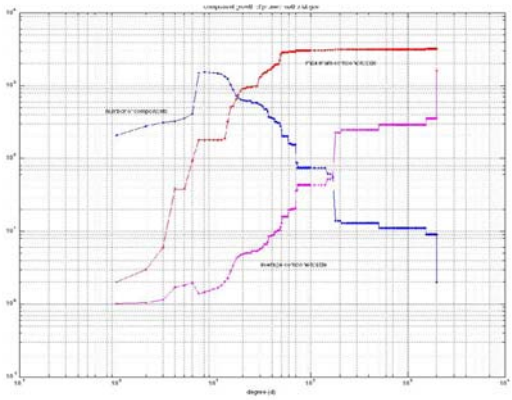

Figure 56. *Isolated communities of nodes with degree 30 or less of the webgraph of http:// math.nist.gov/.*

one turns the degree-threshold parameter, the number of components (communities) starts out small, grows, and finally shrinks down to one. A graph of this phenomenon is shown in Figure 56, which we refer to as a graph isolation profile. This profile provides a characteristic fingerprint of the graph structure that is different from conventional community metrics. We are currently investigating these ideas to develop hybrid metrics which better describe the nature of community structure in graphs.

ITL Program: *Complex Systems*

Network Modeling Toolkit

Brian Cloteaux

Over the past two years, in our research into the measurement and characterization of networks, we have produced a number of new algorithms. In an effort to release this research to the public in a usable form, we are integrating the various versions of our algorithms into a software package for network modeling. We have entitled this the Network Modeling Toolkit.

In the current version, we have implemented several network generating algorithms that create models with constraints such as s-metric or clustering coefficient value. In addition, we are able to build network models which contain a pre-defined subgraph. We also have code to measure certain characteristics of a given network such as number of spanning trees and s-metric and we are able to manipulate degree sequences such as finding the closest graphical sequence to a given non-graphical sequence. We continue to work in adding support for analysis of affiliation networks and to prepare the code base for a release. Accompanying this release will be a paper describing the system and a website for maintaining the code base.

ITL Program: *Complex Systems*

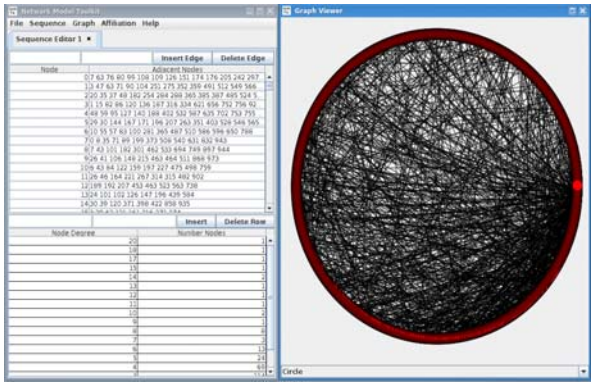

Figure 58. *A display from the Network Modeling Toolkit.*

Network Security Risk Analysis Using Attack Graphs [11]

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Lingyu Wang (Concordia University)
Sushil Jajodia (George Mason University)
Steven Noel (George Mason University)
Duminda Wijesekera (George Mason University)

At present, computer networks constitute the core component of information technology infrastructures in areas such as power grids, financial data systems and emergency communication systems. Protection of these networks from malicious intrusions is critical to the economy and security of our nation. To improve the security of these networked systems, it is necessary to measure the amount of security provided by different network configurations. The objective of our research is to develop a standard model for measuring the security of computer networks. A standard model will enable us to answer questions such as "are we more secure today than yesterday" or "how does the security of one network configuration compare with another one." Also, having a standard model to measure network security will bring together users, vendors and researchers to evaluate methodologies and products for network security.

Good metrics should be measured consistently, be inexpensive to collect, be expressed numerically, have units of measure, and have specific context. We meet this challenge by capturing vulnerability interdependencies among nodes in a network and measuring security in the same way as real attackers do in penetrating the network. Our methodology for security risk analysis is based on the model of attack graphs [3]. We analyze all attack paths through a network, providing a probabilistic metric of the overall system risk. Through this metric, we analyze tradeoffs between security costs and security benefits. Our metric is consistent, unambiguous, and provides context for understanding the security risk of computer networks.

In FY 2010, we developed a new model of security analysis for "zero day" attacks. We proposed a novel security metric called *k zero day safety,* based on the number of unknown zero day vulnerabilities [2]. The metric counts how many (unknown) vulnerabilities would be required to compromise a particular network asset. We also did performance analyses to understand how our method will scale up for enterprise networks consisting of multiple hosts.

In FY 2010, we also developed an ontology for enterprise level security in terms of the entities and relationships among them [1]. This data model can be used to measure the appropriate things needed to un-

[11] This research performed in the ITL Computer Security Division was supported by ACMD funding.

derstand the effectiveness of current security mechanisms and the benefits that they provide.

Numerous papers were published in conferences and workshops based on this work. In FY 2011, we plan to integrate the proposed techniques into existing attack graph based security tools and validate our results. We also plan to make progress on implementation of ontologies for enterprise level security using the Web Ontology Language (OWL).

[1] A. Singhal and D. Wijesekera, Ontologies for Modeling Enterprise Level Security Metrics, in *Proceedings of the Sixth Annual Cyber Security and Information Intelligence Research Workshop (CSIRW'10)*, Oak Ridge National Laboratory, April 21-23, 2010.

[2] L. Wang, A. Singhal, S. Jajodia, S. Noel, k-Zero Day Safety: Measuring the Security of Networks against Unknown Attacks, in *Computer Security – ESORICS 2010*, (D. Gritzalis, B. Preneel, and M. Theoharidou, eds.), Lecture Notes in Computer Science **6345** (2010), Springer, pp. 573-587.

[3] S. Noel, L. Wang, A. Singhal, S. Jajodia, Measuring Security Risk of Networks Using Attack Graphs, *International Journal of Next Generation Computing* **1** (2010).

Vulnerability of Selfish Routing to Attacks

Vladimir Marbukh
Daniel Genin (NIST ITL)
Anastase Nakassis NIST ITL)

An emergent trend in networking is an attempt to resolve inefficiencies of network-defined routing by shifting responsibility for routing from the network to end users. Examples include so-called source routing or overlay routing. Despite the emerging understanding that user-defined routing is much better in addressing specific user concerns, the downside may be the inherent selfish nature of user-centric routing, in which each user attempts to optimize its own performance objective without concern for overall network performance. This selfishness may, in fact, lead to loss in overall network performance.

While the performance limits of network-defined routing can be assessed by using optimization techniques, the performance of selfish routing is typically identified with a Nash equilibrium in a corresponding non-cooperative game-theoretic model. Due to the typical multiplicity of Nash equilibria, loss in overall network performance resulting from user selfishness is defined by the so-called price of anarchy: the worst-case ratio of the aggregate cost of selfish and socially optimal routing. This definition assumes that the network-defined socially optimal routing minimizes aggregate routing cost, and thus the price of anarchy always exceeds or equals one.

This project attempts to gain understanding of the effect of an adversarial presence, i.e., attacker(s), on the performance of selfish routing. To this end we extend the conventional framework for performance evaluation of selfish routing by including a possibility of attacker(s) capable of manipulating the route costs in attempt to maximize the aggregate transportation cost for all or some users. For example, an attacker might damage the physical infrastructure in a transportation network, insert malicious traffic in a denial of service attack on a communication network, or jam links in a wireless network. We propose an extended game-theoretic model, where strategic attacker(s) are modeled as separate agent(s) with the corresponding utilities and limits on ability to manipulate route costs reflecting attacker power.

Previous work on the effect of malicious agents on selfish routing by legitimate users assumed that neither attackers nor legitimate users have an "agility advantage", i.e., they operate on the same time scale. The corresponding loss in performance, called "price of malice" was calculated based on the worst-case scenario Nash equilibrium of the corresponding game. The key difference between these previously studied models and our model [1] is that we assume "agile" adversaries capable of observing and exploiting strategies employed by the legitimate agents. To investigate the effect of this agility we consider a Stackelberg game with legitimate user(s) being the leader(s) and attacker(s) being the follower(s).

Quite surprisingly, our initial results [1] indicate that an agile attacker of very limited power can inflict significant damage on overall network performance. The reason for this disproportional effect is that an adversarial presence creates incentive for selfish users to avoid being attacked by making other users more appealing targets for attacker(s). This incentive may create positive feedback eliminating the socially optimal equilibrium and driving selfish users to a very inefficient equilibrium. Also, the presence of attacker(s) can make Braess's paradox[12] more pronounced.

These initial results demonstrate the importance of further research on the effect of adversarial actions on selfish routing, including the possibility of mitigating this effect while preserving the distributed nature of resource allocation. One of the issues currently under investigation is developing a tractable model of at-

[12] Braess's paradox states that adding additional capacity to a network can sometimes actually decrease performance if network routing is based on the selfish choices of users.

tacker(s) with controlled agility relative to legitimate users. This model would provide an opportunity to investigate the effect of the attacker(s) ability to acquire and exploit system information on system performance. Our initial results suggest that such a model should be interdisciplinary, combining elements of both game and information theories.

[1] D. Genin, V. Marbukh, and A. Nakassis, Vulnerability of Selfish Routing to Attacks: A Game-theoretic Model and Initial Results, in *Proceedings of 2010 International Conference of Information Security and Internet Engineering*, World Congress on Engineering 2010 (WCE 2010), June 30, 2010.

Analysis of a Distributed Protocol for a Multiple User Access Network

Fern Y. Hunt
Vladimir Marbukh

Congestion control is critical to the smooth functioning of modern communication networks in particular and the Internet in general. The goal of a congestion protocol is to allow many users to share network resources without overloading the system. In addition it is desirable to use as much of the available network capacity as possible while ensuring fairness in the allocation of bandwidth. It was first shown by Frank Kelly and later by many others that these objectives can be achieved by protocols that are based on solving a global optimization problem for maximizing system utility, where some notion of fairness is expressed by a choice of utility function. The implication is that the operation of a protocol can be characterized and studied mathematically by analyzing the dynamics of a distributed algorithm for solving the optimization problem. As the need for system robustness has grown amidst cybersecurity concerns, this paradigm has been extended to the problem of designing and characterizing protocols that control routing as well as congestion.

Recently Hunt and Marbukh analyzed a protocol for allocating traffic that assigns routes randomly to users with prescribed path diversity. The entropy of the distribution of routes defined by an allocation is introduced in the corresponding utility maximization problem as a constraint so that users cannot use a single cheapest route as in the OSPF (open shortest path first) allocation. Introducing this feature reduces the risk of instability that arises in the uncontrolled use of this protocol. In previous work on example networks with a single source and destination [2, 3], we showed that maximum utility could be achieved with an allocation of traffic that minimizes the mean route cost. In that work we analyzed the dynamics of the prices of constituent links that make up the routes.

This year we extended our work to a network topology with multiple and possibly large numbers of sources with a single destination. Such a topology could model multiple users (each associated with a source) accessing a single trunk line. Each source has two possible routes, a direct link to the destination and a second route that employs links connecting to its nearest neighbor. To aid the tractability of the problem, route allocations for each source are assumed to be fixed in time but, as in our previous work, we associate a distribution entropy with this allocation.

Some justification for fixing the allocations can be made based on our work on a two link topology. For an arbitrary number of users we find sufficient conditions for the existence and uniqueness of an optimal solution and global convergence of the algorithm. The optimal utility of a source depends in general on the choice of entropies of all the sources and the capacities of the links joining them. Of interest is the behavior of the optimal utility as a function of the source entropies. For example when all the source entropies are the same some rather surprising results are observed numerically. Depending on the value of the entropy, the source utilities are heterogeneous or homogeneous. In the heterogeneous case, the utilities break up into clusters depending on their position in a circular network. At a critical value of the entropy, the utilities collapse into a single utility curve, as if the network collapsed into a single source and destination. This phenomenon seems to be independent of the number of sources [1]. Gaining better understanding of this transition is our current focus

Future work will center on developing ways of measuring the overall performance of a network under various route allocation regimes by calculating the total optimal system utility as a function of the allocation entropy.

[1] F.Y. Hunt and V. Marbukh, A Mathematical Model of Congestion Control with Multiple Sources, Dynamics Days Conference 2010, Bristol, UK, September 2010.

[2] F.Y. Hunt and V. Marbukh, A Model of Joint Congestion Control and Routing Through Random Assignment of Paths, NISTIR 7590, February 2010.

[3] F.Y. Hunt and V. Marbukh, Measuring the Utility/Path Diversity Trade-Off in Multipath Protocols, in *Proceedings of the 4th International Conference on Performance Evaluation Methodologies and Tools*, Pisa, Italy, 2009.

ITL Program: *Complex Systems*

Modeling Failure Scenarios in Large Scale Computing Systems

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In recent years, the advent of large-scale distributed systems such as computing grids and cloud systems has made mass computing services available to large populations of users. These systems are dynamic, heterogeneous and, due to the interactions of many components, subject to the emergence of unpredictable system-wide behaviors that can have deleterious consequences. Their rapid growth and increasing economic importance underline the need for tools and methodologies that enable understanding and prediction of complex system behavior in order to insure the availability and reliability of these services. Key questions are the effect of changes in workload, system design, and other operational parameters on overall system performance. For example, studies of alternative economic strategies and system failure scenarios have shown that small variations in system parameters can lead to large differences in performance (see references in [1]).

By large scale simulation we mean discrete event simulations that follow in detail the various stages encountered by an individual task being processed by a system over time. While large-scale simulations used in such studies are more practical than operational testbeds, computational expense rises dramatically with model size, a critical roadblock to investigation of dynamical behavior in large scale systems.

To address this situation, we introduced in earlier work [3] a succinct Markov chain representation of the dynamics of a large scale grid system over time. The chain simulates the progress of a large number of computing tasks from the time they are submitted by users to the time they either complete or fail. The evolution of the Markov chain itself occurs in discrete time through a set of transition probability matrices (TPMs). Each TPM simulates the grid system over a distinct time period, and thus the Markov chain is piece-wise homogeneous. Changes in system parameters can be modeled by perturbing the TPMs of the Markov chain. The corresponding sample paths are altered and represent altered system execution paths that arise as a result of perturbed parameters [3].

Through systematic perturbation of the TPM matrices followed by simulation of the resulting perturbed Markov chain we were able to identify scenarios that led to degradations of system performance and system-wide failure. Our results compared very favorably with large scale simulation results while being obtained with a substantial reduction in computational cost (hours vs. weeks of simulation) [3]. Nevertheless, as the number of states of the Markov chain grows, the computational cost of this method significantly increases. Thus it is very difficult to quickly identify the set of perturbed TPMs that lead to system deterioration or failure when the number of states is large. Prediction and control of these systems will depend on the ability discover such scenarios quickly. This is the motivation of the work that is described in the report [1].

This paper summarizes our work on graph theory and Markov chain methods for discovering perturbations in operational parameters that lead to decreases in system performance and system failure. They are based on efficiently identifying cut sets in the graph of the Markov Chain on the one hand, and use of the spectral representation theorem and properties of the absorbing Markov Chain on the other. See [1] for more detailed discussion and derivation of our method.

Our contribution based on the spectral properties of the Markov Chain is in two parts. The first is a method for quickly generating the time course of a key variable of the system, the proportion of tasks completed for arbitrary system parameters. The second is a method for measuring the effect of perturbations on the spectral properties of the matrices associated with the Markov chain. Elevated levels of the quantities computed in the second method correlate well with deterioration in the number of tasks completed. We were able to identify all of the failure scenarios found by large scale simulations; however the correlation is not perfect. In a few cases, elevated values occurred without any sign of a decrease in system performance.

Nevertheless, we believe that this methodology offers a promising first step toward the development of scalable and efficient methods. The use of Markov Chains to approximate the dynamics of systems is well known. However most applications involve the use of time homogeneous systems that reach steady state. Grid and cloud computing systems are both *time inhomogeneous* and *absorbing*. Thus much of the literature on perturbations of Markov chains does not apply.

Papers describing the work on the spectral approach are [2] and the graph theory approach [4].

[1] C. Dabrowski, F. Hunt, and K. Morrison, Improving Efficiency of Markov Chain Analysis of Complex Distributed Systems, *NISTIR 7744*, November 2010.

[2] F. Hunt, C. Dabrowski, K. Morrison, Identifying Failure Scenarios in Large Scale Systems Using Absorbing Markov Chains, in preparation.

[3] C. Dabrowski and F. Hunt, Markov Chain Analysis for Large-Scale Grid Systems, *NISTIR 7566*, April 2009.

[4] C. Dabrowski and F. Hunt, Using Markov Chain and Graph Theory Concepts to Analyze Behavior in Complex Distributed Systems, ASME 2011 Pressure Vessels and Piping Conf., Symposium on Risk Informed Online Monitoring of Aging Complex Systems, Oct. 2010.

ITL Program: *Complex Systems*

Visualization and Analysis of the National Vulnerability Database

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http://www.nist.gov/itl/math/hpcvg/nvdvis.cfm

The National Vulnerability Database[13] (NVD) is a continuously updated U.S. government repository of computer security vulnerability management data represented using the Security Content Automation Protocol[14] (SCAP). This year we have developed a tool, NVDvis that allows interactive analysis of the National Vulnerability Database.

Using our tool, the user can choose the NVD's Common Vulnerabilities and Exposures (CVE) 2.0 or CVE 1.2 databases. The tool does an initial analysis that is displayed in the Data Analysis pane of the tool; see Figure 59. It displays which CVE database was selected and how many entries there were. It provides the average vulnerability score as well as the distribution of the scores. It shows the number of elements, as well as the percentage for each value of the six attributes that make up the score, the part, Common Weakness Enumeration ID (CWE-ID), and distribution of date-time. The data is visualized with a Parallel Coordinate plot; see Figure 60. The tool enables the user to do the following.

1. Filter the data in a variety of ways. NVDvis can filter on the vulnerability score as well as the six attributes that contribute to the score: Access vector, access complexity, authentication, confidentiality impact, integrity impact, and availability impact. It also provides access to Part (application, hardware, operating system), CWE-ID, date-time, and vendor. After each filtering operation, the Data Analysis pane is updated as well as the visualization.
2. Generate Parallel Coordinate plots. These are a way to visualize multidimensional data. Our visualization can be viewed both on the desktop as well as in our immersive environment.
3. Output data in a variety of formats:

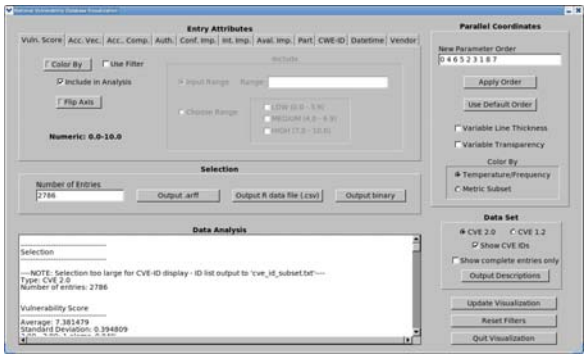

Figure 59. *The NVDvis interface.*

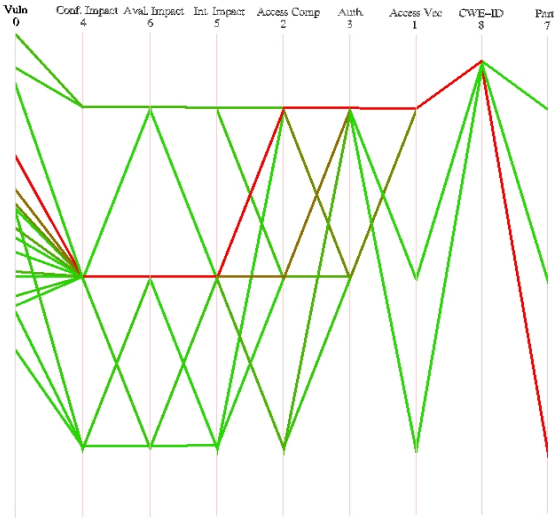

Figure 60. *NVDvis parallel coordinate plot.*

- csv format (comma separated values). Easily read by the R Statistical Package. R provides access to many analysis techniques as well as other visualization packages. This format is also read by many other packages.
- arff format. Read by the Weka open source data mining software. This format is also read by other machine learning software packages.
- Binary format. Enables a user to pick up where he or she left off.
- Descriptions to enable text mining.

This year we performed an examination of the distribution of SQL Injection Vulnerability Scores Relative to the 7.5 Standardized Score. We studied the distribution of XSS Vulnerability Scores Relative to the 4.3 Standardized Score.

We gave NVDvis demos and ran requested scenarios using the tool at the 6th Annual IT Security Automation Conference, September 27-29, 2010 in Baltimore.

[13] http://nvd.nist.gov/
[14] http://scap.nist.gov/

Visualization of Large Complex Networks

Clement Rey
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Terence Griffin

One of the fundamental challenges in complex systems is understanding the nature and structure of large-scale networks. These are often in the form of information networks (like the World Wide Web), biological networks (like protein-protein interactions, food webs), social networks (like online social sites, personal interactions, criminal rings, terrorist cells), and engineering networks. Such networks can be abstracted to graphs typically exhibiting thousands to millions of nodes and about 10 times as many edges. Given the rapid growth of electronic data, networks with billions of nodes will soon be readily available for analysis, providing opportunity for insight into large-scale system behavior.

To the aid the understanding of such systems, we have developed visualization techniques that utilize the latest immersive and 3D environments, together with state-of-the-art graph layout algorithms, so that researchers can walk around and examine these structures interactively.

This year, we developed a portable stand-alone version of this viewer, LightViewer, which can run on various platforms, requiring only an Open Scene Graph (OSG) library. This allows visualizations to be conducted on remote workstations, as well as local 3D immersive environments. One can rotate, zoom, pan, and fly through the graph interactively. By clicking on a node, one can see its annotations (for example, the page's URL for web graphs). The OSG library is available for Linux, Windows, and Mac OS X platforms.

For example, Figure 61 illustrates the visualization of a web graph were nodes are individual web pages of math.nist.gov. In this instance, we have highlighted the community structure by using a fatpoint shader

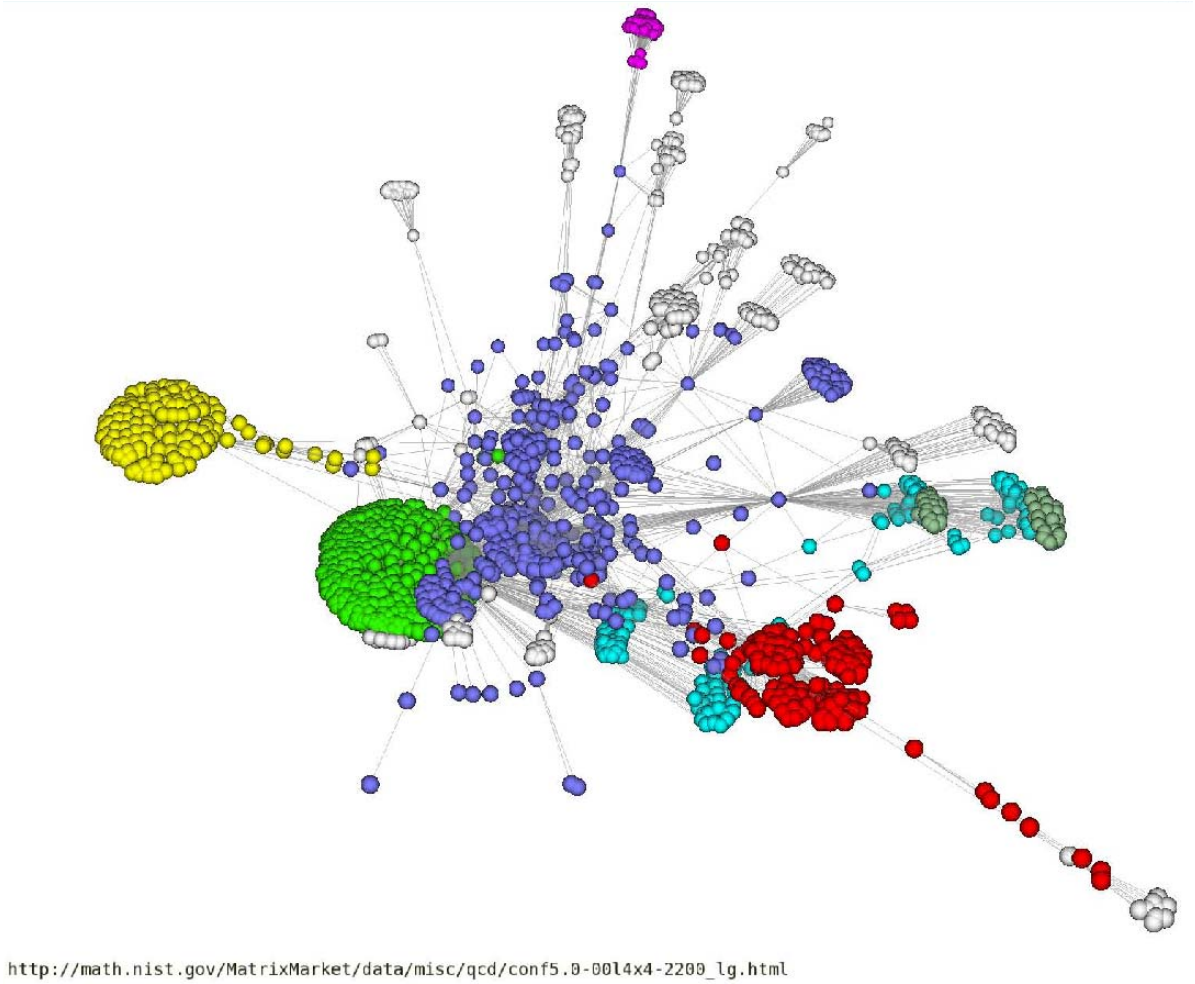

Figure 61. *Three-dimensional visualization of the community structure of a reduced Web graph corresponding to math.nist.gov. Each node is a separate Web page and the colors indicate different community groups. The graph is navigated in real time (pan, zoom, rotate) and the URL is displayed for a selected node, allowing researchers to study its structure interactively.*

(with an interactive size control) to render the nodes of the graph. The largest groups (7 in this case) are colored individually. The set of small groups (179 in this case) is colored a transparent grey. An individual node can be selected using a cross-hair glyph and its URL displayed in a box tethered to the node with lines. In addition, the web page that the node represents can be displayed, so researchers can investigate its content.

ITL Program: *Complex Systems*

Advanced Combinatorial Testing for Systems

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http://csrc.nist.gov/groups/SNS/acts/index.html

A combinatorial interaction fault is a software defect that may cause a complex system to fail when particular values of certain inputs combine with particular values of other inputs. Such faults remain dormant until the unfortunate combination of values is encountered in practice. Many critical system failures in recent times have been traced to interaction faults in the underlying software. Eradicating such faults is critical to ensure trustworthy software in business, industrial, medical, scientific, and transport systems.

To test for interaction faults one must check all possible combinations of input parameters. This is impossibly difficult for any real-world system. There are just too many combinations to check. Combinatorial testing is an approach to detecting interaction faults based on the observation that most such faults involve only a relatively few parameters. Thus, one effective strategy is to devise a testing plan in which all interactions between small numbers of parameters are tested in a minimum number of trial runs. For example, a system with 10 parameters, each with two possible values, would require 1024 trial runs to test every possible combination of inputs. However, a judicious selection of just 13 input sets is sufficient to cover all possible 3-way combinations. Unfortunately, in general, automatically generating testing plans with a minimum number of runs is itself very computationally challenging.

Most combinatorial testing has until recently been limited to pair-wise (2-way) testing in which all interactions involving two parameters are detected. Software testing tools have not been available for higher strength testing. The goal of this project is to advance combinatorial testing technology from pair-wise to higher order (strength) testing and to demonstrate successful applications of high strength combinatorial testing.

In Octover 2010 we released version 2 of the ACTS (Advanced Combinatorial Testing System) tool to generate high strength test suites based on covering arrays. The major features of ACTS tool are:

- *t-way test set generation:* given a set of parameters and values, ACTS can generate a test set that achieves t-way coverage for t = 1 to 6. (For t = 1, base choice coverage is implemented, which is more meaningful than naïve 1-way testing.)
- *Constraint support:* ACTS allows the user to specify constraints among different parameters, and then generates a t-way test set that satisfies these constraints.
- *Mixed-strength support:* ACTS allows the user to create groups of parameters with different strengths, and then generates a test set that satisfies the different coverage strengths.
- *Test set augmentation:* given a test set that does not satisfy t-way coverage, ACTS can generate additional tests to make this test set complete.
- *Coverage check:* ACTS can check the coverage of a test set, with or without constraints. It also allows the user to graph coverage increments against each test.
- *Expected output specification:* ACTS allows expected output to be specified for each test.
- *Accessible user interfaces:* ACTS provides both command-line and graphic user interfaces. Generating test suits which allow for complex constraints among parameter values in software testing is very challenging problem.

The current version includes an innovative method of generating constrained test sets. We revised constraint parser to provide better error reporting about constraint specification. The current version computes coverage correctly when there are constraints. The GUI version of ACTS allows multiple systems to be opened at the same time. We have distributed (as of December 8, 2010), 540 copies of ACTS tool to individuals. We put no restrictions of those individuals to re-distribute to others. The users include US government agencies, global corporations including Microsoft, Lockheed Martin, Cisco, SAP, AT&T, Intel, and SAIC. The number of users is believed to some multiple of 500. Based on the feedback received we continue to improve the ACTS tool.

Since the project's inception, we have published nine papers in refereed publications and four magazine

articles. This year we published a refereed article in the Proceedings of Modeling and Simulation World 2009 [3]. We also wrote an article for *LogiGear Magazine* [6]. This issue also includes an interview of Rick Kuhn by LogiGear, a company based in San Mateo, California dedicated to improving software test efficiency. Our NIST Special Publication 800-142, "Practical Combinatorial Testing," [5] has been downloaded by about 5,000 people since its release in October 2010.

In FY 2010 NIST and the Lockheed Martin Corporation signed a cooperative research and development agreement (CRADA) on combinatorial testing (CT). Under this CRADA, Lockheed Martin will apply CT to one or more application areas and NIST will provide R&D assistance. The results will be described in a white paper for public release. We are also collaborating with the Food and Drug Administration, and the Johns Hopkins Applied Physics Lab, the US Air Force, and the US Army. We are investigating applications in computer security [7], health care, GUI based applications, web-applications, and for optimization and testing of simulations of complex systems.

[1] R. C. Bryce, Y. Lei, D. R. Kuhn, and R. Kacker, Combinatorial Testing, Chapter 14, in *Handbook of Research on Software Engineering and Productivity Technologies: Implications of Globalization*, M. Ramachandran and R. Atem de Carvalho, eds., IGI Global, 2010.

[2] B. Johnasson, R. Kacker, R. Kessel, C. McLean, and R. Sriram, Utilizing Combinatorial Testing to Detect Interactions and Optimize a Discrete Event Simulation Model for Sustainable Manufacturing, in *Proceedings of the ASME 2009 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference*, IDETC/CIE 2009, San Diego, CA, Aug. 30 - Sept. 2, 2009, CD-ROM Paper I: DETC2009-86522.

[3] D. R. Kuhn, R. N. Kacker and Y. Lei, Random vs. Combinatorial Methods for Discrete Event Simulation of a Grid Computer Network, in *Proceedings of ModSim World 2009*, Virginia Beach, VA, Oct. 14-17, 2009.

[4] W. Wang, Y. Lei, S. Sampath, R. Kacker, D. R. Kuhn and J. Lawrence, A Combinatorial Approach to Building Navigation Graphs for Dynamic Web Applications, in *Proceedings of 25th IEEE International Conference on Software Maintenance*, ICSM, Edmonton, Alberta, Canada, Sept. 20-26, 2009, pp. 211-220.

[5] D. R. Kuhn, R. Kacker and Y. Lei, Practical Combinatorial Testing, NIST Special Publication 800-142, October 2010.

[6] D. R. Kuhn, R. Kacker and Y. Lei, What is Combinatorial Testing and Why Should Testers Care, *LogiGear Magazine*, November 2010.

[7] R. Kacker, Y. Lei, D. R. Kuhn, and W. Wang, A Combinatorial Approach to Detecting Buffer Overflow Vulnerabilities, in review.

ITL Program: *Trustworthy Information Systems*

Towards Self-organizing Mobile Sensor Networks

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Amir G. Aghdam (Concordia University)
Hamid Mahboubi (Concordia University)
Ahmadreza Momeni (Concordia University)

Mobile sensor networks (MSNs) are envisioned to enable a novel set of applications in detecting, monitoring and tracking people, targets or events in pervasive computing environments. Locations of sensors in a MSN affect both their ability to acquire information on the intended targets and events, as well as their ability to communicate this information to the intended recipients. Information acquisition needs, which require proximity to targets, could potentially compete with communication needs, which require proximity to intended recipients of the sensor information. Communication ability can be improved if sensors are capable of forming and optimizing a multi-hop *Mobile Ad-hoc NETwork* (MANET) with some sensors relaying the other sensor information possibly in addition to transmitting their own information.

In [1] we consider a network of collaborative sensors tracking a single target. The objective is to compute (in real time) the effective sensing and communication radii of sensors as well as their location at each time instant, such that a set of prescribed specifications are achieved. These specifications include end-to-end connectivity preservation from the target to a fixed destination, while durability of sensors is maximized and the overall energy consumption is minimized. The problem is formulated as a constrained optimization problem, and a procedure is presented to solve it. Simulation results demonstrate the effectiveness of the proposed techniques. However, the formulation in [1] is based on a number of simplifying assumptions, including flat terrain, energy-free sensor relocation, etc.

Due to the difficulty of incorporating these and other inherent traits of MSNs, such as lack of centralized control, a variety of performance criteria, operational uncertainties, etc., into a conventional optimization framework, we suggest in [2] a unified pricing/evolutionary framework for MSN self-organization. Framework [2] involves sensor cooperation in data acquisition and communication, as well as sensor relocation in a general non-flat terrain, and accounts for the energy expenditure for sensor relocation. Decentralized MSN optimization is achieved through socially optimal pricing, which internalizes the effect of each sensor action on overall MSN performance. Results of a MSN tracking a single target are presented

in [2] that suggest the viability of the proposed framework for prolonging MSN life-span.

The first step in developing a co-evolutionary framework for MSN self-organization is identifying "socially optimal" individual sensor fitness/utility landscapes in the inherently distributed environment of a MSN. Social optimality implies that each sensor maximization of its individual fitness results in overall performance optimization of the network. This is a challenging problem since MSN performance critically depends on sensors cooperation, while "selfish" sensors behavior typically results in drastic deterioration of overall performance. For example, selfish sensor positioning can quickly deplete some sensor battery power, resulting in the network's inability to carry out its mission.

Framework [2] builds on extending pricing-based *network utility maximization* (NUM) framework for MSN distributed optimization that includes sensor location. The appeal of this unified MSN NUM framework is that while system utility maximization over sensor information flow rates in a "fast" time scale yields the optimal cross-layer design of the MSN MANET, system utility maximization over sensor locations in a "slow" time scale controls sensors motion. Major issues discussed in [2] are information asymmetry, cost of sensor relocation, and simulated annealing for MSN optimization.

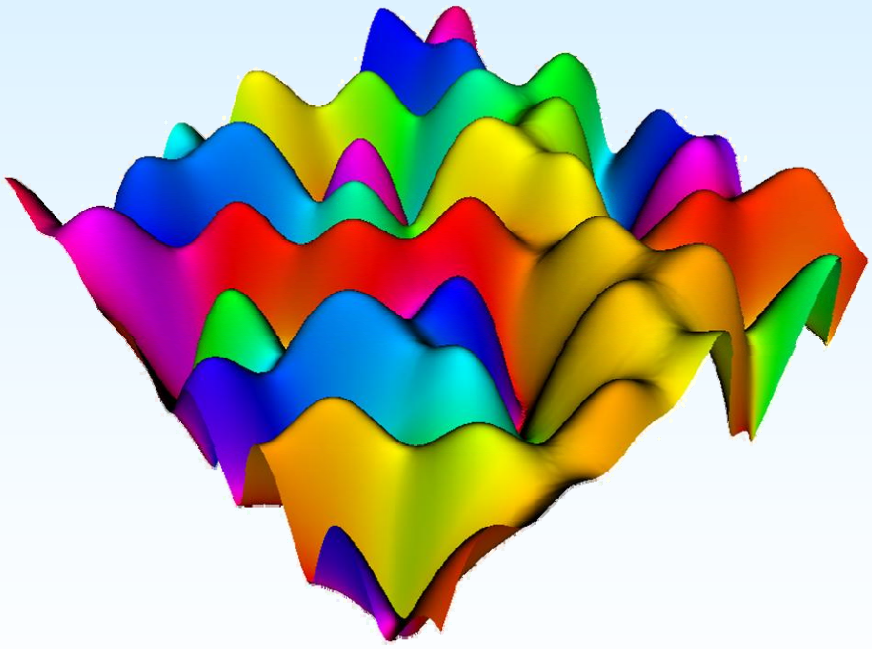
[1] H. Mahboubi, A. Momeni, A. G. Aghdama, K. Sayrafian-Pour, and V. Marbukh, Minimum cost routing with controlled node mobility for target tracking in mobile sensor networks, in *Proceedings of the 2010 American Control Conference* (ACC2010), USA, 2010.

[2] V. Marbukh, K. Sayrafian-Pour, H. Mahboubi, A. Momeni, and Amir G. Aghdam, Towards evolutionary-pricing framework for mobile sensor network self-organization, in *Proceedings of the 2010 IEEE World Congress on Computational Intelligence*, Barcelona, Spain, 2010

ITL Program: *Pervasive Information Technology*

Part IV

Activity Data



Publications

Appeared

Refereed Journals

1. D. M. Anderson, G. B. McFadden, S. R. Coriell, and B. T. Murray, "The Solidification of an Ideal Ternary Alloy in a Mushy Layer," *Journal of Fluid Mechanics* **647** (2010), pp. 309-333.
2. I. Beichl, B. Cloteaux, and F. Sullivan, "An Approximation Algorithm for the Coefficients of the Reliability Polynomial," *Congressus Numerantium* **197** (2010), pp. 143-151.
3. J. D. Benson, C. C. Chicone, and J. K. Critser, "Optimal Control of Cryoprotective Agent Addition and Removal Protocols," *Cryobiology* **59** (3) (December 2009), p. 382.
4. W. J. Boettinger and G. B. McFadden, "Bending of a Bimetallic Beam Due to the Kirkendall Effect," *Journal of Phase Equilibria and Diffusion* **31** (2010), pp. 6-14.
5. G. W. Bryant, M. Zieliński, N. Malkova, J. S. Sims, W. Jaskólski, and J. Aizpurua, "Effect of Mechanical Strain on the Optical Properties of Quantum Dots: Controlling Exciton Shape, Orientation, and Phase with a Mechanical Strain," *Physical Review Letters* **105** (6) (2010), article 067404 (4 pages).
6. J. W. Bullard, E. Enjolras, W. L. George, S. G. Satterfield, and J. E. Terrill, "A Parallel Reaction-transport Model Applied to Cement Hydration and Microstructure Development," *Modeling and Simulation in Materials Science and Engineering* **18** (2) (March 2010), article 025007 (16 pages).
7. T. J. Burns, S. P. Mates, R. L. Rhorer, E. P. Whitenton, D. Basak, and R. H. McFadden, "Modeling of the Temperature Field in the Chip and in the Tool in High-speed Machining of a Carbon Steel: Effect of Pearlite to Austenite Phase Transition in AISI 1075," *International Journal of Material Forming* **3** (Supplement 1) (June 17, 2010), pp. 491-494.
8. A. Carasso, "Bochner Subordination, Logarithmic Diffusion Equations, and Blind Deconvolution of Hubble Space Telescope Imagery and Other Scientific Data," *SIAM Journal on Imaging Sciences* **3** (2010), pp. 954-980.
9. B. Cloteaux and N. Serova, "Matching Observed Alpha Helix Lengths to Predicted Secondary Structure," *International Journal of Computational Bioscience* **1** (2010), pp. 103-110.
10. R. V. Datla, R. Kessel, A. W. Smith, R. N. Kacker, and D. B. Pollock, "Uncertainty Analysis of Remote Sensing Optical Sensor Data: Guiding Principles to Achieve Metrological Consistency," *International Journal of Remote Sensing* **31** (4) (2010), pp. 867-880.
11. M. J. Donahue, "Parallelizing a Micromagnetic Program for Use on Multi-processor Shared Memory Computers," *IEEE Transactions on Magnetics* **45** (2009), pp. 3923-3925.
12. P. R. Garabedian and G. B. McFadden, "The DEMO Quasisymmetric Stellarator," *Energies* **3** (2010), pp. 277-284
13. T. Gerrits, S. Glancy, T. S. Clement, B. Calkins, A. E. Lita, A. J. Miller, A. L. Migdall, S. W. Nam, R. P. Mirin, E. Knill, "Generation of Optical Coherent-State Superpositions by Number-Resolved Photon Subtraction from the Squeezed Vacuum," *Physical Review A* **82** (2010), article 031802 (4 pages).
14. A. I. Glazar, S. F. Mullen, J. Liu, J. D. Benson, J. K. Critser, E. L. Squires, and J. K. Graham, "Osmotic Tolerance Limits and Membrane Permeability Characteristics of Stallion Spermatozoa Treated with Cholesterol," *Cryobiology* **59** (2) (October 2009), pp. 201-206.
15. C. L. Holloway, A. Dienstfrey, E. F. Kuester, J. F. O'Hara, A. E. Azad, and A. J. Taylor, "A Discussion on the Interpretation and Characterization of Metafilms/Metasurfaces: The Two-dimensional Equivalent of Metamaterials," *Metamaterials* **3** (2009), pp. 100-112.
16. R. D. Johnson III, K. K. Irikura, R. Kacker, and R. Kessel, "Scaling Factors and Uncertainties for ab-initio Anharmonic Vibrational Frequencies," *Journal of Chemical Theory and Computation* **6** (9) (2010), pp. 2822-2828
17. R. N. Kacker and J. F. Lawrence, "Rectangular Distribution Whose End-points Are Not Exactly Known: Curvilinear Trapezoidal Distribution," *Metrologia* **47** (3) (March 11, 2010), pp. 120-126.
18. S. Kim, M. I. Aladjem, G. B. McFadden, and K. W. Kohn, "Predicted Functions of MdmX in Fine Tuning the Response of p53 to DNA Damage," *PLoS Computational Biology* **6** (2010), pp. 1-18.
19. E. Knill, "News and Views Q&A: Quantum Computing," *Nature* **463** (January 21, 2010), pp. 441-443.
20. K. M. Lebecki and M. J. Donahue, "Comment on 'Frustrated Magnetization in Co Nanowires: Competition between Crystal Anisotropy and

Demagnetization Energy,'" *Physical Review B* **82** (2010), article 096401 (4 pages).

21. A. Lewandowski, D. F. Williams, P. D. Hale, J. C. M. Wang, and A. Dienstfrey, "Covariance-Based Vector-Network-Analyzer Uncertainty Analysis for Time-and Frequency-Domain Measurements," *IEEE Transactions on Microwave Theory and Techniques* **58** (7) (2010), pp. 1877-1887.
22. L. Ma, O. Slattery, and X. Tang, "Detection and Spectral Measurement of Single Photons in Communication Bands Using Up-conversion Technology," *Laser Physics* **20** (5) (April 2, 2010), pp. 1244-1250.
23. L. Ma, O. Slattery and X. Tang, "Single Photon Level Spectrum Measurement at Fiber Communication Band Using Frequency Up-conversion Technology," *Laser Physics* **20** (7) (May 27, 2010), pp. 1612-1617.
24. N. S. Martys, D. Lootens, W. L. George, P. Hebraud, "Spatio-temporal Organization of Colloids in Start-up Flows," *Physical Review E* **80** (3) (2009), article 031401 (7 pages).
25. N. S. Martys, W. L. George, B.-W. Chun, and D. Lootens, "A Smoothed Particle Hydrodynamics Based Fluid Model with a Spatially Dependent Viscosity: Application to Flow of a Suspension with a Non-Newtonian Fluid Matrix," *Rheologica Acta* **49** (10) (2010).
26. G. B. McFadden, S. R. Coriell, and P. A. Lott, "Onset of Convection in Two Layers of a Binary Liquid," *Journal of Fluid Mechanics* **647** (2010), pp. 105-124.
27. H. Min, R. D. McMichael, M. J. Donahue, J. Miltat, M. D. Stiles, "Effects of Disorder and Internal Dynamics on Vortex Wall Propagation," *Physical Review Letters* **104** (2010), article 217201 (4 pages).
28. W. F. Mitchell, "The *hp*-Multigrid Method Applied to *hp*-Adaptive Refinement of Triangular Grids," *Numerical Linear Algebra with Applications* **17** (March 16, 2010), pp. 211-228.
29. J. Obrzut, A. Anopchenko, J. F. Douglas, and B. W. Rust, "Relaxation and Antiplasticization Measurements in Trehalose Glycerol Mixtures – A Model for Protein Preservation," *Journal of Non-Crystalline Solids* **356** (2010), pp. 777-781.
30. C. S. Pande and G. B. McFadden, "Self-similar Grain Size Distribution in Three Dimensions: A Stochastic Treatment," *Acta Materialia* **58** (2010), pp. 1037-1044.
31. F. Potra and E. Simiu, "Multi-hazard Design: A Structural Approach," *Journal of Optimization Theory and Applications* 144 (2010), pp. 120-136.
32. M. T. Rakher, L. Ma, O. Slattery, X. Tang, and K. Srinivasan, "Quantum Transduction of Telecommunications-band Single Photons from a Quantum Dot by Frequency Upconversion," *Nature Photonics* **4** (2010), pp. 786-791.
33. K. Sayrafian-Pour, W.-B. Yang, J. Hagedorn, J. Terrill, K. Y. Yazdandoost, and K. Hamaguchi "Channel Models for Medical Implant Communication," *International Journal of Wireless Information Networks* **17** (2010), pp. 105-112.
34. J. S. Sims and S. A. Hagstrom, "Hy-CI Study of the 2^2S Ground State of Neutral Lithium and the First Five Excited ^{2}S States," *Physical Review A* **80** (2009), article 052507 (8 pages).
35. H. Stamerjohanns, M. Kohlhase, D. Ginev, C. David, B. Miller, Transforming Large Collections of Scientific Publications to XML, *Mathematics in Computer Science* **3** (2010), pp. 299-307.
36. H. Vasconcelos, L. Sanz, and S. Glancy, "All-optical Generation of States for 'Encoding a Qubit in an Oscillator'," *Optics Letters* **35** (2010), pp. 3261-3263.
37. L. Yan, L. Ma, and X. Tang, "Bragg-grating enhanced Narrowband Spontaneous Parametric Down-conversion," *Optics Express* **18** (6) (2010), p. 5957- 5963.
38. Y. Zhang, E. Knill, and S. Glancy, "Statistical Strength of Experiments to Reject Local Realism with Photon Pairs and Inefficient Detectors," *Physical Review A* **81** (March 2010), article 032117 (7 pages).

Journal of Research of NIST

1. D. E. Gilsinn, B. R. Borchardt, and A. Tebbe, "Estimating Volumes of Near-Spherical Molded Artifacts," *Journal of Research of the NIST* **115** (3) (May-June 2010), pp. 149-177.

Books

1. M. E. Kilmer and D. P. O'Leary, eds., *G. W. Stewart: Selected Works with Commentaries*, Birkhauser Press, Boston (2010).
2. F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W Clark, eds., *NIST Handbook of Mathematical Functions*, Cambridge University Press, New York, 2010.

Book Chapters

1. R. C. Bryce, Y. Lei, D. R. Kuhn, and R. Kacker, "Combinatorial Testing," Chapter 14, in *Handbook of Research on Software Engineering and Productivity Technologies: Implications of Globalization*, M. Ramachandran and R. Atem de Carvalho, eds., IGI Global, 2010.
2. L. Ma, O. Slattery, and X. Tang, "NIR Single Photon Detectors with Up-conversion Technology and Its Applications in Quantum Communication Systems" Chapter 15 in *Advances in Lasers and Electro Optics*, INTECH, April 2010, pp. 315-336.
3. B. W. Rust, D. P. O'Leary, and K. M. Mullen, "Modelling Type Ia Supernova Light Curves," in *Exponential Data Fitting and its Applications*, Victor Pereyra and Godela Scherer, eds., Bentham Electronic Books, 2010, pp. 145-164.

Conference Proceedings

1. D. Banerjee, J. Gross, P. Reddy Gaddam, M. Olano, W. Hess, J. Terrill, T. Griffin, J. Hagedorn, J. Kelso, and S. Satterfield, "An Integrated Interactive Visualization and Analysis Environment to Study the Impact of Fire on Building Structures," in *Proceedings of SIGGRAPH'10*, ACM SIGGRAPH 2010 Posters, Los Angeles, CA, July 25-29, 2010, article 149 (1 page).
2. I. Beichl and B. Cloteaux, "A Structural Approach to the Temporal Modeling of Networks," in *Proceedings of the Winter Simulation Conference (WSC09)*, Austin, TX, December 13-16, 2009, pp. 788-796.
3. T. J. Burns, S. P. Mates, R. L. Rhorer, E. P. Whitenton, D. Basak, and R. H. McFadden, "Modeling of the Temperature Field in the Chip and in the Tool in High-speed Machining of a Carbon Steel: Effect of Pearlite to Austenite Phase Transition in AISI 1075," in *Proceedings of ESAFORM 2010*, Brescia, Italy, April 7-9, 2010.
4. T. J. Burns, S. P. Mates, R. L. Rhorer, E. P. Whitenton, and D. Basak, "On Modeling the Peak Temperature on the Tool-Chip Interface during High-Speed machining of AISI 1045 Steel," in *Proceedings of the Eigth International Conference on High Speed Machining*, Metz, France, December 8-10, 2010.
5. J. Chalfoun, A. Dima, A. Peskin, J. Elliot and J. Filliben, "A Human Inspired Local Ratio-Based Algorithm for Edge Detection in Fluorescent Cell Images," in *Advances in Visual Computing*, *(*G. Bebis, et al., eds.), Lecture Notes in Computer Science **6453** (2010), pp. 23-34.
6. B. Cloteaux and N. Serova, "Matching Observed Alpha Helix Lengths to Predicted Secondary Structure," in *Proceedings of the 2009 IEEE International Conference on Bioinformatics and Biomedicine Workshops*, Bethesda, MD, November 1-4, 2009, pp. 113-119.
7. B. Cloteaux, "Modeling Affiliations in Networks," in *Proceedings of the Winter Simulation Conference (WSC10)*, Baltimore, MD, December 5-8, 2010, pp. 2958-2967.
8. J. M. Conroy, J. D. Schlesinger, P. A. Rankel, and D. P. O'Leary, "CLASSY 2010: Summarization and Metrics," in *Proceedings of the Text Analysis Conference (TAC) 2010 Workshop*, NIST, November 15-16, 2010.
9. G. Dogan, "A Flexible and Efficient Numerical Framework for Image Segmentation by Energy Minimization," in *Proceedings of the Workshop on Applications of Digital Geometry and Mathematical Morphology,* Istanbul, Turkey, August 22-23, 2010.
10. J. T. Fong and P. V. Marcal, "Artificial Intelligence Tools for Failure Event Data Management and Probabilistic Risk Analysis for Failure Prevention," in *Proceedings of the Materials Science & Technology 2009 Conference*, Pittsburgh, PA, Oct. 25-29, 2009, Charles R. Morin Memorial Symposium on Failure Analysis and Prevention, R. Parrington and D. McGarry, eds., American Ceramic Society, Association for Iron & Steel Technology, ASM International, and Minerals, Metals & Materials Society (2009).
11. E. Garboczi, J. Bullard, N. Martys, and J. Terrill, "The Virtual Cement and Concrete Testing Laboratory: Performance Prediction, Sustainability, and the CSHub," in *Proceedings of the National Ready Mixed Concrete Association Concrete Sustainability Conference*, Tempe, AZ, April 13-15, 2010.
12. D. Genin, V. Marbukh, and T. Nakassis, "Vulnerability of Selfish Routing to Attacks: A Game-theoretic Model and Initial Results," in *Proceedings of 2010 International Conference of Information Security and Internet Engineering, World Congress on Engineering 2010* (WCE 2010), June 30, 2010.
13. P. D. Hale and A. Dienstfrey, "Waveform Metrology and a Quantitative Study of Regularized Deconvolution," in *Proceedings of the Instrumentation and Measurement Technology Conference (I2MTC)*, Austin, TX, May 3-6, 2010, pp. 386-391.
14. F. Hunt and V. Marbukh, "Measuring the Utility/Path Diversity Tradeoff In Multipath

Protocols," in *Proceedings of the 4th International Conference on Performance Evaluation Methodologies and Tools*, Pisa, Italy, Oct. 20-22, 2009.

15. B. Johnasson, R. Kacker, R. Kessel, C. McLean, and R. Sriram, "Utilizing Combinatorial Testing to Detect Interactions and Optimize a Discrete Event Simulation Model for Sustainable Manufacturing," in *Proceedings of the ASME 2009 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference*, IDETC/CIE 2009, San Diego, CA, Aug. 30-Sept. 2, 2009, CD-ROM Paper I: DETC2009-86522.
16. R. N. Kacker, R. Kessel, K.-D. Sommer, and X. Bian, "Comparison of Statistical Consistency and Metrological Consistency," in *Proceedings of the XIX IMEKO World Congress on Fundamental and Applied Metrology*, Lisbon, Portugal, Sept. 6-11, 2009.
17. R. Kacker, R. Kessel, and K.D. Sommer, "Metrological Compatibility and Statistical Consistency," in *Proceedings of the Tenth International Symposium on Measurement and Quality Control*, Osaka, Japan, September 5-9, 2010, article 157.
18. R. Kessel and R. N Kacker, "Correlation in Uncertainty of Measurement - A Discussion of State of the Art Techniques," in *Proceedings of the XIX IMEKO World Congress on Fundamental and Applied Metrology*, Lisbon, Portugal, Sept. 6-11, 2009.
19. R. Kessel, R. Kacker and K.D. Sommer, "A More General Type A Evaluation," in *Proceedings of the Tenth International Symposium on Measurement and Quality Control*, Osaka, Japan, September 5-9, 2010, article 35.
20. D. R. Kuhn, R. N. Kacker and Y. Lei, "Random vs. Combinatorial Methods for Discrete Event Simulation of a Grid Computer Network," in *Proceedings of ModSim World 2009*, Virginia Beach, VA, Oct. 14-17, 2009.
21. L. Ma, O. Slattery and X. Tang, "Ultra Sensitive NIR Spectrometer Based on Frequency Upconversion Detector," *Proceedings of the SPIE* **7680** (April 7, 2010), article 76800 (10 pages).
22. L. Ma, O. Slattery, and X. Tang, "Study on Noise Reduction in Up-conversion Single Photon Detectors," *Proceedings of the SPIE* **7815** (2010), article 781508 (8 pages).
23. L. Ma, O. Slattery, and X. Tang, "Optimization of the Optical Gating Width in Up-conversion Single Photon Detectors," in *Proceedings of the SPIE* **7815** (2010), article 781508 (8 pages).
24. V. Marbukh, H. Mahboubi, A. Momeni, A.G. Aghdama, and K. Sayrafian-Pour, "Optimal Target Tracking Strategy with Controlled Node Mobility in Mobile Sensor Networks," in *Proceedings of 2010 American Control Conference (ACC2010)*, June 30, 2010.
25. V. Marbukh, H. Mahboubi, A. Momeni, A. G. Aghdama, and K. Sayrafian-Pour, "Towards Evolutionary-pricing Framework for Mobile Sensor Network Self-organization," in *Proceedings of the IEEE World Congress on Computational Intelligence (WCCI2010)*, Barcelona, Spain, July 18-23, 2010.
26. A. Peskin, K. Kafadar, and A. Dima, "A Quality Pre-Processor for Biological Cell Images," in *Advances in Visual Computing*, Part I, (G. Bebis, et al., eds.), Lecture Notes in Computer Science **5875** (2009), pp. 1051-1062.
27. A. Peskin, A. Dima, J. Chalfoun and J. Elliot, "Predicting Segmentation Accuracy for Biological Cell Images," in *Advances in Visual Computing*, Part I, (G. Bebis, et al., eds.), Lecture Notes in Computer Science **6453** (2010), pp. 549-560.
28. A. Peskin and A. Dima, "Modeling Clinical Tumors to Create Reference Data for Tumor Volume Measurement," in *Advances in Visual Computing*, Part II, (G. Bebis, et al., eds.), Lecture Notes in Computer Science **6454** (2010), pp. 736-746.
29. M. T. Rakher, L. Ma, O. Slattery, X. Tang, K. Srinivasan, "Quantum Transduction of Telecommunications-band Single Photons from a Quantum Dot by Frequency Upconversion", in *Proceedings of Frontiers in Optics 2010*, Rochester, New York, October 24-28, 2010.
30. B. Saunders and Q. Wang, "Tensor Product B-Spline Mesh Generation for Accurate Surface Visualization in the NIST Digital Library of Mathematical Functions", in *Mathematical Methods for Curves and Surfaces,* (M. Dæhlen, et al., eds.), Lecture Notes in Computer Science **5862** (2010), pp. 385-393.
31. X. Tang, L. Ma and O. Slattery, "Ultra Low Dark-count-rate Up conversion Single Photon Detector," in *Proceedings of the 2010 IEEE Photonics Society Annual Meeting*, Denver, CO, November 7-11, 2010, IEEE catalog: CFP10LEO-CDR.
32. W. Villanueva, W. J. Boettinger, G. B. McFadden, and J.A. Warren, "A Multicomponent and Multiphase Model of Reactive Wetting," *Proceedings of the 7th International Conference on Multiphase Flows* (ICMF 2010), Tampa, FL, May 30-June 4, 2010.

33. W. Wang, Y. Lei, S. Sampath, R. Kacker, R. Kuhn and J. Lawrence, "A Combinatorial Approach to Building Navigation Graphs for Dynamic Web Applications," in *Proceedings of 25th IEEE International Conference on Software Maintenance*, ICSM, Edmonton, Alberta, Canada, Sept. 20-26, 2009, pp. 211-220.
34. J. C. Wu, A. F. Martin, R. Kacker and C. R. Hagwood, "Significance Test in Operational ROC Analysis" in *Proceedings of SPIE Defense, Security, and Sensing Conference*, Orlando FL, April 5-9, 2010, article 76670I (15 pages).
35. W.-B. Yang, K. Sayrafian-Pour, J. Hagedorn, J. Terrill, and K. Y. Yazdandoost, "Simulation Study of Body Surface RF Propagation for UWB Wearable Medical Sensors," in *Proceedings of the 2nd International Symposium on Applied Sciences in Biomedical and Communication Technologies*, Bratislava, Slovak Republic, November 24-27, 2009.
36. L. Yan, L. Ma, and X. Tang, "Narrow-band Photon Pairs Generated from Spontaneous Parametric Down Conversion in a Bragg-grating Enhanced Waveguide," in *Proceedings of the SPIE* **7815** (2010), article 781511 (7 pages).

Other Formal Publications

1. I. Beichl, "Where the Rubber Meets the Road," *Computing in Science & Engineering* **11** (5) (Sept.-Oct. 2009), p. 3.
2. I. Beichl, "Ephemera," *Computing in Science & Engineering* **12** (1) (January 2010), p. 3.
3. I. Beichl, "You Say You Want a Revolution," *Computing in Science & Engineering* **12** (2) (March 2010), p. 5.
4. I. Beichl, "Good Policy Makes Good Science," *Computing in Science & Engineering* **12** (3) (May 2010), p. 5.
5. I. Beichl, "Revitalizing Work in CiSE," *Computing in Science & Engineering* **12** (5) (September 2010), p. 4.
6. W. L. George, "Modeling the Rheological Properties of Concrete," in *High End Computing at NASA - Highlights of Science and Engineering Achievements on NASA's Supercomputers* (2007-2008), pp. 112-113.
7. R. Kessel and T. Hewison, "Common Reference Channels for Metrological Comparability," *Global Space-based Inter-Calibration Systems Quarterly* **4** (4) (2010), pp. 1-2.
8. D. R. Kuhn, R. Kacker and Y. Lei, What is Combinatorial Testing and Why Should Testers Care, *LogiGear Magazine*, November 2010.

Technical Reports

1. J. Bernal, "Linking Canny Edge Pixels with Pseudo-watershed Lines," NISTIR 7673, March 2010.
2. R. F. Boisvert (ed.), "Mathematical and Computational Sciences Division, Summary of Activities for Fiscal Year 2009", NISTIR 7671, February 25, 2010 (110 pages).
3. A. Carasso and A. Vládár, "Fractional Diffusion, Low Exponent Levy Stable Laws, and Slow Motion Denoising of Helium Ion Microscope Nanoscale Imager," NISTIR 7727, September 2010 (20 pages).
4. C. Dabrowski, F. Hunt and K. Morrison "Improving Efficiency of Markov Chain Analysis of Complex Distributed Systems," NISTIR 7744, November 2010.
5. D. E. Gilsinn, K. Bhadriraju, J. T. Elliott, "Biological Cell Feature Identification by a Modified Watershed-Merging Algorithm", NISTIR 7750, November 2010 (47 pages).
6. F. Hunt and V. Marbukh, "A Model of Joint Congestion Control and Routing Through Random Assignment of Paths," NISTIR 7590, February 2010.
7. R. Kuhn, R. Kacker and Y. Lei, "Practical Combinatorial Testing," NIST Special Publication 800-142, October 2010.
8. W. F. Mitchell, "A Collection of 2D Elliptic Problems for Testing Adaptive Algorithms," NISTIR 7668, March 5, 2010.
9. S. Ramamurti and D. Gilsinn, "Bicubic B-spline Surface Approximation of Invariant Tori", NISTIR 7731, October 20, 2010.
10. J. C. Wu, A. F. Martin, C. S. Greenberg, and R. N. Kacker, „Measurement Uncertainties in Speaker Recognition Evaluation," NISTIR 7722, September 15, 2010 (16 pages).

Accepted

1. J. D. Benson, C. C. Chicone, and J. K. Critser, "A General Model for the Dynamics of Cell Volume, Global Stability, and Optimal Control," *Journal of Mathematical Biology*.

2. J. D. Benson, A. Bagchi, X. Han, J. K. Critser, and E.J. Woods, "Melting Point Equations for the Ternary System Water-sodium Chloride-ethylene Glycol Revisited," *Cryobiology*.

3. J. W. Bullard, C. F. Ferraris, E. J. Garboczi, N. S. Martys, P. E. Stutzman, J. E. Terrill, "Virtual Cement and Concrete," *Innovations in Portland Cement Manufacturing*.

4. J. W. Bullard, E. J. Garboczi, W. L. George, N. S. Martys, S. G. Satterfield, J. E. Terrill, "Advancing the Materials Science of Concrete with Supercomputers," *Concrete International*.

5. T. J. Burns, S. P. Mates, R. L. Rhorer, E. P. Whitenton, D. Basak, "Dynamic Properties for Modeling and Simulation of Machining: Effect of Pearlite to Austenite Phase Transition on Flow Stress" *AISI 1075 Steel, Machining Science and Technology*.

6. B. Cloteaux, "Approximating the Number of Bases for Almost All Matroids," *Congressus Numerantium*.

7. V. R. Coffman, J. P. Sethna, J. Bozek, A. Ingraffea, N. P. Bailey and E. I. Barker, "Challenges in Continuum Modeling of Intergranular Fracture," *Strain*.

8. A. A. Dima, J. T. Elliott, J. J. Filliben, M. Halter, A. Peskin, J. Bernal, B. L. Stottrup, M. Kociolek, M. C. Brady, H. C. Tang, and A. L. Plant, "Comparison of Segmentation Algorithms for Fluorescence Microscopy Images of Cells," *Cytometry Part A*.

9. V. Marbukh, H. Mahboubi, A. Momeni, A.G. Aghdama, and K. Sayrafian-Pour "Self-Deployment Algorithms for Coverage Problem in a Network of Mobile Sensors with Un-identical Sensing Range" *IEEE Globecom 2010*.

10. A. Mink, L. Ma, B. Hershman and X. Tang "An Application of Quantum Networks for Secure Video Surveillance," in *Video Surveillance,* I-TECH Education and Publishing, Vienna, Austria.

11. W. F. Mitchell and M. A. McClain, "A Survey of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations," *Annals of the European Academy of Sciences*.

12. B. W. Rust, "Atmospheric Retention of Man-made CO_2 Emissions," *Mathematics and Computers in Simulation*.

13. J. S. Sims, G. W. Bryant, W. L. George, T. G. Griffin, J. G. Hagedorn, J. T. Kelso, T. M. Olano, A. P. Peskin, S. G. Satterfield, and J. D. Terrill, "Computation and Visualization of Nano-structures and Nano-optics," *Computing and Visualization in Science*.

14. J. S. Sims and S. A. Hagstrom, "Hylleraas-configuration-interaction Study of the Singlet S Ground State of Neutral Beryllium*," Physical Review*.

In Review

1. G. S. Abo, Y. K. Hong, B. C. Choi, S. Bai, J. Jalli, J. H. Park, J. J. Lee, M. J. Donahue, M. H. Park, and S. H. Gee, "Micromagnetic Computer Simulated Scaling Effect of S-shaped Permalloy nano-element on Operating Fields for AND or OR Logic."

2. I. Beichl, "Working in Computational Science."

3. I. Beichl, "Dystopia."

4. J. D. Benson, C. C. Chicone, and J. K. Critser, "An Optimal Method for the Addition and Removal of Cryoprotective Agents."

5. J. D. Benson, "Stability Analysis of Several Non-dilute Multiple Solute Transport Equations."

6. J. D. Benson, C. T. Benson, and J. K. Critser, "Mathematical Model Formulation and Validation of Water and Cryoprotective Agent Transport in Whole Hamster Pancreatic Islets."

7. R. Braun, R. Usha, G. McFadden, T. Driscoll, L. P. Cook and P. King-Smith, "Thin Film Dynamics on a Prolate Ellipsoid with Application to the Cornea."

8. A. Carasso and A. Vladár, "Fractional Diffusion, Low Exponent Levy Stable Laws, and 'Slow Motion' Denoising of Helium Ion Microscope Nanoscale Imagery."

9. V. R. Coffman, A. C. E Reid, S. A. Langer, and G. Dogan, "OOF3D: An Image-based Finite-element Solver for Materials Science."

10. C. Dabrowski and F. Hunt, "Using Markov Chain and Graph Theory Concepts to Analyze Behavior in Complex Distributed Systems."

11. G. Dogan and R. Nochetto, "First Variation of the General Curvature-dependent Surface Energy."

12. D. Duthinh and F. Potra, "Probabilistic and Optimization Considerations in Multi-hazard Engineering."

13. D. Gilsinn, K. Bhadriraju, J. Elliott, "Biological Cell Feature Identification by a Modified Watershed-Merging Algorithm."

14. X. Han, Y. Liu, J. D. Benson, and J. K. Critser, "A Calorimetric Method to Measure Water-cryoprotectant Mutual Diffusivity in Biological Tissues at Both Super- and Sub-zero Temperatures."
15. D. Harris, F. Sullivan, and I. Beichl, "Fast Sequential Importance Sampling to Estimate the Graph Reliability Polynomial."
16. R. Kacker and J. Lawrence, "Derivation of Isosceles Trapezoidal Distributions."
17. R. Kacker, Y. Lei, D. R. Kuhn, and W. Wang, "A Combinatorial Approach to Detecting Buffer Overflow Vulnerabilities."
18. R. Kessel, R. Kacker, and J. Lawrence, "Effective Degrees of Freedom for Correlated Input Quantities."
19. R. Kessel and T. Hewison, "Treatment of Spectral Response in Inter-calibration."
20. J. Lawrence, R. Kacker, Y. Lei, D. R. Kuhn, and M. Forbes, "A Survey of Binary Covering Arrays."
21. J. D. D. Melo and J. T. Fong, "A New Approach to Creating Composite Materials Elastic Property Database with Uncertainty Estimation Using a Combination of Mechanical and Thermal Expansion Tests."
22. D. P. O'Leary and B. W. Rust, "Variable Projection for Nonlinear Least Squares Problems."
23. L. Ma, J. C. Bienfang, O. Slattery and X. Tang, "Multi-wavelength Pumping Technique for Up-conversion Single-photon Detectors."
24. L. Ma, J. C. Bienfang, O. Slattery and X. Tang, "Up-conversion Single-photon Detector using Multi-wavelength Sampling Techniques."
25. J. S. Pelc, C. R. Phillips, C. Langrock, Q. Zhang, L. Ma, O. Slattery, X. Tang, and M. M. Fejer, "Single-Photon Detection at 1550 nm via Upconversion Using a Tunable Long-Wavelength Pump Source."
26. M. T. Rakher, L. Ma, O. Slattery, X. Tang, and K. Srinivasan, "Upconversion of Triggered Single Photon Emission from a Telecommunications-band Semiconductor Quantum Dot."
27. P. E. Shah, J. D. D. Melo, C. A. Cimini, and J. T. Fong, "Composite Material Property Database Using Smooth Specimens to Generate Design Allowables with Uncertainty Estimation."
28. W. Wang, Y. Lei, D. Liu, D. Kung, C. Callner, D. Zhang, R. Kacker and R. Kuhn, "A Combinatorial Approach to Detecting Buffer Overflow Vulnerabilities."

Presentations

Invited Talks

1. J. D. Benson, "Basic Principles of Sperm Cryopreservation," European Society for Human Reproduction and Embryology (ESHRE), Granada, Spain, March 25-26, 2010.
2. A. Carasso, "Randomizing the Time in the Heat Equation and Blind Deconvolution of Galaxy Images," AMS-SIAM Minisymposium "Frontiers in Geomathematics," American Mathematical Society Annual Meeting, San Francisco, CA, January 13, 2010.
3. A. Carasso, "Bochner Subordination, Logarithmic Diffusion Equations, and Blind Deconvolution of Hubble Space Telescope Imagery and Other Scientific Data," Applied Analysis Seminar, Department of Mathematics, Yale University, New Haven, CT, January 27, 2010.
4. A. Carasso, "Bochner Subordination, Logarithmic Diffusion Equations, and Blind Deconvolution of Hubble Space Telescope Imagery and Other Scientific Data," Department of Mathematics Colloquium, George Mason University, Fairfax, VA, March 26, 2010.
5. A. Carasso, "Randomizing the Time Variable in Brownian Motion and Blind Deconvolution of Hubble Telescope Imagery," SIAM Conference on Imaging Science, Chicago, IL, April 13-15, 2010.
6. V. Coffman, "Object-Oriented Finite Elements (OOF) for Modeling Materials Behavior," 21st NIST Computer Modeling Workshop, Gaithersburg, MD, August 12, 2010.
7. A. Dienstfrey, "Numerical Solution of Riemann-Hilbert Problems Related to Random Matrix Theory and the Painlevé Equations," International Center for Mathematical Sciences Workshop on the Numerical Solution of the Painlevé Equations, Edinburgh, UK, May 10-15.
8. A. Dienstfrey, "Uncertainty Quantification for Scientific Computation," National Academy of Sciences Committee on Mathematical Science Foundations of Verification, Validation, and Uncertainty Quantification, Albuquerque, NM, June 11, 2010.
9. F. Hunt, "A Model of Routing in a Computer Network," Oxtoby Centennial Conference, Bryn Mawr College, October 30, 2010.

10. J. Fong, "Aging Plant Risk-Informed In-Service Inspection (RI-ISI) Methods and Artificial Intelligence Tools for Probabilistic Risk Assessment," Department of Aeronautics and Astronautics Seminar, Stanford University, Stanford, CA, Oct. 7, 200**9.**
11. J. Fong, "Artificial Intelligence Tools for Failure Event Data Management and Probabilistic Risk Analysis for Failure Prevention," Materials Science & Technology 2009 Conference, Pittsburgh, PA, Oct. 25-29, 2009, Charles R. Morin Memorial Symposium on Failure Analysis and Prevention, sponsored by the American Ceramic Society, Association for Iron & Steel Technology, ASM International, and Minerals, Metals & Materials Society, Oct. 27, 2009.
12. J. Fong, "Application of Artificial Intelligence (AI) Tools to Failure Event Data Management and Probability Risk Analysis for Failure Prevention," Department of Mechanical & Aerospace Engineering Seminar, George Washington University, Washington, DC, Nov. 23, 2009.
13. J. Fong, "Application of Artificial Intelligence (AI) Tools to On-line Monitoring of Aging Structures, and Research Opportunities at National Institute of Standards & Technology," Department of Mechanical Engineering Seminar, Stanford University, Stanford, CA, Dec. 8, 2009.
14. F. Hunt, "How to Write A Grant Proposal," Infinite Possibilities Conference, Institute for Pure and Applied Mathematics, UCLA, Las Angeles, CA, March 18-20, 2010.
15. F. Hunt, "A Mathematician Looks at Hollywood, DNA and Paint," Career Workshop on Minorities and Applied Mathematics, Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, MN, March 25-27, 2010.
16. E. Knill, "Building Quantum Computers," Indiana University, Bloomington, IN, Nov. 21, 2009
16. P. A. Lott, "Fast Solvers for Models of Fluid Flow with Spectral Elements," Applied and Computational Math Seminar, George Mason University, Washington, DC, Dec. 4 2009.
17. P. A. Lott, "Fast Solvers for Models of Fluid Flow with Spectral Elements," Differential Equations Seminar, University of Maryland Baltimore County, Dec. 7 2009.
18. P. A. Lott, "Fast Solvers for Models of Fluid Flow with Spectral Elements," Department of Mathematics Colloquium Howard University, Washington, DC, Feb. 2010.
19. P. A. Lott, "Fast Solvers for Models of Fluid Flow with Spectral Elements," Center for Applied Scientific Computing, Lawrence Livermore National Lab, Livermore, CA, Feb. 2010.
20. P. A. Lott, "Fast Solvers for Models of Fluid Flow with Spectral Elements," Computer Science and Mathematics Division Seminar, Oak Ridge National Lab, Oak Ridge, TN, May 6, 2010.
21. D. Lozier, "Public Release of the NIST DLMF and Handbook," Workshop on Numerical Solution of the Painlevé Equations, International Centre for Mathematical Sciences, Edinburgh, Scotland, May 10-14, 2010.
22. G. B. McFadden, "QAS Design of the DEMO Reactor," 17th International Stellarator/Heliotron Workshop, Princeton Plasma Physics Laboratory, Princeton, NJ, October 12-16, 2009.
23. G. McFadden, "Phase-field Modeling of Reactive Wetting**,"** SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, May 22 - May 26, 2010.
24. B. Saunders, "Applying Numerical Grid Generation to the Visualization of Complex Function Data," Institute for Mathematics and its Applications/Minnesota Center for Industrial Mathematics (IMA/MCIM) Industrial Problems Seminar, University of Minnesota, Minneapolis, MN, April 9, 2010.
25. B. Saunders, "Creating Interactive 3D Graphs for a Digital Library: So How Is This Math?" Kappa Mu Epsilon Honorary Mathematics Society, Stevenson University, Stevenson, MD, September 21, 2010.
26. W.-B. Yang, K. Sayrafian-Pour, J. Hagedorn, J. Terrill, and K. Y. Yazdandoost, "Simulation Study of Body Surface RF Propagation for UWB Wearable Medical Sensors," in *Proceedings of the 2nd International Symposium on Applied Sciences in Biomedical and Communication Technologies*, November 24-27, 2009, Bratislava, Slovak Republic.

Conference Presentations

1. D. Banerjee, J. Gross, P. R. Gaddam, M. Olano, W. Hess, J. Terrill, T. Griffin, J. Hagedorn, J. Kelso, and S. Satterfield, "An Integrated Interactive Visualization and Analysis Environment to study the Impact of Fire on Building Structures," SIGGRAPH 2010, Los Angeles, CA, July 25-29, 2010.

2. J. D. Benson, "Exact and Numerical Boundary Control of the Diffusion Equation in Cryobiology," Annual International Meeting of the Society for Cryobiology, Bristol, UK, July 2010.
3. B. Cloteaux, "Matching Observed Alpha Helix Lengths to Predicted Secondary Structure," Computational Structural Bioinformatics Workshop 2009, Bethesda, MD, November 1, 2009.
4. B. Cloteaux, "A Structural Approach to the Temporal Modeling of Networks," Winter Simulation Conference 2009, Austin, TX, December 14, 2009.
5. B. Cloteaux, "Approximating the Number of Bases for Almost All Matroids," 41st Southeastern International Conference on Combinatorics, Graph Theory, and Computing 2010, Florida Atlantic University, Boca Raton, FL, March 11, 2010.
6. V. R. Coffman, "OOF3D: An Image-based Finite Element Solver for Materials Science," SEM Annual Conference and Exposition on Experimental and Applied Mechanics, Indianapolis, IN, June 10, 2010.
7. G. Dogan, "Image-Based Analysis of Microstructures with OOF," SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, May 25, 2010.
8. G. Dogan, "A Flexible and Efficient Numerical Framework for Image Segmentation by Energy Minimization," Workshop on Applications of Discrete Geometry and Mathematical Morphology, Istanbul, Turkey, August 22, 2010.
9. M. Donahue, "Accurate Computation of the Demagnetization Tensor for Finite Difference Micromagnetics," Joint Intermag/MMM 2010 Conference, Washington, DC, January 20, 2010.
10. E. Garboczi, J. Bullard, N. Martys, and J. Terrill, "The Virtual Cement and Concrete Testing Laboratory: Performance Prediction, Sustainability, and the CSHub," National Ready Mix Cement Association Concrete Sustainability Conference, Tempe, AZ, April 13-15.
11. W. George, N. Martys, S. Satterfield, J. Hagedorn, M. Olano, J. Terrill, and E. Garboczi, "Simulation of Non-Newtonian Suspensions: Shear Thinning Case," animation, International Conference for High Performance Computing, Networking, Storage, and Analysis (SC09), Portland, OR, November 2009.
12. F. Hunt, "Measuring the Utility/Path Diversity Tradeoff In Multipath Protocols," 4th International Conference on Performance Evaluation Methodologies and Tools, Pisa, Italy, October 20-22, 2009.
13. F. Hunt, "A Mathematical Model of Congestion Control in a Network with Multiple Sources," Dynamics Days Conference, University of Bristol, Bristol, UK, September 9, 2010.
14. E. Knill, "Building Quantum Computers," SURF Seminar, Boulder, CO, June 24, 2010.
15. P.A. Lott, "Fast Solvers for Models of Fluid Flow with Spectral Elements," SIAM Conference on Applied Linear Algebra, Monterey, CA, October 26-29, 2009.
16. A. Lott, "Fast Solvers for Models of Fluid Flow with Spectral Elements," AMS/MAA Joint Mathematics Meetings, San Francisco, CA, January 14, 2010.
17. A. Lott, "Fast Solvers for Models of Thermosolutal Convection," APS/AAPT Joint Physics Meeting, Washington, DC, February 15, 2010.
18. A. Lott, "Fast Solvers for Models of Fluid Flow with Spectral Elements," 11th Copper Mountain Conference on Iterative Methods, Copper Mountain, CO, April 5, 2010.
19. L. Ma, O. Slattery, and X. Tang, "NIR Spectrometer Based on Frequency Up-conversion Technology," American Physical Society March Meeting 2010, Portland, OR, March 15–19, 2010.
20. V. Marbukh, D. Genin, and T. Nakassis paper "Vulnerability of Selfish Routing to Attacks: A Game-theoretic Model and Initial Results" 2010 International Conference of Information Security and Internet Engineering, World Congress on Engineering 2010 (WCE 2010), London, UK, June 30 – July 2, 2010.
21. V. Marbukh, H. Mahboubi, A. Momeni, A. G. Aghdama, and K. Sayrafian-Pour, "Towards Evolutionary-pricing Framework for Mobile Sensor Network Self-organization," IEEE World Congress on Computational Intelligence (WCCI2010), Barcelona, Spain, July 18-23, 2010.
22. N. S. Martys, W. George, S. Satterfield, D. Lootens, P. Hebraud, and J. Hagedorn, "A Smoothed-particle-hydrodynamics-based Fluid Model with a Local Shear-rate Dependent Viscosity: Application to flow of a Suspension with a Non-Newtonian Fluid Matrix," Society for Rheology 81st Annual Meeting, Madison, WI, October 18-22, 2009.
23. N. S. Martys, D. Lootens, W. L. George, and P. Hebraud, "Contact and Stress Anisotropies in the Start-up Flow of Colloidal Suspensions," 2009 Society of Rheology Meeting, Madison, WI, October 18-22, 2009.

24. A. Meier, "Using and Extending Randomized Benchmarks for Trapped-Ion Quantum Computing," 41st Annual Meeting of the Division of Atomic, Molecular, and Optical Physics (DAMOP), Houston, TX, May 26, 2010.
25. W. F. Mitchell, Some Computational Results with *hp*-Adaptive Refinement, SIAM Conference on Parallel Processing for Scientific Computing, February 2010.
26. W. Mitchell, "A Summary of *hp*-Adaptive Finite Element Strategies," Workshop on Adaptive Finite Elements and Domain Decomposition Methods, Milano, Italy, June 17-19, 2010.
27. W. Mitchell, "A Summary of *hp*-Adaptive Finite Element Strategies," 2nd European Seminar on Coupled Problems, Pilsen, The Czech Republic, June 28-July 2, 2010.
28. M. Mullan, "A Numerical Quantum and Classical Adversary," 10th Canadian Summer School on Quantum Information and the associated Workshop on Quantum Algorithms, Computational Models, and Foundations of Quantum Mechanics, Vancouver, Canada, July 17-30, 2010.
29. A. Peskin, K. Kafadar, and A. Dima, "A Quality Pre-Processor for Biological Cell Images," poster presentation, Computational Bioimaging 2009, 5th International Symposium on Visual Computing, Las Vegas, NV, November 30 – December 2, 2009.
30. A. Peskin, A. Dima, J. Chalfoun and J.J. Filliben, "Accuracy in Cell Image Segmentation Algorithms" The International Symposium on Business and Industrial Statistics (IBIS), Portoroz, Slovenia, July 5-9, 2010.
31. A. Peskin, A. Dima, J. Chalfoun and J. Elliot, "Predicting Segmentation Accuracy for Biological Cell Images," Bioimage Informatics 2010, Pittsburg, PA, September 17-19, 2010.
32. B. W. Rust, "Using Confidence Ellipsoids to Choose the Regularization Parameter for Ill-Posed Problems," SIAM Conference on Applied Linear Algebra, Monterey, CA, October 26-29, 2009.
33. B. Saunders, "B-Spline Mesh Generation for the Visualization of Complex Function Data" Seventh International Conference of Curves and Surfaces, Avignon, France, June 24-30, 2010.
34. W.-B. Yang, K. Sayrafian-Pour, J. Hagedorn, J. Terrill, and K.Y. Yazdandoost, "Simulation Study of Body Surface RF Propagation for UWB Wearable Medical Sensors," 2nd International Symposium on Applied Sciences in Biomedical and Communication Technologies, Bratislava, Slovak Republic, November 24-27, 2009.
35. Y. Zhang, "The Statistical Strength of Experiments to Reject Local Realism with Photon Pairs and Inefficient Detectors," 41st Annual Meeting of the Division of Atomic, Molecular, and Optical Physics (DAMOP), Houston, TX, May 28, 2010.

Web Services

1. Digital Library of Mathematical Functions[15]: a repository of information on the special functions of applied mathematics.
2. Guide to Available Mathematical Functions[16]: a virtual repository of mathematical software components.
3. Matrix Market[17]: a repository of matrices for testing of algorithms and software for numerical linear algebra.
4. SciMark[18]: a benchmark for scientific computing in Java.

Software Released[19]

1. f90gl[20]: Fortran 90 interface for the OpenGL graphics library. Version 1.2.15 (December 2, 2009). – *W. Mitchell*
2. Network Graph Toolkit[21]: a suite of applications for graph files for analysis, visualization, conversion between graph formats. Version 3.2 (December 2, 2010). – *R. Pozo*
3. NGraph[22]: a simplified C++ graph library for analysis of complex networks. Version 3.5 (December 2, 2010). – *R. Pozo*
4. OOF2[23]. Object Oriented Finite Elements, modeling of materials with complex microstructures. Version 2.0.5a11 (May 17, 2010). - *S. Langer*
5. PHAML[24]: Parallel Hierarchical Adaptive Multi Level, general purpose software for 2D elliptic

[15] http://dlmf.nist.gov/
[16] http://gams.nist.gov/
[17] http://math.nist.gov/matrixmarket/
[18] http://math.nist.gov/scimark/
[19] In cases where multiple versions have been released during the year we only list the last.
[20] http://math.nist.gov/f90gl
[21] http://math.nist.gov/~RPozo/ngraph/ngraph_toolkit_index.html
[22] http://math.nist.gov/pozo/ngraph
[23] http://www.ctcms.nist.gov/oof/
[24] http://math.nist.gov/phaml/

partial differential equations. Version 1.8.0 (April 2010). – *W. Mitchell*

6. Tcl/Tk[25]: Tool Command Language and Toolkit. Version 8.5.9, (September 8, 2010). – *D. Porter*
7. PCrawler[26]: suite of Python modules to build network graphs by crawling the World Wide Web. Version 2.1 (December 3, 2010). – *R. Pozo*

Conferences, Minisymposia, Lecture Series, Shortcourses

MCSD Seminar Series

1. S. Jordan (California Institute of Technology), "Approximating Topological Invariants on a Quantum Computer," February 3, 2010.
2. H. Elman (University of Maryland), "Numerical Methods for Partial Differential Equations with Random Data," June 24, 1010.
3. E. Cox (Purdue University), "Constrained Regularization for Lagrangian Actinometry," Sept. 21, 2010.
4. J. Benson (NIST), Modeling and Optimization in Cryobiology, Oct. 19, 2010.
5. I. Saniee (Bell Laboratories), The Large Scale Curvature of Networks and Its Implications for Network Management and Security, Nov. 9, 2010.
6. M. Cromer, Jr. (University of Delaware), Modeling and Simulation of a Complex Fluid: Wormlike Micellar Solutions, Nov. 30, 2010.

Hosted Public Events

1. R. Boisvert, Member, Organizing Committee, From Quantum Information and Complexity to Post Quantum Information Security, University of Maryland, October 27-29, 2010.
2. R. Boisvert, Chair, Organizing Committee, IFIP Working Conference on Uncertainty Quantification in Scientific Computing, Boulder, CO, Aug. 1-4, 2011.
3. A. Dienstfrey, Chair, Program Committee, IFIP Working Conference on Uncertainty Quantification in Scientific Computing, Boulder, CO, Aug. 1-4, 2011.
4. D. Lozier, Member, Organizing Committee, International Conference on Special Functions in the 21st Century: Theory and Applications, Washington, DC, April 6-8, 2011.

External Events Organization

1. M. Donahue, Member, Organizing Committee, 6th SIAM meeting on Mathematical Aspects of Materials Science, Philadelphia, PA, May 23-26, 2010.
2. M. Donahue, Minisymposium Organizer, Micromagnetic Modeling and Computation, 6th SIAM meeting on Mathematical Aspects of Materials Science, Philadelphia, PA, May 23-26, 2010.
3. J. Fong, Minisymposium Organizer, Pressure Vessels and Piping Failure Databases, Probability of Failure Prediction, Consequence of Failure Estimation, and Risk Analysis for Aging Plants, ASME PVP Conference, Bellevue, WA, July 19-23, 2010.
4. E. Knill, Member, Organizing Committee, From Quantum Information and Complexity to Post Quantum Information Security, University of Maryland, October 27-29, 2010.
5. D. P. O'Leary, Member, Organizing Committee, SIAM Annual Meeting, Pittsburgh, PA, July 12-16, 2010.
6. D. P. O'Leary, Member, Organizing Committee, Numerical Linear Algebra: Perturbation, Performance, and Portability, Conference in honor of G. W. Stewart, Austin, TX, July 19-20, 2010.
7. D. P. O'Leary, Member, Organizing Committee, SIAM Conference on Applied Linear Algebra (LA12), Valencia, Spain, June 18-22, 2012.
8. B. Miller, Member, Program Committee, 9th Mathematical Knowledge Management Conference, Paris, France, July 2010.
9. B. Miller, Program Committee, 10th Mathematical Knowledge Management Conference, Bertinoro, Italy, July 18-22, 2011.
10. W. F. Mitchell, Member, Scientific Committee, International Conference of Numerical Analysis and Applied Mathematics, Rhodes, Greece, September 19-25, 2010.
11. Y. Parker and J. Terrill, Organizers, NIST Exhibit and Demonstration Booth, SC10, the 2010 International Conference for High Performance Computing, Networking, Storage and Analysis, New Orleans, November 13-19, 2010.
12. B. Rust and K. Mullen (MML), Minisymposium Organizers, Recent Advances in Separable

[25] http://tcl.sourceforge.net/
[26] http://math.nist.gov/~RPozo/ngraph/webcrawler.html

Nonlinear Least Squares, International Congress on Industrial and Applied Mathematics, Vancouver, July 18-22, 2011.

Other Professional Activities

Internal

1. I. Beichl, Member, NIST Research Advisory Committee.
2. I. Beichl, Co-organizer, ITL Summer Undergraduate Research Fellowship (SURF) program.
3. R. Boisvert, Member, NIST Scientific Computing Steering Group.
4. R. Boisvert, Member, ITL Diversity Committee.
5. D. Gilsinn, Division Safety Representative (term ended October 2010).
6. Barry Hershman, Division Safety Representative (term began October 2010).
7. W. Mitchell, Chair, ITL Awards Committee.
8. A. O'Gallagher, Organizer, ITL Diversity Book Club.
9. A. O'Gallagher, Member, Boulder Labs Diversity Council,
10. A. O'Gallagher, Member, ITL Diversity Committee.
11. A. Peskin, Member, Boulder Research Advisory Council.
12. O. Slattery, Member, NIST Laser Safety Committee.
13. O. Slattery, Member, NIST Safety Operational Committee.

External

Editorial

1. I. Beichl, Editor-in-Chief, *Computing in Science & Engineering*.
2. J. Benson, Associate Editor, *CryoLetters*.
3. R. Boisvert, Associate Editor, *ACM Transactions on Mathematical Software*.
4. R. Boisvert, Editor, Numerical Analysis, Mathematical Software, and Computational Engineering, Finance, and Science areas of the Computing Research Repository (CoRR) preprint service hosted by www.arXiv.org.
5. D. Lozier, Associate Editor, *Journal of Numerical Analysis, Industrial and Applied Mathematics*.
6. G. McFadden, Associate Editor, *Journal of Crystal Growth*.
7. G. McFadden, Associate Editor, *Interfaces and Free Boundaries*.
8. G. McFadden, Guest Co-editor, Special issue of the *Journal of Fluid Mechanics* in honor of the 70th birthday of the main editor, Professor Stephen H. Davis, of the Engineering and Applied Sciences Department at Northwestern University.
9. W. Mitchell, Associate Editor, *Journal of Numerical Analysis, Industrial and Applied Mathematics*.
10. D. P. O'Leary, Editor-in-Chief, *SIAM Journal on Matrix Analysis and Applications*.
11. D. P. O'Leary, Member, Editorial Board, Education Section, *SIAM Review*.
12. D. P. O'Leary, Member, Editorial Board, *SIAM Books*.
13. D. P. O'Leary, Member, Editorial Board, SIAM book series on "Fundamentals of Algorithms."
14. D. P. O'Leary, Member, Editorial Board, *Computing in Science & Engineering*.
15. D. Porter, Guest Editor, *IEEE Transactions on Magnetics,* November 2009 (Selected papers from the 2009 Hysteresis and Micromagnetic Modeling Symposium).
16. R. Pozo, Associate Editor, *ACM Transactions on Mathematical Software*.

Boards and Committees

1. I. Beichl, Member, IEEE Electronic Products and Services Subcommittee.
2. R. Boisvert, Chair, International Federation for Information Processing's (IFIP) Working Group 2.5 on Numerical Software.
3. R. Boisvert, Co-chair, Publication Board, Association for Computing Machinery (ACM).
4. R. Boisvert, Ex-Officio Member, Association for Computing Machinery (ACM) Council.
5. R. Boisvert, Member, Program Review Committee, Center for Computing Sciences, Institute for Defense Analysis.
6. R. Boisvert, Member, External Review Committee, Computer Science Department, George Washington University.

7. D. Lozier, Secretary, Activity Group on Orthogonal Polynomials and Special Functions, Society for Industrial and Applied Mathematics (SIAM).
8. D. Lozier, Founding Member, Painlevé Project[27].
9. G. McFadden, Member, Nomination Committee, SIAM Activity Group on Mathematical Aspects of Materials Science.
10. B. Miller, Member, Math Working Group, World Wide Web Consortium (W3C).
11. D. P. O'Leary, Member, Oversight Committee, Gene Golub SIAM Summer School.
12. D. P. O'Leary, Member, Advisory Committee, SIAM Linear Algebra Activity Group International Summer School on Numerical Linear Algebra.
13. D. P. O'Leary, Chair, Committee on Committees, Association for Women in Mathematics.
14. D. Porter, Member, Tcl Core Team.
15. B. Saunders, Member, Mathematics Advisory Panel, Department of Mathematics and Statistics, American University, Washington, DC.
16. B. Saunders, Member, Advisory Group, NSF CoSMIC Scholars Program, Towson University.
17. J. Terrill, Member, Federal High End Computing Implementation Task Force.
18. J. Terrill, Member, High End Computing Research and Development, and Infrastructure Interagency Working Groups, Networking and Information Technology R&D (NITRD) National Coordination Office.

Reviewing

Division staff members referee manuscripts for a wide variety of journals and conferences including *ACM Transactions on Mathematical Software, Annals of the European Academy of Sciences, Computing in Science & Engineering, CryoLetters*, *IEEE/ACM Transactions on Networking, IEEE Transactions on Magnetics, International Journal of Computer Mathematics, Inverse Problems, Journal of Applied Physics, Journal of Computing and Information Science in Engineering, Journal of Fluid Mechanics, Journal of Numerical Analysis, Industrial and Applied Mathematics, Journal of Physics B: Atomic, Optical and Molecular Physics, Journal of Supercomputing, Linear Algebra and its Applications*, *Mathematical Reviews*, *Nature*, *New Journal of Physics*, *Nonlinear Dynamics, Physical Review A, Physical Review B, Physical Review Letters*, *Reviews of Modern Physics, SIAM Journal on Scientific Computing.*

MCSD staff reviewed proposals for the following agencies/competitions during FY 2010: Canada Research Chairs, DOE, NSF, NIST ARRA Measurement Science and Engineering Grants Program.

External Contacts

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

Industrial Labs

Achronix Semiconductor
ADVR Inc.
Alcatel-Lucent Bell Laboratories
Deepwoods Software
Lepton Technologies Inc.
Lockheed Martin
Marintek (Norway)
Microsoft
Morson Projects Ltd. (UK)
Motorola
Northrup Grumman
NVIDIA
Orbital Sciences Corporation
Palantir Technologies
RSA
Toptica Photonics
Wipro Technologies

Government/Non-profit Organizations

Army Research Laboratory
Association for Computing Machinery
Food and Drug Administration
IDA Center for Computing Sciences
Institut Geographique National (France)
Institute for Defense Analysis
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Moscow Engineering Physics Institute (Russia)
NASA
National Institutes of Health
National Security Agency
Naval Research Laboratory
Perimeter Institute for Theoretical Physics (Canada)
Sandia National Laboratories
Santa Fe Institute
Society for Industrial and Applied Mathematics
SP Technical Research Institute of Sweden
US Air Force
US Army

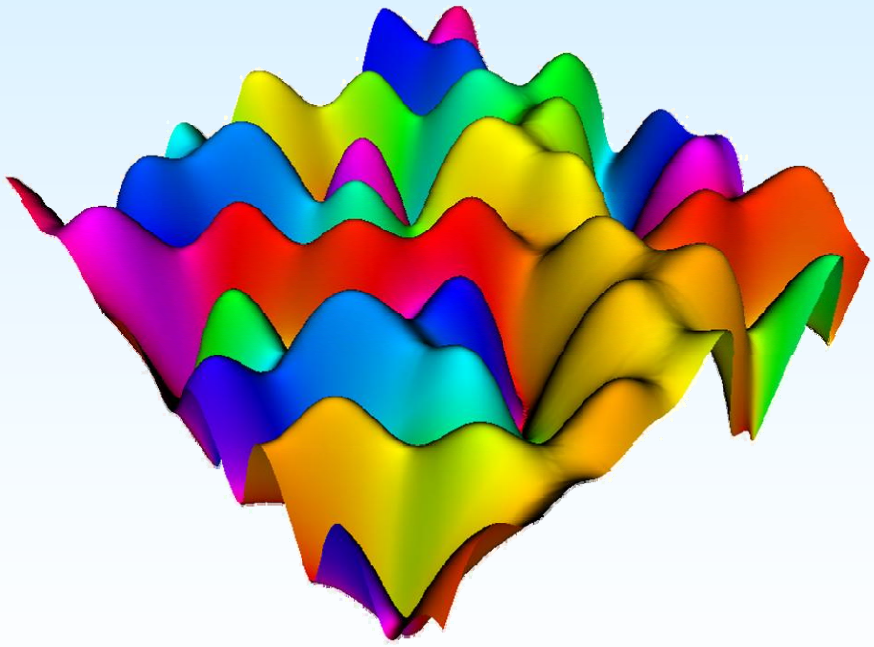
[27] http://math.nist.gov/~lozier/PainleveProject/

Universities

Abo Akademi University (Finland)
Aalto University (Finland)
Albion College
Boston University
California Institute of Technology
California State University
Concordia University (Canada)
Clemson University
Colorado State University
École Supérieure de Physique et de Chimie Industrielles (France)
George Mason University
George Washington University
Indian Institute of Technology (India)
Indiana University
Johns Hopkins University Applied Physics Lab
Nicolaus Copernicus University (Poland)
Kettering University
King Abdullah Univ. of Sci. and Tech. (Saudi Arabia)
Nancy University (France)
Nottingham University
Ohio State University
Princeton University
Purdue University
Royal Institute of Technology (Sweden)
Saint Mary's College
Stanford University
SUNY Binghamton
Technische Univ. Bergakademie Freiberg (Germany)
Tulane University
Universidade Federal do Rio Grande do Sul (Brasil)
Universidade Federal do Ceará (Brazil)
Universidade Federal de Uberlândia (Brazil)
University of Antwerp (Belgium)
University of California at Berkeley
University of the Basque Country (Spain)
University of California at Irvine
University of Central Florida – Orlando
University of Colorado
University of Delaware
University of Edinburgh (Scotland)
University of Hawaii
University of Maryland
University of Maryland Baltimore County
University of Montana
University of Nebraska – Lincoln
University of Nevada – Reno
University of Texas at Arlington
University of Palermo (Italy)
University of Utah
University of Vienna (Austria)
University of Virginia
University of Washington
University of Wisconsin
Vassar College
Virginia Tech
Yale University

Part V

Appendix



Staff

ACMD consists of full time permanent staff located at NIST laboratories in Gaithersburg, MD and Boulder, CO. This is supplemented with a variety of faculty appointments, guest researchers, postdoctoral appointments, and student appointments. The following list reflects all appointments held during any portion of the reporting period. (*) Denotes staff at the NIST Boulder Laboratory.

Division Staff

Ronald Boisvert, *Chief*, Ph.D. (Computer Science), Purdue University, 1979
Robin Bickel, *Secretary*
Robert Bohn, Ph.D. (Physical Chemistry), University of Virginia, 1991
Alfred Carasso, Ph.D. (Mathematics), University of Wisconsin, 1968
Roldan Pozo, Ph.D. (Computer Science), University of Colorado at Boulder, 1991
Christopher Schanzle, B.S. (Computer Science), University of Maryland Baltimore County, 1989

Mathematical Analysis and Modeling Group

Timothy Burns, *Leader*, Ph.D. (Mathematics), University of New Mexico, 1977
*Bradley Alpert, Ph.D. (Computer Science), Yale University, 1990
Javier Bernal, Ph.D. (Mathematics), Catholic University, 1980
*Andrew Dienstfrey, Ph.D. (Mathematics), New York University, 1998
Jeffrey Fong, Ph. D. (Applied Mechanics and Mathematics), Stanford University, 1966
David Gilsinn, Ph.D. (Mathematics), Georgetown University, 1969
Fern Hunt, Ph.D. (Mathematics), New York University, 1978
Raghu Kacker, Ph.D. (Statistics), Iowa State University, 1979
Anthony Kearsley, Ph.D. (Computational and Applied Mathematics), Rice University, 1996
Peter Ketcham. M.S. (Mathematics), University of Minnesota, 1997
Geoffrey McFadden, *NIST Fellow,* Ph.D. (Mathematics), New York University, 1979
*Agnes O'Gallagher, M.S. (Applied Mathematics), University of Colorado at Boulder, 1991
Bert Rust, Ph.D. (Astronomy), University of Illinois at Urbana-Champaign, 1974

NRC Postdoctoral Associates
James Benson, Ph.D. (Mathematics), University of Missouri – Columbia, 2009
P. Aaron Lott, Ph.D. (Mathematics), University of Maryland, 2008

Faculty Appointee (Name, Degree / Home Institution)
Daniel Anderson, Ph.D. / George Mason University
Saul Gass, Ph.D. / University of Maryland College Park
Dianne O'Leary, Ph.D. / University of Maryland College Park
Florian Potra, Ph.D. / University of Maryland Baltimore County

Guest Researchers (Name, Degree / Home Institution)
Mirit Aladjem, Ph.D. / National Institutes of Health
Richard Braun, Ph.D. / University of Delaware
Guillaume Bousquet / ISIMA, Campus de Clermont-Ferrand, France
David Cotrell, Ph.D. / Lawrence Livermore National Laboratory
*John Gary, Ph.D. / NIST (retired)
Katharine Gurski, Ph.D. / George Washington University
Rüdiger Kessel, Ph.D. / Metrodata GmbH, Germany
Sohyoung Kim, Ph.D. / National Institutes of Health
Yu (Jeff) Lei, Ph.D. / University of Texas at Arlington

Bruce Murray, Ph.D. / SUNY Binghampton
Sita Ramamurti, Ph.D. / Trinity Washington University
Christoph Witzgall, Ph.D., *NIST Scientist Emeritus*

Students (Name / Home Institution)
Nathan Jacobson / Hood College

Mathematical Software Group

Daniel Lozier, *Leader,* Ph.D. (Applied Mathematics), University of Maryland, 1979
Michael Donahue, Ph.D. (Mathematics), Ohio State University, 1991
Stephen Langer, Ph.D. (Physics), Cornell University, 1989
Marjorie McClain, M.S. (Mathematics), University of Maryland College Park, 1984
Bruce Miller, Ph.D. (Physics), University of Texas at Austin, 1983
William Mitchell, Ph.D. (Computer Science), University of Illinois at Urbana-Champaign, 1988
Donald Porter, Ph.D. (Electrical Engineering), Washington University, 1996
Bonita Saunders, Ph.D. (Mathematics), Old Dominion University, 1985

NRC Postdoctoral Associates
Valerie Coffman, Ph.D. (Physics), Cornell University, 2006
Howard Cohl, Ph.D. (Mathematics), University of Auckland, 2010

Contractors
Andrew C.E. Reid, Ph.D. (Physics), Queen's University, Kingston, Ontario, 1994
Gunay Dogan, Ph.D. (Applied Math and Scientific Computing), University of Maryland, 2006

Faculty Appointees (Name, Degree / Home Institution)
Frank Olver, D.Sc. / University of Maryland College Park
G.W. Stewart, Ph.D. / University of Maryland College Park
Abdou Youssef, Ph.D. / George Washington University

Guest Researchers (Name, Degree / Home Institution)
Leonard Maximon, Ph.D. / George Washington University
Qiming Wang / NIST (retired)

Computing and Communications Theory Group

Ronald Boisvert, *Acting Leader*
Isabel Beichl, Ph.D. (Mathematics), Cornell University, 1981
Brian Cloteaux, Ph.D. (Computer Science), New Mexico State University, 2007
*Scott Glancy, Ph.D. (Physics), University of Notre Dame, 2003
Barry Hershman, A.A. (Electronics Engineering), Capitol College, 1979
*Emanuel Knill, *NIST Fellow,* Ph.D., (Math), University of Colorado at Boulder, 1991
Vladimir Marbukh, Ph.D. (Mathematics) Leningrad Polytechnic University, 1986
Alan Mink, Ph.D. (Electrical Engineering), University of Maryland, 1980.
Oliver Slattery, M.S. (Electrical Engineering), Johns Hopkins University, 2008
Xiao Tang, Ph.D (Physics), Chinese Academy of Sciences, 1985

NRC Postdoctoral Associates
*Bryan Eastin, PhD. (Physics), University of New Mexico, 2007
Elizabeth Moseman, Ph.D. (Mathematics), Dartmouth College, 2007

Contractors
Lijun Ma, Ph.D. (Optical Engineering), Tsinghua University, 2001

Faculty Appointees (Name, Degree / Home Institution)
James Lawrence, Ph.D. / George Mason University

Guest Researchers (Name, Degree / Home Institution)
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Glossary of Acronyms

AAPT	American Association of Physics Teachers
ACM	Association for Computing Machinery
ACMD	NIST/ITL Applied and Computational Mathematics Division
ACTS	Advanced Combinatorial Test Suites (software)
ACS	Advanced Camera for Surveys
AISI	American Iron and Steele Institute
AMS	American Mathematical Society
APD	avalanche photo diode (photon detector)
APS	American Physical Society
ASME	American Society of Mechanical Engineers
BLAS	Basic Linear Algebra Subprograms
CI	configuration interaction
CiSE	Computing in Science & Engineering
CMM	coordinate measuring machine
CMOS	complementary metal-oxide semiconductor
CNST	NIST Center for Nanoscale Science and Technology
CODATA	Committee on Data for Science and Technology
CPU	central processing unit
CRADA	Cooperative Research and Development Agreement
CT	computed tomography
CVE	Common Vulnerabilities and Exposures
CY	calendar year
DARPA	DOD Defense Advanced Research Projects Agency
DIVERSE	Device Independent Virtual Environments — Reconfigurable, Scalable, Extensible (software)
DLMF	Digital Library of Mathematical Functions
DNA	deoxyribonucleic acid
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
DPD	dissipative particle dynamics
EL	NIST Engineering Laboratory
EM	electromagnetic
EM	expectation maximization
EPG	error probability per gate
ETSI	European Telecommunications Standards Institute
FDA	Food and Drug Administration
FDS	Fire Dynamics Simulator
FFT	fast Fourier transform
FMM	fast multipole method
FY	fiscal year
F90gl	Fortran 90 interface to OpenGL graphics standard
GAMS	Guide to Available Mathematical Software
GUI	graphical user interface
HEC	high-end computing
HIM	helium ion microscope
HTML	hypertext markup language
Hy-CI	Hylleraas-Configuration Interaction technique
IDA	Institute for Defense Analysis
IEEE	Institute of Electronics and Electrical Engineers
IETF	Internet Engineering Task Force
IFIP	International Federation for Information Processing
IMS	Innovations in Measurement Science
INCITE	Innovative and Novel Computational Impact on Theory and Experiment (DOE Program)
IR	infrared
ISIMA	Institut Supérieur d'Informatique, de Modélisation et de leurs Applications (France)

IT	information technology
ITL	NIST Information Technology Laboratory
IWG	Interagency Working Group
JAMA	Java Matrix package (software)
LANL	Los Alamos National Laboratory
LAPACK++	software for numerical linear algebra in C++
LaTeXML	LaTeX to MathML translator
LTP	Live Tables Project
MAA	Mathematical Association of America
MANET	mobile ad-hoc network
MathML	Mathematical Modeling Language (W3C standard)
MCMC	Markov Chain Monte Carlo
MKM	mathematical knowledge management
MML	NIST Material Measurement Laboratory
MMM	magnetism and magnetic materials
MPI	Message Passing Interface
MRAM	magneto-resistive random access memory
MRI	magnetic resonance imaging
MSN	mobile sensor network
μmag	Micromagnetics Activity Group
NASA	National Aeronautics and Space Administration
NBS	National Bureau of Standards
NCNR	NIST National Center for Neutron Research
NIH	National Institutes of Health
NIR	near infrared
NIST	National Institute of Standards and Technology
NISTIR	NIST Internal Report
NITRD	Networking and Information Technology Research and Development
NRC	National Research Council
NSF	National Science Foundation
NUM	network utility maximization
NUMA	non-uniform memory access
NVD	National Vulnerability Database
NYU	New York University
OOF	Object-Oriented Finite Elements (software)
OOMMF	Object-Oriented Micromagnetic Modeling Framework (software)
OSG	Open Scene Graph
OSPF	open shortest path first
OTF	optical transfer function
OWL	Web Ontology Language
PDE	partial differential equation
PHAML	Parallel Hierarchical Adaptive Multi Level (software)
PML	NIST Physical Measurement Laboratory
PPLN	periodically poled lithium niobate
PREP	Professional Research Experience Program
QD	quantum dot
QDPD	quarternion-based dissipative particle dynamics
QI	quality index
QIS	quantum information science
QKD	quantum key distribution
QPM	quasi phase matching
R&D	research and development
PDE	partial differential equation
REGEN	software for modeling of cryocoolers
SAVG	MCSD Scientific Applications and Visualization Group
SBIR	Small Business Innovative Research
SCAP	Security Content Automation Protocol

SciDAC	Scientific Discovery through Advanced Computing (DOE Program)
SHIP	NIST Summer High School Internship Program
SIAM	Society for Industrial and Applied Mathematics
SIGGRAPH	ACM Special Interest Group on Graphics
SIS	sequential importance sampling
SparseLib++	software for spare linear algebra in C++
Spblas	sparse basic linear algebra subprograms
SPIE	International Society for Optical Engineering
STEP	NIST Student Temporary Employment Program
SUNY	State University of New York
SURF	Student Undergraduate Research Fellowship
TES	transition-edge sensor
TIP	NIST Technology Innovation Program
TNT	Template Numerical Toolkit (software)
TRC	NIST Thermodynamics Research Center
TV	total variation
UCLA	University of California at Los Angeles
UMBC	University of Maryland Baltimore County
URL	universal resource locator
VCCTL	Virtual Cement and Concrete Testing Laboratory
VRML	virtual reality modeling language
W3C	World Wide Web Consortium
X3D	Extensible 3D
XML	Extensible Markup Language
ZPE	zero-point energy