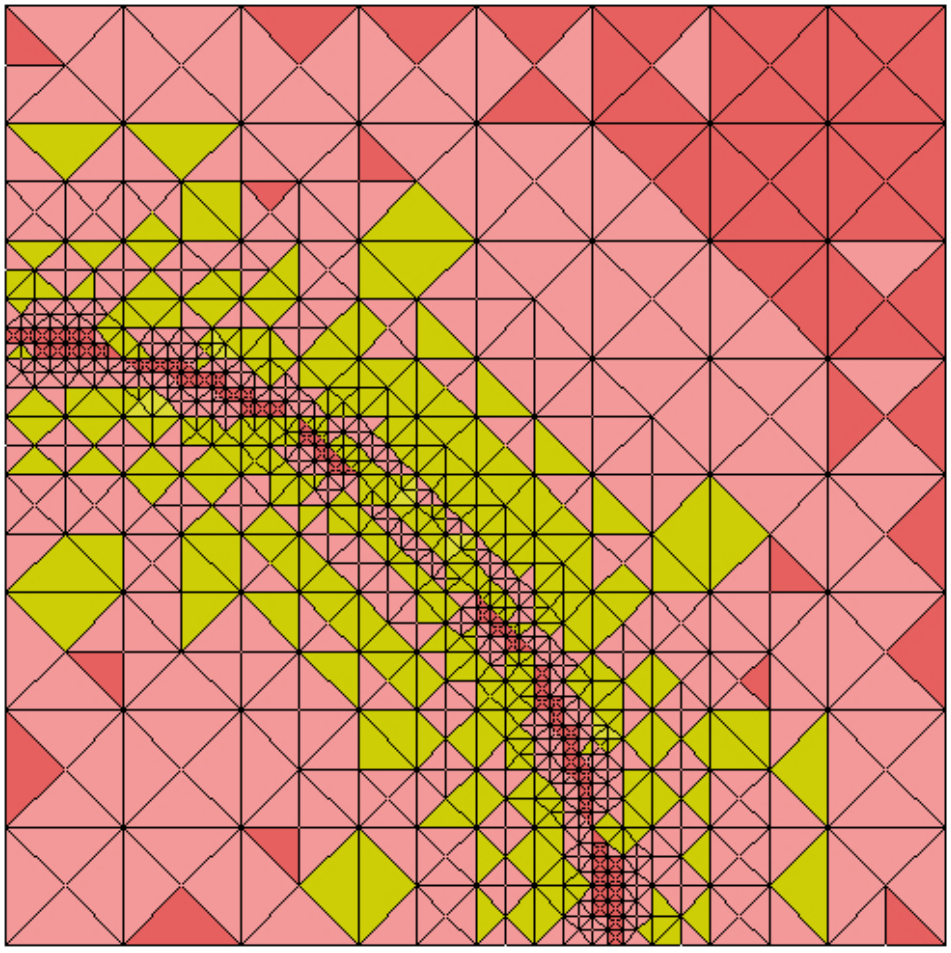
NISTIR 7856

Applied and Computational Mathematics Division

Summary of Activities for Fiscal Year 2011



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

NISTIR 7856

Applied and Computational Mathematics Division

Summary of Activities for Fiscal Year 2011

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

May 2012

U.S. Department of Commerce
John E. Bryson, 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 2010 through December 2011.

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 computational grid for an elliptic boundary value problem whose solution has a mild circular wave front. The colors represent the polynomial degree of approximation over each element. The grid comes from a comparative study of automated grid refinement strategies. The strategies studied utilize a combination of refinement in space (h) and in polynomial degree (p), termed hp-refinement. The study was undertaken by William Mitchell and Marjorie McClain. For details, see page 27.

Acknowledgement: We are grateful to Robin Bickel for collecting the information and organizing the first draft of this report. Thanks also to Timothy Burns and Ashit Talukder for carefully reading through the document and providing corrections.

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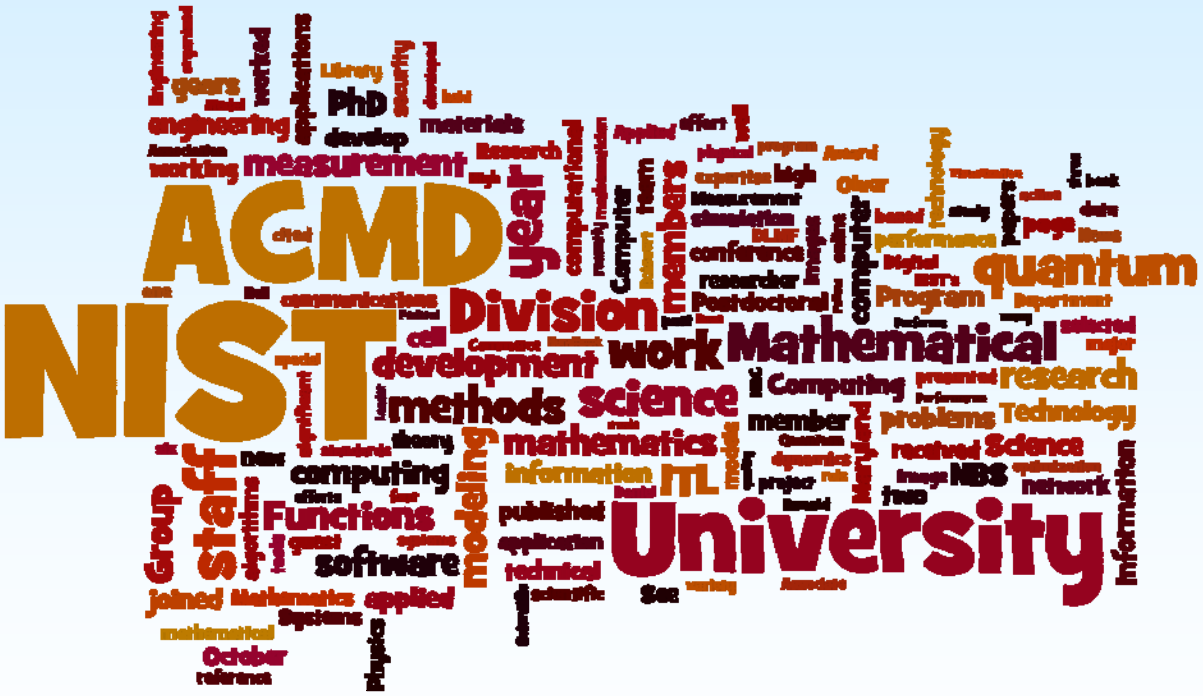
Part I

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 and user facilities 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 ACMD 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 groups and external organizations 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 addition, ITL has several cross-cutting programs to which the Division contributes:

- *Virtual Measurement Systems.* A virtual measurement is a quantitative result and its associated uncertainty, obtained by a computer simulation or computer-assisted measurements. This Program introduces metrology constructs, standard references, uncertainty characterization, and traceability into scientific computation and computer-assisted measurements to enable predictive computing with quantified reliability.

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 to 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.* Complex Systems are composed of large interrelated, interacting entities which taken together, exhibit a macroscopic behavior which may not be predictable by examining the components. This Program seeks to understand the fundamental science of these systems and develop rigorous mathematical and statistical descriptions that enable prediction and control of their behavior.
- *Pervasive Information Technology.* Pervasive information technology is the trend towards increasingly ubiquitous connected computing sensors, devices, and networks that monitor and respond transparently to human needs. This Program creates the mathematical and statistical foundations that facilitate the creation of standards for sensor communication, networking interoperability, and sensor information security.

In Part III of this document we provide outlines of most ongoing technical projects of the Division. These are organized by thematic area. ITL Programs to which the project contributes are also identified.

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 notable technical accomplishments with significant impact. Further details are provided in Part II (Features) and Part III (Project Summaries).

Digital Library of Mathematical Functions. The DLMF[1], a major online reference on the special functions of applied mathematics, which, along with its print companion, the *NIST Handbook of Mathematical Functions*, was released in May 2010, continues to garner significant attention. The work has seen favorable reviews in *SIAM News*, *SIAM Review*, *Notices of the American Mathematical Society*, *Optics and Photonics News*, and the *International Statistical Review*. After just 19 months Google Scholar has already identified 166 citations to the print edition. In late 2011 the work was recognized with two significant awards: the Department of Commerce Gold Medal and the *Government Computer News* award for IT achievement in government. **(See page 74.)**

On April 6-8, 2011 ACMD hosted a major conference on this topic. More than 60 researchers in the field of special functions from 10 countries and the U.S. participated in the International Conference on Special Functions in the 21st Century: Theory and Applications, which was held in Washington, DC. The conference provided a forum for the exchange of expertise, experience and insights among world leaders on the subject. The conference highlighted the recent release of the DLMF and was dedicated to its Mathematics Editor, Frank W. J. Olver. Six plenary and 34 contributed talks were presented. The plenary speakers were Roderick Wong (City University of Hong Kong), Leonard Maximon (George Washington University), Nalini Joshi (University of Sydney), Michael Berry (University of Bristol), William Reinhardt (University of Washington), and Richard Askey (University of Wisconsin). The City University of Hong Kong, the University of Maryland, and SIAM were co-sponsors. Daniel Lozier of ACMD Chaired the Organizing Committee.

Mathematics of Metrology. ACMD was the host of a second major conference this year, which was associated with the ITL Virtual Measurement Systems program. A virtual measurement is a measurement made using a computer simulation model. As in physical measurement, characterizing the uncertainty in the measured quantity is of prime concern. This was the main subject of the Working Conference on Uncertainty Quantification in Scientific Computing[2] held in Boulder, CO on August 1-4, 2011, where 76 participants representing 10 countries gathered to consider the role of metrology in mathematical modeling and computer simulation. Among the keynote speakers were Pasky Pascual of the US Environmental Protection Agency, William Kahan of the University of California at Berkeley, Scott Ferson of Applied Biomathematics, and Maurice Cox of the National Physical Laboratory (UK). Applications discussed included cosmology, weather/climate modeling, atmospheric chemistry, hydrology, nuclear energy/safety, fluid dynamics, engineering mechanics, manufacturing processes, medicine, toxicology, and computer security. Proceedings will be published by Springer. **(See page 51.)**

The ITL Virtual Measurement Systems Program also received a boost this year from an interagency initiative in materials science: the Materials Genome Initiative (MGI). The MGI, which was announced by the President in June[3], seeks to develop the computational modeling and simulation infra-

[1] http://dlmf.nist.gov/
[2] http://www.nist.gov/itl/math/ifip-woco-10.cfm
[3] http://www.whitehouse.gov/blog/2011/06/24/materials-genome-initiative-renaissance-american-manufacturing

structure needed to significantly accelerate the process by which new materials are developed and deployed. One of four participating Federal agencies[4], NIST is expected to play a critical role in several areas, including the curation of materials property data, standards for data and software interoperability, and the technology and tools for the assessment of quality of computational results. ACMD's long experience in materials modeling, scientific software development, and its growing competence in uncertainty quantification in scientific computing will position it well to make contributions to this effort in the coming years.

Scientific Software. ACMD, in collaboration with the NIST Materials Measurement Laboratory, this year released a new version of its OOF2 software system for modeling materials with complex microstructures. Such materials are composed of many small regions, or grains, with different compositions or crystalline orientations. The microscopic shape and arrangement of the grains affects the macro scale properties of the material. Users start with a micrograph, which gives the geometry of the grains, and use OOF2 to generate a finite element mesh which is then used to calculate various physical properties of the material as a whole. The new version, 2.1, can solve for nonlinear and time dependent physical properties, including coupled elasticity, thermal conductivity, and dielectricity, on two dimensional material images. A three dimensional version is under development. OOF2 was developed by Valerie Coffman, Gunay Dogan, and Stephen Langer of ACMD and Andrew Reid of MML. OOF2 can be downloaded[5] at no cost. **(See page 70.)**

This year ACMD's software system, PHAML[6], for parallel solution of elliptic partial differential equations[7] (PDEs) based on adaptive grid refinement and multigrid methods, was used as a platform for a major survey of methods for so-called *hp* adaptive grid refinement. Adaptive methods are essential for successfully attacking the most challenging modeling problems based on PDEs. *h*-based methods improve their solution estimates by refining in space (i.e., reducing size of triangles), while *p*-based methods refine by increasing the polynomial order of approximation on fixed-size grid elements. *hp* methods combine the two. Many heuristics have been proposed for implementing such a refinement strategy. 13 separate strategies were evaluated on a battery of 12 test problems. Not only do the results provide useful data on the comparative performance of the methods, but they also provide insight on practical tradeoffs between efficiency and performance. **(See page 72.)**

High Performance Computing and Visualization. Our effort to develop a high fidelity modeling capability for the simulation of dense suspensions continues. Our model, QDPD, which was developed in collaboration with the NIST Engineering Lab, is based on a dissipative particle dynamics approach. This is currently being applied to the study of rheometers for measuring flow properties of concrete. A typical simulation for this problem may entail keeping track of up to 100,000 solids of varying shape and size. The resulting computational complexity requires the use of parallel processing. Our parallel implementation scales well up to 32,000 processors on the Blue Gene/P supercomputer at Argonne National Laboratories. Late last year we were awarded an additional 22 million CPU hours for this effort from the Department of Energy's INCITE program[8]. **(See page 34.)**

We continue to refine our growing expertise in image analysis, which is becoming an increasingly important tool in metrology. This year, for example, we worked with colleagues at the National Institutes of Health who are studying the migration of cancer cells which can lead to metastasis. Large sequences of images are collected to study cell migration, but these are difficult to process manually, and existing image segmentation and tracking methods are largely ineffective on cell imagery. We have developed novel image segmentation and cell tracking algorithms for this application. **(See page 38.)**

Quantum Information. We continue our efforts to assess both the opportunities and the risks posed by quantum engineering. The opportunities include the development of specialized computing de-

[4] The others are the Department of Energy, the Department of Defense, and the National Science Foundation.
[5] http://www.ctcms.nist.gov/oof/oof2
[6] http://math.nist.gov/phaml/
[7] Ellipic PDEs are ubiquitous in mathematical modeling of numerous processes, including electrostatics, steady-state diffusion, pressure fields in fluid flow, and quantum mechanics.
[8] http://www.doeleadershipcomputing.org/incite-program/

vices which can solve heretofore intractable problems. A significant risk is that fast quantum algorithms for factoring and computing discrete logarithms break the public key infrastructure that is the basis for secure online commerce. An important Division effort is the development and application of experimental benchmarks for evaluating the practical capability of the many physical systems which have been proposed to effectively quantum compute. One such method for determining an error per unit gate (EPG) for one-qubit computations has been implemented on an increasing number of platforms. This year Division staff participated in a new implementation of this benchmark in a NIST ion trap where the qubits are manipulated with microwaves instead of laser light. This implementation successfully demonstrated EPGs below the critical value of 0.0001, which is believed to be necessary for practical scalable quantum computing. **(See page 78.)**

Division staff played a critical role in an important demonstration of quantum optical engineering critical to future quantum computing applications. In a collaborative effort with NIST's Center for Nanoscale Science and Technology, Division staff demonstrated for the first time 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. Quantum dots have potential both as qubit storage devices, as well as reliable photon sources. Converting the color of an emitted photon in this way enables highly efficient detection by commercially available detectors. Division staff developed the highly sensitive and efficient upconversion detectors used in this study, which was reported in *Nature Photonics*. **(See page 40.)**

Our effort to characterize the true power of quantum computers was given a significant boost this year with the hiring of two experts in quantum algorithms and complexity theory. One interest will be the analysis of computational problems which could serve as a basis for public key cryptosystems which are immune to attack by quantum computers.

Foundations of Measurement Science for Information Systems. We continue to make progress in this ACMD initiative which began in FY2007. Our work focuses on characterizing the structure and dynamics of networked information systems. The goal is to understand how these influence network performance, e.g., reliability and security. The tools for this work include graph theory, combinatorics, discrete dynamics, optimization, and game theory. Examples of our work include the development of Monte Carlo approximation methods for combinatorially difficult counting problems, such as computing the reliability polynomial of a large graph, the evaluation of methods for community detection in graphs, modeling of network routing algorithms, and the optimization of network bandwidth assignments. Finally, we are considering some application areas, such as software testing. **(See page 84.)**

This year we kicked-off a new collaboration with Bell Laboratories by sponsoring a joint workshop. Some two dozen researchers in a newly emerging subfield of network science gathered together at Bell Labs in Murray Hill, NJ on April 26, 2011, at a joint Bell Labs-NIST Workshop on Large-Scale Geometry of Networks. The meeting highlighted current work on fundamental geometric methods in the modeling and optimization of complex networks. A particular focus was the hyperbolicity of network graphs and its possible impact on network performance, reliability, robustness and security, with the eventual goal of creating new metrics for such network characteristics. The workshop featured eight technical presentations from researchers at the University of California at Santa Cruz, the University of Southern California, the Cooperative Association for Internet Data Analysis (CAIDA) at UCSD, Rutgers, Bell Labs, and NIST. Researchers from AT&T Labs also attended. Eight ACMD staff members participated. The meeting was co-organized by Iraj Saniee of Bell Labs and Vladimir Marbukh of ACMD.

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 22 articles appearing in peer-reviewed journals, two book chapters, 33 papers in conference proceedings, and nine magazine articles. Thirty-one additional papers have been accepted for publication, while 24 others are undergoing review. Division staff members gave 54 invited technical talks and presented 40 others in conferences and workshops.

Table 1. *Downloads of Selected Division Software Packages During CY 2011*

Package	Description	Downloads
JAMA	Linear algebra in Java	33,499
TNT	Linear algebra using C++ templates	8,900
OOMMF	Modeling of nano-magnetic phenomena	5,000
f90gl	Fortran 90 interface to OpenGL graphics	1,945
spblas	Sparse basic linear algebra components	1,388
OOF	Modeling materials with complex microstructure	1,314
REGEN	Modeling of cryocoolers	1,227
PHAML	Parallel adaptive solution of partial differential equations	843
Ngraph	Basic graph algorithms; web crawler	540

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 (CY) 2011, the division web server satisfied more than 10.3 million requests for pages from more than 40,000 distinct hosts. In total, there have been more than 304 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 113 such papers which were published in CY 2011 alone (more than 1,230 such papers have been identified since 2001).

Members of the Division are also active in professional circles. Staff members hold a total of 14 editorial positions in peer-reviewed journals. They are also active in conference organization, serving on 10 organizing/steering/program committees. Staff members organized four 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. In addition, staff members serve on committees of the IEEE Computer Society, the Mathematical Association of America, the Association for Women in Mathematics, and the Society for Cryobiology. 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, Bruce Miller is a member of W3C's Math Working Group, and Sandy Ressler is a member of the Declarative 3D for the Web Architecture Community 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. Robert Bohn is Co-Chair of the NITRD Program's Faster Administration of Science and Technology Education and Research (FASTER) Community of Practice.

For further details, see Section IV, Activity Data.

Administrative News

The past year also saw many staffing changes. Among these are the following.

Arrivals

Stephen Jordan joined ACMD in April 2011. Jordan comes to ACMD from Caltech, where he was a Postdoctoral Fellow in John Preskill's Quantum Information Group. His thesis, "Quantum Computation beyond the Circuit Model," was done at MIT under the advising of Edward Farhi. At NIST he works on quantum computation and post-quantum cryptography.

Yi-Kai Liu joined the ACMD staff in May 2011. Liu earned a PhD in Computer Science from the University of California at San Diego where he worked with Russell Impagliazzo and David Meyer on quantum complexity theory. Before coming to NIST he held postdoctoral appointments at Caltech and the University of California at Berkeley. At NIST Liu will be working on the theory of post-quantum cryptography as well as quantum state tomography.

Sandy Ressler, Manager of ITL's Complex Systems Program for the past three years, transferred into ACMD's High Performance Computing and Visualization Group in October 2010. A 25-year NIST veteran, Ressler is an expert in visualization technology. His work has been instrumental in the development and standardization of web-based 3D graphics. In ACMD he will develop information visualization techniques, tools, and applications.

Howard Cohl joined NIST as an NRC Postdoctoral Associate in January 2011. 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 $\boldsymbol{R}^d$ and $\boldsymbol{H}^d$. Cohl also holds a PhD in Physics from Louisiana State. At NIST he is working with Daniel Lozier on rotationally-invariant expansions for solving linear inhomogeneous partial differential equations.

James Shook joined NIST as an NRC Postdoctoral Associate in July 2011. Shook has a Ph.D. in mathematics from the University of Mississippi where he worked on combinatorics and graph theory. In ACMD Shook is working with Brian Cloteaux and Isabel Beichl on the characterization of affiliations in networks.

Asha Nurse joined NIST in January 2011 as a Postdoctoral Fellow supported through the NIST ARRA Fellowship Program administered by the University of Maryland. (ARRA is the American Recovery and Reinvestment Act.) Nurse comes to NIST from Brown University where she obtained a PhD in solid mechanics. Her thesis dealt with the driving forces for self-assembly of cell clusters and cluster stability. At NIST she will be working with Geoffrey McFadden on fluid dynamics applications.

Assane Gueye, a recent PhD in Computer Science from the University of California at Berkeley, joined NIST in the spring of 2011 as a Postdoctoral Fellow supported through the NIST ARRA Fellowship Program. Gueye's thesis research utilized game-theoretic approaches to study communications security. At NIST he will work on game-theoretic models of network dynamics and computer security with Vladimir Marbukh.

Paulina Kuo of the Joint Quantum Institute (a cooperative venture of NIST and the University of Maryland) joined ACMD in October 2011 as a Guest Researcher. Kuo received undergraduate degrees in Physics and Materials Science from MIT. In 2008 she received a PhD in Applied Physics from Stanford University. She also served as an NRC Postdoctoral Associate in PML. An expert in nonlinear optics, Kuo will be contributing to the Division's experimental efforts in quantum communications.

Ismet Sahin began a term in ACMD as an ARRA Senior Fellow in October 2011. Sahin has a PhD in Electrical and Computer Engineering from the University of Pittsburgh (2006). He was most recently a Guest Researcher in the NIST National Center for Neutron Research. Sahin will be working with Anthony Kearsley on optimization methods applied to waveform time delay estimation algorithms that are used in seismology, radar, sonar, and biomedical science.

Dennis Backhaus from Fachhochschule Wiesbaden (University of Applied Sciences, Wiesbaden, Germany) began work as a Guest Researcher in the ACMD High Performance Computing and Visualization Group.

Departures

David Gilsinn has retired from NIST after 40 years of Federal service. After obtaining a PhD in mathematics from Georgetown University in 1969, Gilsinn joined the NBS Technical Analysis Division where he worked on railroad crossing risk analysis, flow models for predicting national air cargo and oil pipeline flow, models supporting simulation of fires on LP tankers on railcars, and a firehouse location master plan for Dade County, Florida. In 1974 he joined the NBS Institute of Computer Science and Technology, where he led a team developing conformance tests for commercial BASIC compilers. He also represented

NIST on the ANSI BASIC subcommittee, leading to the Minimal BASIC Standard in 1978. That year he moved to the NBS Precision Engineering Division to work on models of surface roughness, optical scattering from rough surfaces, and image acquisition from scattered laser light. He was also project mathematician for the development of the NIST Molecular Measuring Machine. In 1991 he began work in the NIST Automated Production Technology Division where, among other things, he worked on mathematical models of machine tools. After 30 years as a mathematician serving in the trenches on foreign soil, Gilsinn finally came home to the math division in 2000. In ACMD he worked on computational geometry, L_1 spline surface fitting, urban terrain modeling, surface models from LADAR data, and construction object recognition. In the last few years he has been working on image processing for medical and biological applications. Gilsinn received the DOC Bronze Medal and the NIST Applied Research Award. He produced more than 60 publications, along with the 2009 Springer Book, *Delay Differential Equations: Recent Advances and New Directions*[9] by Balakumar Balachandran, Tamás Kalmár-Nagy, and David E. Gilsinn. He also served on the Editorial Board of the *ASME Journal of Computational and Nonlinear Dynamics.* Gilsinn remains a guest researcher in ACMD.

Alan Mink, a long time NIST staff member, most recently a member of ACMD's Computing and Communications Theory Group, retired from NIST in early April 2011. He leaves with an incredible 41 years of Federal service. Mink earned a PhD in electronics and communications engineering from the University of Maryland, where he also taught courses in computer architecture. At NIST he worked on a wide variety of projects in computer aided design, networking, parallel processing, computer performance measurement, cluster computing, digital TV, and quantum communications. Mink is a co-winner of the DOC Bronze (2005) and Silver (2008) Medals, the NIST Allen Astin Measurement Science Award (1990) as well as the co-recipient of two prestigious R&D 100 Awards (1988 and 2007). He continues to contribute to ACMD programs as a guest researcher.

Valerie Coffman, a former NRC Postdoctoral Associate in ACMD and most recently a term appointee, resigned from NIST in July 2011 to devote her energies to her own startup company. In ACMD Coffman was a key contributor to the OOF project, which develops software for the modeling of materials with complex microstructure. Coffman was leading the development of OOF3D. She has a PhD in Physics from Cornell University.

Peter Ketcham resigned from NIST in October 2011 after service as a mathematician at NIST for 14 years. During the late 1990s Ketcham worked with David Feder of the NIST Physics Lab and others to develop visualizations of models of the newly discovered Bose Einstein condensate. These striking images made their way to the covers of *Physics Today, Optics and Photonics News, Parity*, and the lead illustration in a *Scientific American* article. In 2000 Ketcham was a joint recipient of the NIST Bronze Medal.

James Benson completed his tenure as a NIST NRC Postdoctoral Associate, accepting a position in the Mathematics Department of Northern Illinois University. At NIST Benson worked with Anthony Kearsley on optimal control of heat and mass transfer problems with to application to cryobiology, such as the improvement of cell cryopreservation protocols.

Ruediger Kessel completed a three-year term as a Guest Researcher in ACMD, returning to his hometown of Braunschweig, Germany, to join the staff of the Physikalisch-Technische Bundesanstalt (PTB), NIST's sister institution in Germany. While at NIST Kessel was active in a wide variety of projects, including calibration of optical sensing devices in satellites, combinatorial testing, definitions of metrological consistency, and the development of software for propagating uncertainties using Monte Carlo methods.

Lijun Ma, an ITL guest researcher for seven years, left in October 2011 to take a position as a research assistant professor in the Biomedical Engineering Department at Washington University in St. Louis. An expert in quantum optics, Ma was a significant contributor to ITL's experimental efforts in quantum communications. An incredibly productive researcher, Ma co-authored 52 papers in journals and confer-

[9] http://www.amazon.com/Delay-Differential-Equations-Advances-Directions/dp/0387855947

ence proceedings during his six years at NIST. Ma received his PhD in Physics from Tsinghua University in China in 2001. He recently became a permanent resident in the US.

Pradeep Reddy Gaddam, guest researcher from Suvojit Chanda, in Navi Mumbai, India, and **Clement Rey and Guillaume Bousquet**, guest researchers from Institut Supérieur d'Informatique, de Modélisation et de leurs Applications (ISIMA) in Clermont-Ferrand, France, completed their internships in ACMD.

Table 2. *Student Interns in ACMD*

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
Marlene Hildebrand	Polytech (France)	G	Guest Researcher	J. Terrill A. Peskin	Visualization of medical images
Gregory Rami	ISIMA (France)	G	Guest Researcher	J. Terrill	Impact of fire on building structures
Jean-Loup Traore	Univ. Blaise Pascal (France)	G	Guest Researcher	J. Terrill	Cement hydration modeling
Adam Meier	University of Colorado	G	PREP	E. Knill	Quantum computer simulation
Michael Mullan	University of Colorado	G	PREP	E. Knill	Quantum computing theory
Yanbao Zhang	University of Colorado	G	PREP	E. Knill	Tests of local realism
William Hess	Purdue University	U	STEP	J. Terrill	Lighting in the Immersive Visualization Environment
Kevin Rawlings	Carnegie Mellon Univ.	U	STEP	J. Terrill	Visualization and analysis of the National Vulnerability Database
Anshu Rustagi	University of Illinois	U	STEP	W. George	Screen Saver Science
Halley Coplin	Rensselaer Poly. Institute	U	SURF	S. Ressler	Using the immersive platform to study RF propagation from medical implants
Gregory Herpel	St. Mary's College	U	SURF	W. George	Analysis of a high performance flow of suspension code
Brady O'Connell	University of Maryland	U	SURF	R. Bohn	Implementation of Use Cases for NIST Cloud Computing Program
Nadezhda Serova	UMBC	U	SURF	J. Terrill	Dynamics of breaking glass
Matthew Du	Thomas S. Wooton H.S.	HS	SHIP	J. Terrill	Spatial distribution of spin in nanostructures
Kevin Harrison	Poolesville H.S.	HS	SHIP	J. Terrill	Impact of fire on building structures

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

During FY 2011 ACMD was able to support the work of 17 student interns, including four in the Student Undergraduate Research Fellowship (SURF) program, three graduate students in Boulder's Professional Research Experience Program (PREP), and two high school volunteers. We also hosted four 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.

Recognition

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

The NIST Digital Library of Mathematical Functions (DLMF) was selected for recognition as an **Outstanding Information Technology Achievement in Government** for 2011 by Government Computer News (GCN). The DLMF is the online interactive successor to the classic NBS Handbook of Mathematical Functions (M. Abramowitz and I. Stegun, eds.) published in 1964. The DLMF provides reference data on the special functions of applied mathematics in a concise, usable form needed in a wide variety of fields, from the physical sciences to engineering, biology and finance. The online reference features interactive graphics, math-aware search capabilities, and a rich set of internal and external links. According to GCN, these awards "have come to symbolize the best and most notable IT accomplishments in advancing the work of government agencies." Ten projects were selected for recognition this year from more than 200 nominations. The selection was based on "the degree of innovation in the technology plan carried out, the quality of the leadership that carried the project to fruition", and "the degree to which a given IT project improved an agency's ability to operate more efficiently or serve the public more effectively." Other awardees this year include an app from the City of Boston that enables citizens to request city services from their smartphones and the IT infrastructure that supports the TSA's secure flight program. NIST staff members cited for the DLMF achievement are Daniel Lozier, Frank Olver, Ronald Boisvert, Bruce Miller, Bonita Saunders, Marjorie McClain, Abdou Youssef, and Qming Wang of ACMD, Brian Antonishek of the ITL Information Access Division, and Charles Clark of the NIST Physical Measurement Laboratory. The project team was formally honored at the 24th Annual GCN Awards Gala, October 19, 2011, at the Ritz-Carlton Tysons Corner in McLean, Va.

Figure 1. *The Digital Library of Mathematical Functions Team garnered two major recognitions this year. They were cited for producing one of the top 10 IT acheivements in government by Government Computer News. They also received the Department of Commerce Gold Medal. From left to right: Charles Clark (PML), Brian Antonishek, Marjorie McClain, Frank Olver, Qiming Wang, Daniel Lozier, Bonita Saunders, Ronald Boisvert, Bruce Miller, Abdou Youssef.*

The DLMF team members were also recipients of the **Department of Commerce Gold Medal** for 2011. The Gold Medal is the highest honor conferred by DOC. The team was cited for "the development of the NIST Digital Library of Mathematical Functions, an unprecedented reference on the special functions of applied mathematics." The award was presented by Secretary of Commerce John Bryson on December 13, 2011.

Figure 2. *Adele Peskin won a Bronze Medal for her work on cell image analysis.*

Adele Peskin of ACMD was part of a team selected to win the **Department of Commerce Bronze Medal** for 2011. The team was cited for "developing innovative techniques that improved the accuracy in measurements associated with live cell tracking and image acquisition in cell biology." The innovations attributed to the team include a

bivariate metric for the evaluation of image segmentation quality, a novel morphological object separation technique, a technique for predicting segmentation accuracy for cell images, an accurate overlap-based cell tracker, and new techniques for segmenting static and live cell images.

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.

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** in October 2010. Frank Olver was similarly honored in October 2011. 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.

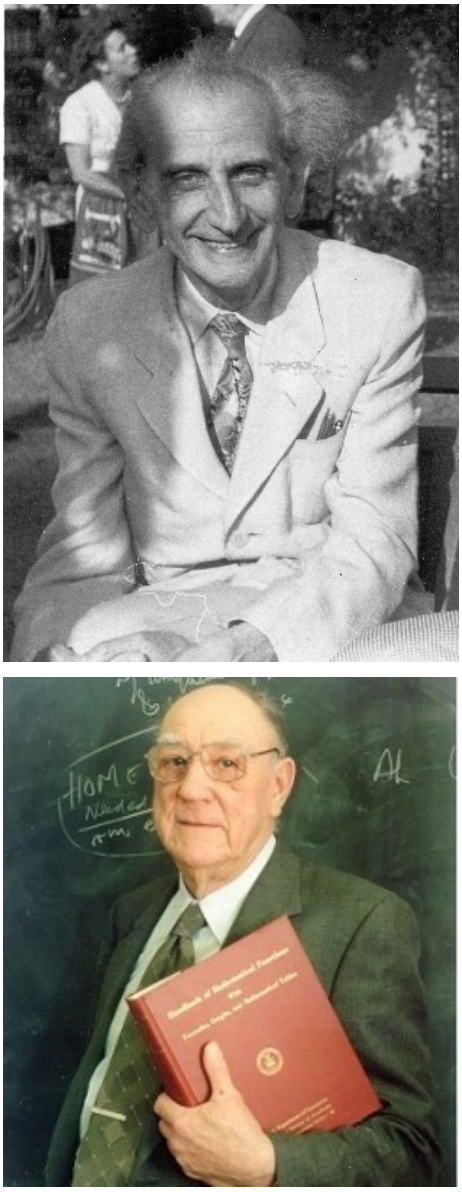


Figure 3. *Cornelius Lanczos (top) and Frank Olver (bottom) were inducted into the Portrait Gallery of Distinguished NIST Alumni.*

Olver was recruited by Milton Abramowitz in 1961 to be the author of the chapter "Bessel Functions of Integer Order" in the *NBS Handbook of Mathematical Functions* (M. Abramowitz and I. Stegun, eds., 1964), a publication which went on to become the most widely distributed and most highly cited publication in NIST's history. Olver left NIST for the University of Maryland in 1986, though he returned to NIST in 1986 as a guest researcher. He is currently a faculty appointee in ACMD. Olver is particularly known for his extensive work in the study of the asymptotic solution of differential equations. He is author of six books (three as editor), two book chapters, 72 journal articles, 27 papers in proceedings, and nine book reviews. His well-known and well-regarded book, *Asymptotics and Special Functions*, originally published by Academic Press in 1974 and translated into Russian in 1978, was reprinted in the AKP Classics Series by AK Peters in 1997. In 2000, a 1,074-page commemorative volume *Selected Papers of F.W.J. Olver, Parts 1 and II* was published by World Scientific Publishing Co. More than half of the 56 reprinted papers, originally published from 1949 through 1999, cite an NBS affiliation. More recently he served as the Editor-in-Chief and Mathematics Editor of the online *NIST Digital Library of Mathematical Functions* and its 966-page print companion, the *NIST Handbook of Mathematical Functions* (Cambridge University Press, 2010).

Three ACMD staff members were honored in ITL's annual awards ceremony in 2011:

- Alfred S. Carasso received the **ITL Best Journal Paper Award** based on the single authored manuscript, "Bochner Subordination, Logarithmic Diffusion Equations, and Blind Deconvolution of

Hubble Space Telescope Imagery and Other Scientific Data," which appeared in the refereed journal *SIAM Journal of Imaging Sciences,* Volume 3, Number 4, 2010, pp. 954-980.

- The inter-Divisional team of Dr. Daniel Genin (ITL/ANTD), Dr. Vladimir Marbukh (ACMD), and Dr. Anastase Nakassis (ITL/ANTD) received the **ITL Best Conference Paper Award** based on the manuscript, "Vulnerability of Selfish Routing to Attacks: Game-theoretic Models and Initial Results," which was presented at the 2010 International Conference of Information Security and Internet Engineering held in London on June 30 – July 2, 2010.
- Oliver Slattery of ACMD received the **Outstanding Contribution to ITL Award** for his outstanding efforts in safety, both as a member of the NIST laser safety committee as well as for his leadership in laboratory safety within ITL.

Figure 4. *ACMD Faculty Appointee Dianne O'Leary was named Norbert Weiner Lecturer by Tufts University.*

Dianne O'Leary, Professor of Computer Science at the University of Maryland and a faculty appointee in ACMD, was selected as the **Norbert Wieier Lecturer** by Tufts University for 2011. The Norbert Wiener Lectures were instituted to celebrate one of Tuft's most well-known alumni. A world renowned mathematician, Norbert Wiener may be most well-known for founding the science of cybernetics. The term he coined is the root of now common neologisms such as cyberspace and cybersecurity. As the Wiener Lecturer, O'Leary presented three lectures on consecutive days, beginning on March 29. The lectures were entitled "Mathematics in Words and Images: The role mathematics plays in searching the web and in restoring blurred images," "Uncertainty Quantification for Ill-posed Problems," and an undergraduate seminar "Where Am I? Position from incomplete distance information, from Gauss's geodesy problems to protein structures." Previous Wiener Lecturers have included Persi Diaconis (Stanford), Nick Trefethen (Oxford), Jim Yorke (University of Maryland), and Margaret Wright (NYU).

Florian Potra, Professor of Mathematics at the University of Maryland Baltimore County and a faculty appointee in ACMD, was recognized in a **special commemorative session** at the 2011 Spring Southeastern Section Meeting of the American Mathematical Society held at Georgia Southern University on March 12-13, 2011. The session, which was entitled, "Advances in Optimization," was organized in honor of Potra's 60th birthday. The session spanned two days of the conference. Potra presented the first one-hour lecture, which was entitled "Interior point methods in wide neighborhoods of the central path;" this was followed by 14 30-minute presentations on current research in optimization theory and applications.

Figure 5. *ACMD Faculty Appointee Florian Potra's 60th birthday was commemorated by a special session of the AMS' Southeast Section meeting.*

The paper: J. Bullard, E. Enjolras, W. George, S. Satterfield and J. Terrill, "A Parallel Reaction-Transport Model Applied to Cement Hydration and Microstructure Development," *Modelling and Simulation in Materials Science and Engineering,* volume 18 (2010), article 025007 (16pp), was selected as one of the 10 **highlights of the journal** for 2010 and collected together on a highlights page[10]. According to IOP Publishing, the paper was one of the most frequently downloaded of the year, and "exemplifies the high standard of research that MSMSE attracts." George, Satterfield, and Terrill are ACMD staff members. Enjolras was an ACMD guest researcher.

[10] http://iopscience.iop.org/0965-0393/page/Highlights%20of%202010

A **biography** of and an extensive interview with ACMD mathematician Fern Hunt have appeared as a chapter in the new book, *Fascinating Mathematical People: Interviews and Memoirs*, edited by Donald Albers and Gerald Alexanderson, and published this year by Princeton University Press[11]. Hunt is one of 16 mathematicians profiled in the volume. In her interview she describes what it was like to be among the first black women to earn a PhD in mathematics. Others profiled include Tom Apostol (Caltech), Jean Taylor (Rutgers), and Don Saari (University of California at Irvine). Apostol is the author of a chapter in the NIST Digital Library of Mathematical Functions, while Taylor and Saari are former frequent visitors to NIST.

Figure 6. *Fern Hunt's biography is featured in a new book.*

[11] http://press.princeton.edu/titles/9527.html

Part II

Features

hp-Adaptive Finite Element Methods

The numerical solution of partial differential equations is the most compute-intensive part of a wide range of scientific and engineering applications. So the development and application of faster and more accurate methods for solving partial differential equations is a very important field that has received much attention in the past fifty years. Many of the applications at the cutting edge of research are extraordinarily challenging. These problems necessitate the use of the most advanced numerical techniques including adaptive grid refinement and high order finite elements. Recent research on adaptive grid refinement has resulted in several approaches to the so-called hp version of the finite element method. We have studied these methods and performed an extensive numerical experiment to compare their convergence rates and determine which methods are most effective in different situations.

William F. Mitchell

To solve partial differential equations (PDEs) numerically one divides the domain of the problem into small subregions called elements and approximates the solution over each element with a polynomial. To resolve difficult features in the solution such as steep fronts, highly oscillatory regions, or singularities, the elements must be small and/or the polynomial degree must be large, but if one does this uniformly over the whole domain the number of algebraic equations (degrees of freedom) explodes and the problem becomes intractable. It is necessary, then, to use high degree and/or small elements only where required. Unfortunately, to optimize the element size and degree one must know the solution to the PDE. An alternative is adaptive grid refinement: start with a coarse, low degree grid, compute a solution, estimate the error in each element, subsubdivide elements with unacceptably large error, and repeat. This process, known as *h*-adaptive refinement because *h* represents the size of the elements, has been studied for many years and is widely used in practice today. Recent research has improved this algorithm by allowing the option of increasing the polynomial degree, denoted *p*, in an element instead of subdividing it. This is known as *hp*-adaptive refinement. The attraction of *hp* adaptivity is that, with a suitably chosen *hp* grid, the error can converge exponentially in the number of degrees of freedom, *N*, i.e.,

$$\left\| e_{hp} \right\| \le C_1 e^{-C_2 N^{1/3}}$$

for some C_1 and $C_2>0$ independent of *N*, as opposed to a polynomial rate for *h*-adaptive refinement with fixed *p*, i.e.,

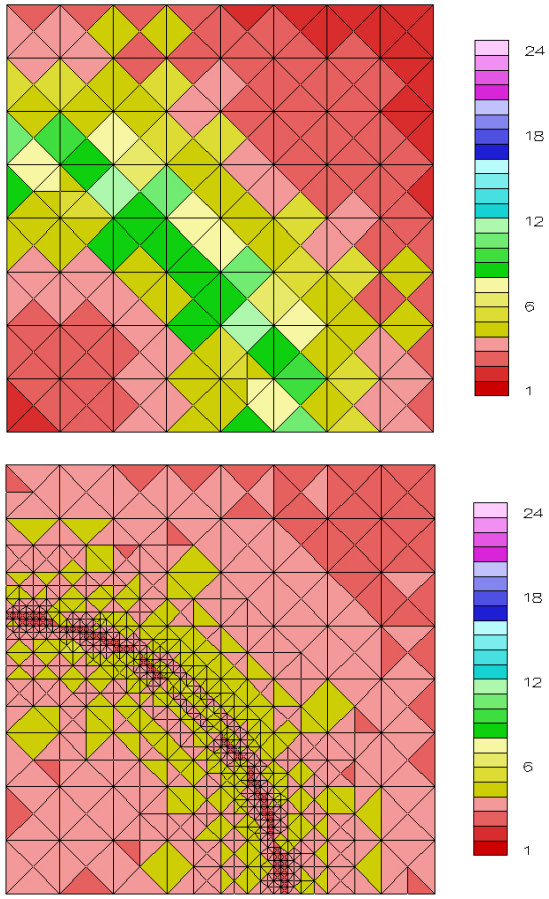


Figure 7. *Example hp-adaptive grids for two strategies for a solution with a mild circular wave front. The colors represent the polynomial degree over each element. Notice that one strategy was heavily biased toward p-refinement while the other was biased toward h-refinement.*

$$\left\| e_h \right\| \le C_2 e^{N^{-p/2}}.$$

This implies that one can use a much smaller value of *N* for a given error tolerance, and hence solve the problem much more quickly.

The difficulty is in determining how to suitably choose the *hp* grid. The local error estimate can be used to determine *which* elements should be refined, the same as in *h*-adaptive refinement, but it cannot simultaneously determine *how* to refine the element, i.e. whether it should be subdivided (*h*-refined) or have the polynomial degree increased (*p*-refined). Methods for making that determination are called *hp*-adaptive strategies, and have been the subject of considerable research. We identified 13 *hp*-adaptive strategies in the literature.

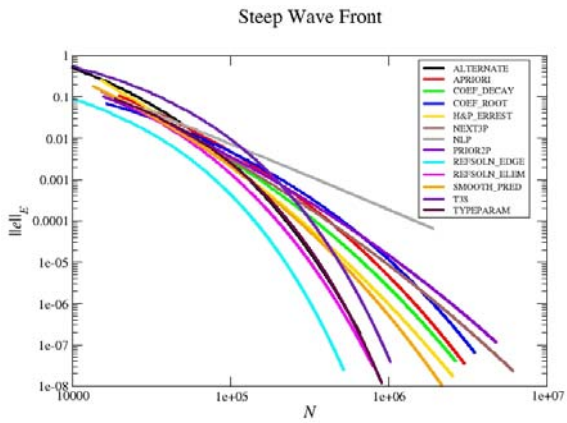


Figure 8. *The convergence plots for all strategies for the problem with a very steep wave front.*

Many of the strategies are based on the premise that one should use *h*-refinement near singularities and other strong features, and *p*-refinement where the solution is smooth. If one has *a priori* knowledge of these features in the solution, it is easy to guide the refinement in this way, but this is rarely the case. Several strategies attempt to approximate the smoothness of the solution. This is done by examining error estimates for approximations with different polynomial degree, and using them in a mathematical expression based on the theoretical convergence rates.

Other strategies use a number of different ideas on how to estimate which type of refinement will be most effective. One of them attempts to formulate the decision globally as an optimization problem: minimize the error subject to several constraints, such as placing an upper bound on the number of degrees of freedom, and requiring that the polynomial degree be positive. Unfortunately the optimization problem is NP hard and contains unknown quantities (e.g. the error), so many approximations must be made to formulate a tractable problem. Another strategy separates the *h* and *p* refinement by performing just *h*-refinement until the estimated error has been reduced by a given amount, and then just *p*-refinement until the final tolerance is reached. Another strategy uses error estimators to estimate whether *h*-refinement or *p*-refinement of an element will reduce the error the most. Two strategies compute a reference solution by performing uniform *h*- and *p*-refinement of the entire grid, and project that solution onto several candidate refinements to estimate which candidate is most effective in an error reduction vs. increased cost measure. These strategies are different than the others in that they allow for decreasing the polynomial degree in elements that are *h*-refined.

The PDE solver PHAML developed by William Mitchell of ACMD is based on adaptive refinement and contains an implementation of all these *hp*-adaptive strategies. We used this code to perform a numerical experiment to compare the effectiveness of the strategies in terms of accuracy vs. degrees of freedom. For this experiment we gathered a collection of 12 test problems [1], most of which came from the numerical results section of papers on *hp*-adaptive refinement. These contain a variety of difficulties including singularities, sharp peaks, wave fronts, oscillations and boundary layers. Most of them are parameterized to adjust the problems in the experiment.

Figure 7 illustrates two examples of *hp* grids adapted to a solution that contains a mild circular wave front. The black lines show the elements of the grid and the colors indicate the degree of the polynomial in each element. These grids were generated by different strategies for the same problem, and demonstrate how very different the resulting grids can be.

In anticipation that different strategies would work best in different situations, the results of the experiment are grouped into six categories: problems with a mild difficulty, a strong difficulty, singularities, each at a low accuracy requirement (10^{-2} relative error) and high accuracy requirement (10^{-6} relative error). Summary results will be published in [2], with the full results available in [3]. The experiment showed that which strategies are most effective is dependent on the characteristics of the problem and accuracy requirement. An example is shown in Figure 8. For this problem we see that the REFSOLN_EDGE strategy is clearly superior. But also notice how T3S is the worst strategy at low accuracy, but one of the best at high accuracy.

One interesting result is that the reference solution strategies performed exceptionally well in all categories. However, they are much more computationally expensive than the other strategies, which offsets the reduction in number of degrees of freedom. This suggests that future research on the development of a more effective *hp*-adaptive strategy should be directed towards using some aspects of these methods to obtain their convergence rates without having to compute the expensive reference solution.

References

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

[2] W.F. Mitchell and M.A. McClain, A Comparison of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations, submitted.

[3] W.F. Mitchell and M.A. McClain, A Comparison of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations (long version), NISTIR 7824, 2011.

Participants

William Mitchell, Marjorie McClain (ACMD).

http://math.nist.gov/phaml/

Unsuspected Nonuniqueness in Solving Parabolic Equations Backward in Time

An iterative procedure originating in the field of spectroscopy has been successfully applied to solve nonlinear parabolic equations backward in time. This has led to the discovery of previously unsuspected one dimensional examples of well-behaved, physically plausible, but ***completely false*** *reconstructions of the initial data at time t=0, given approximate values for the solution at time t=1. Even more striking examples of false reconstructions are likely in multidimensional problems. Such examples are of considerable significance in hydrologic inversion and image deblurring, two important areas of application of backward parabolic equations. These examples indicate that highly detailed prior information about the correct solution is likely to be a necessary ingredient in many backward reconstruction problems. Such detailed prior knowledge may not always be available.*

Alfred Carasso

There has been growing interest in recent years in the development of numerical methods for solving parabolic equations backward in time. Currently, the two most significant areas of application of backward parabolic equations are *hydrologic inversion* and *image deblurring*. In hydrologic inversion, the aim is to identify sources of groundwater pollution by reconstructing the contaminant plume history. This involves solving the *advection dispersion equation* (ADE) backward to time t=0, given the contaminant spatial distribution $g(x,y)$ at the current time t = 1. In scientific and medical applications, images blurred by Gaussian point spread functions are a common occurrence. Deblurring Gaussian blur is mathematically equivalent to solving the heat conduction equation backward in time, with the noisy blurred image $g(x,y)$ as data at time t = 1, and with conduction coefficient $\alpha > 0$ proportional to the point spread variance. Of continuing interest at NIST and other U.S. Government research facilities, is the successful application of time-reversed fractional and logarithmic diffusion equations in blind deconvolution of nanoscale scanning electron microscope imagery, as well as cosmological scale Hubble Space Telescope imagery.

While several useful backward parabolic numerical methods exist, no method can avoid the inherent practical difficulty that only approximate values can generally be known for the solution at the current time t=1. Thus, one must reconstruct the past from **imprecise knowledge of the present**. How such imprecision may affect the reconstruction is seldom considered in practice.

Given a well-posed linear or nonlinear parabolic equation $w_t = Lw$, $t>0$ and approximate data $f(x)$ at time t = 1such that in the L^2 norm,

$$\| w(.,1) - f \| \le \delta$$

where

$$0 < \delta << \| w(.,0) \| \le M \ ,$$

what can be said about the expected accuracy in backward reconstruction from the given data f ? The following **fundamental uncertainty inequality** for the difference of any two possible reconstructions $w^1(x,t)$ and $w^2(x,t)$, from the given approximate data f, is known:

$$\| w^1(.,t) - w^2(.,t) \| \le 2M^{1-\mu(t)}\delta^{\mu(t)}, \quad 0 \le t \le 1$$

Here the dependence of the Hölder exponent $\mu(t)$ on t, shown in Figure 9A, plays a crucial role. In the best possible case, that of a linear self adjoint elliptic operator L with time-independent coefficients (blue line), we have $\mu(t) = t$, so that $\mu(t)$ decays linearly to zero as \$t↓ 0. This implies a progressive loss of accuracy as reconstruction proceeds from t=1 to t=0. Much more severe loss of accuracy may occur in non self adjoint or nonlinear problems (red curve), where the decay in $\mu(t)$ is sublinear. Moreover, no matter how small δ is, no accuracy can be guaranteed at t=0 since $\mu(0) = 0$.

The above inequality necessarily contemplates worst case scenarios that may be too pessimistic in some applications. Indeed, highly useful enhancements of nanoscale electron micrographs and Hubble galaxy images have been documented. Nevertheless, the behavior of $\mu(t)$ in Figure 9A reflects a basic underlying truth about parabolic problems. An iterative procedure has been developed that can illuminate the deeper meaning of the above uncertainty inequality. That iteration can be used to uncover previously unsuspected examples of specific one dimensional parabolic equations with distinct solutions $w^{red}(x,t)$ and $w^{green}(x,t)$, having the property that their traces $w^{red}(x,1)$, $w^{green}(x,1)$ at t=1 are visually indistinguishable, while their corresponding initial values $w^{red}(x,0)$, $w^{green}(x,0)$ are vastly different. Such an example is shown in Figure 9B, and discussed further below.

Van Cittert iteration. Given the linear or nonlinear parabolic equation $w_t = Lw$, $t > 0$, let S be the associated solution operator at time t = 1. Thus, given initial values $h(x)$ at t = 0, $S[h] = w_h(x,1)$, the corresponding solution of the parabolic equation at t = 1.

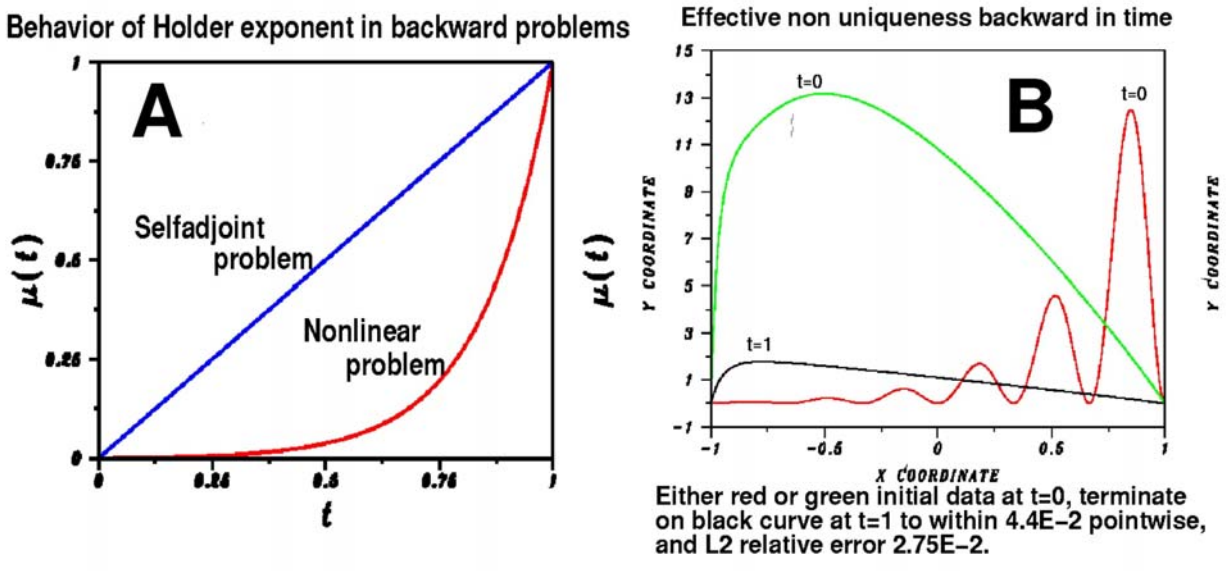


Figure 9. *(A) Linear and sublinear behavior in Hölder exponent. (B) Vastly different red and green initial values at t=0, produce approximately the same result at t=1.*

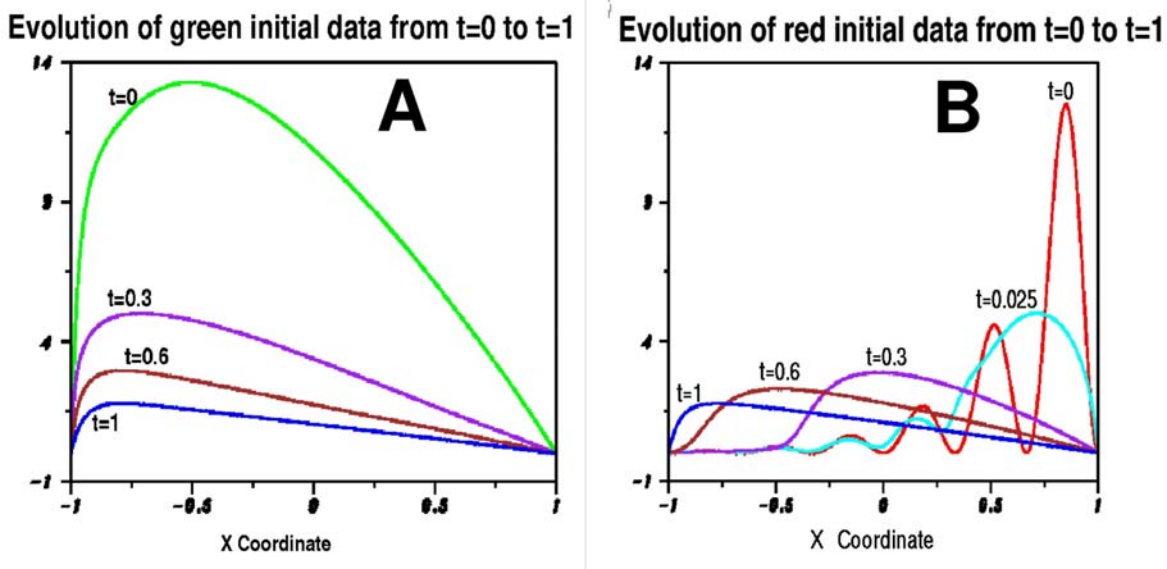


Figure 10. *Distinctly different evolutions of red and green initial values at t = 0 into almost identical blue curve at t = 1.*

Using efficient numerical parabolic solvers, the operation $S[h]$ can be accurately calculated at mesh-points, given any $h(x)$. With approximate data $f(x)$ at $t = 1$ such that

$$\| w(.,1) - f \| \le \delta << \| w(.,0) \| \le M ,$$

we may try to reconstruct the initial value $h(x) = w(x,0)$ through the following iteration:

$$h^{n+1}(x) = h^n(x) + \gamma \{ f(x) - S[h^n(x)] \}, \quad n > 1$$

where $\gamma > 0$ is a fixed relaxation parameter, and $h^1(x) = \gamma f(x)$. The above Van Cittert iterative procedure is often used in spectroscopy, where S is an explicitly known linear convolution operator. The successful application of that procedure in nonlinear parabolic equations, where S is not known explicitly, was unanticipated. In fact, the Van Cittert iteration seldom converges. However, in many cases, the procedure generates a sequence of iterates $h^n(x)$ such that the L^∞ norm of the residual, $\| f - S[h^n] \|_\infty$ decays quasi monotonically to a small value after finitely many iterations.

This is often sufficient for our purpose. If for some positive integer N we find

$$\left\| f - S[h^N] \right\| < \delta, \quad \text{with} \left\| h^N \right\| < M,$$

then $h^N(x)$ is a valid candidate reconstruction of $w(x,0)$, given the approximation $f(x)$ to $w(x,1)$.

Highly Plausible, Yet False Reconstructions. The following numerical experiment is one of dozens of similar experiments that were performed on one dimensional linear and nonlinear parabolic partial differential equations. Here, a strongly nonlinear equation with the initial data $w^{red}(x,0)$ shown in Figure 9B, was accurately solved numerically up to time $t = 1$ to produce $w^{red}(x,1)$, shown as the black curve $f(x)$ in Figure 9B. Using $f(x)$ as given approximate data at $t = 1$, the Van Cittert iteration was pursued for 50 iterations resulting in an L^∞ residual of 4.4×10^{-2}. The last iterate $h^{50}(x) = w_0^{green}(x)$ is the green trace in Figure 9B. We stress that $w_0^{green}(x)$ is a **valid reconstruction** of the unknown initial data, given the approximation $f(x)$ at $t = 1$. Indeed, using $w_0^{green}(x)$ as initial data in our parabolic solver reproduces the black curve at $t = 1$ in Figure 9B to within 4.4×10^{-2} pointwise, and L^2 relative error 2.75×10^{-2}. Given the data error levels δ likely to be found in typical engineering applications, such an L^2 relative error for the reconstruction seems quite reasonable. Moreover, both red and green curves in Figure 9B have an L^∞ norm of about 13.

In Figure 2A, the evolution of $w_0^{green}(x)$ into the blue curve at $t = 1$, is distinctly different from the evolution of $w_0^{red}(x)$ into the almost identical blue curve in Figure 2B. Indeed, given the blue curve at $t = 1$, the green evolution seems highly plausible, while the red evolution seems improbable. We note that smoothness and/or positivity constraints are often applied to regularize backward reconstructions. Here, the reconstructed **false** green evolution is both smooth and positive at all times.

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[1] A.S. Carasso, Reconstructing the Past from Imprecise Knowledge of the Present: Some examples of Non Uniqueness in Solving Parabolic Equations Backward in Time, *Journal of Research of the NIST*, to appear.

Body Area Network Visualization and Analysis

Body Area Networks (BANs) consist of RF-enabled wearable and implantable sensory nodes for short range reliable communication in or around the human body. This technology is poised to be a promising interdisciplinary technology with novel uses in pervasive health information technology. This project provides tools for modeling and visualizing the propagation of the signals on which the networks' wireless communications depend. Our recent work on BAN visualization and analysis is shedding light on: the effect of other types of medical implants on BAN signal propagation; path loss in BAN communications channels; and the creeping wave phenomenon as it affects body surface signal propagation. This work is assisting IEEE standards committees and will help RF engineers to design more effective network devices.

John Hagedorn

Body Area Networks (BANs), which are networks operating near or within the human body, are an emerging technology that has potential in a variety of application areas. Perhaps the most important use for BANs is in pervasive heath IT where they will enable continuous remote monitoring of a person's health status (such as heart rate, blood pressure, etc.) as well as active therapeutic devices such as precision drug delivery. Furthermore, BAN is an important technology for the implementation of electronic health records; data from medical BANs can be sent directly into electric records without the need for human data entry. So, BAN technology is poised to become a significant piece of the health IT puzzle.

We seek to advance the state of BAN technology by providing tools for understanding RF propagation through and near the human body. This understanding is essential in developing the devices and protocols that will be used in BANs. Our work is supporting the IEEE committees that are developing the communications standards for BANs as well as the RF engineers who are designing the network communications devices.

There are two intertwined parts of this work on BAN technology. The first part is the simulation of RF propagation through the human body; the second part is the visualization and analysis of the data produced by these simulations. The work within ACMD is mostly focused on the visualization and analysis.

We perform simulations of RF propagation because experiments involving implanting devices in human subjects are not feasible. The modeling is achieved using a commercially available 3D full-wave electromagnetic field simulator. A detailed 3D human body model is used which includes frequency-dependent dielectric properties of over 300 parts in a male body.

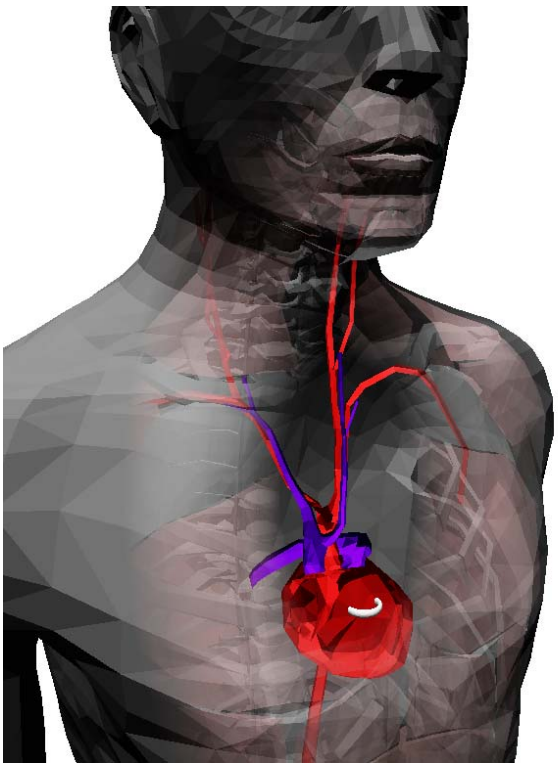

Figure 11. *A metal ring placed in the body model to simulate the presence of an aortic valve replacement.*

We have developed a three dimensional immersive visualization system to support the investigation of these RF propagation results. This system creates a 3D virtual environment that enables the user to interact directly with the body model and the RF data. We have developed interactive tools for quantitatively probing these data. This immersive virtual environment and our interactive tools are described elsewhere [1, 2].

We recently simulated the effect of an artificial aortic heart valve implant on communications among BAN devices on the surface of the body. In Figure 11 we show a visualization of a ring that approximates the metallic portion of an artificial aortic valve.

We performed simulations of ultra-wide band (UWB) signal propagation based on this valve placement and the placement of a BAN transmitter and several receivers on the upper body [3]. The simulations correspond to experiments conducted by our collaborators at the University of Oulu, Finland. Simulations and experiments were run both with and without the aortic implant.

The effect of the aortic implant is clear in both the simulation and experimental data. (See Figure 12 for a

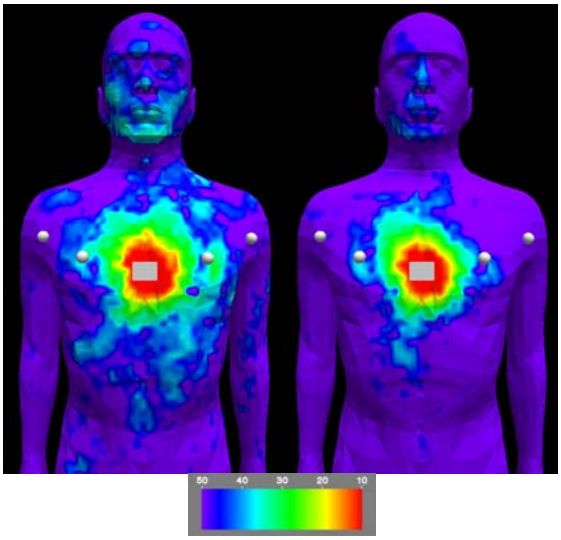

Figure 12. *The image on the left shows simulated path loss without the aortic valve implant. On the right is the same simulation with the valve implant. The rectangle in the middle of the chest is the position of the transmitter and the spheres show the positions of the receivers in the experiments.*

visual comparison of the simulations.) However experimental and simulation data do not exactly match; see our paper [3] for more detailed results. We will continue to investigate the effect of other medical implants on BAN signal propagation.

Another part of this effort has involved the creation of statistical path loss models for BAN communication channels [4]. These models are based on simulations of four near surface and two deep tissue implant applications using our 3D model of the human body. The path loss models obtained in this study have been adopted by the IEEE 802.15 task group TG6. The accuracy and applicability of such models will require further validation and investigation.

Much of our current work centers on applications in which BAN devices are attached or worn on the surface of the body. In this situation, the creeping wave phenomenon comes into play which affects how signals propagate along surfaces. We are investigating how the creeping wave effect may be exploited for on-body BAN devices. This may effect antenna design and device placement decisions.

Our visualizations and analyses of the simulations showed a pronounced creeping wave effect. We then performed simulations using a transmitting antenna design optimized to exploit the creeping wave. The use of these results to compare antenna designs proved problematic. We are currently studying how to resolve these problems.

In addition to the continuing effort on the issues described above, we are pursuing several lines of investigation. We are collaborating with researchers who are doing related experimental work that will help us to validate our simulations. We are also developing methods for placing our 3D body model into various poses so that we can study the effect that positions and body motions have on signal propagation. While this work is in an early stage, these simulations will help researchers and engineers understand the issues that affect BAN communication.

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

Rheology of Dense Suspensions

Understanding the mechanisms of dispersion or agglomeration of particulate matter in complex 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 many different ways. Predicting the flow of such systems via mathematical models represents a great scientific and computational challenge, requiring large scale simulations at a fundamental level. In collaboration with scientists in NIST's Engineering Laboratory (EL), we are developing an application, called QDPD (Quaternion based Dissipative Particle Dynamics), which is capable of performing large scale simulations of dense suspensions. QDPD is highly parallel and has been shown to efficiently scale up to at least 32 thousand processors when running on the DOE supercomputer Intrepid at Argonne National Laboratory. Our goal in this project is to advance our understanding of the flow properties of a specific system, fresh concrete, a dense suspension composed of cement, water, sand, and rocks.

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Nicos Martys

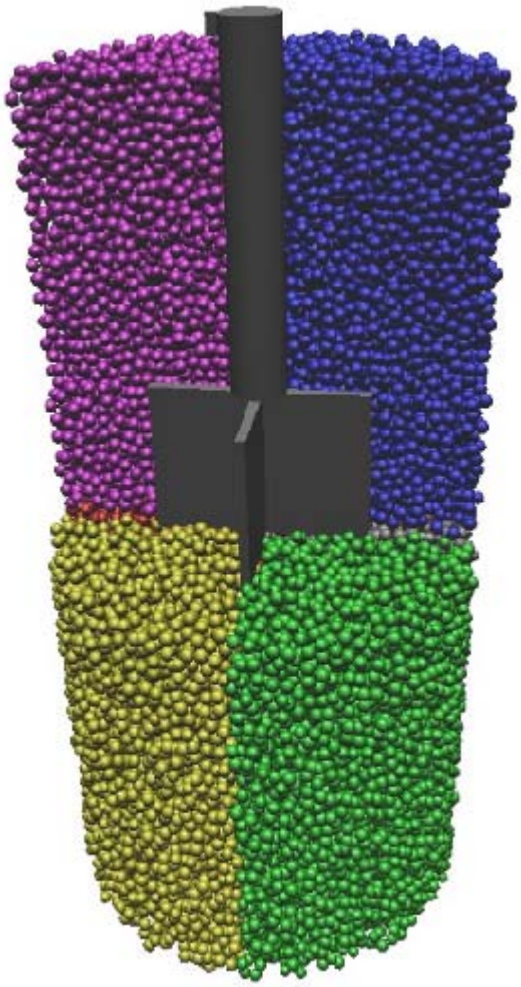

Figure 13. *Snapshot of a simulation of a 4-blade vane rheometer with a suspension of hard spheres. The hard spheres are colored by the octant in which it is initially located within the rheometer. Spheres from two of these octants have been omitted to show the blades of the rheometer. This is the original configuration of a simulation of a mortar.*

Concrete is the most widely used building material in the world, representing a 100 billion dollar industry in the US that is 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, is responsible for about 8% to 10% of global CO_2 production.) As new mixture designs of concrete are developed to meet these needs, it is important to measure and 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 months of delay by having to correct previous errors.

Often fluids are characterized by the properties yield stress and viscosity, which are a function of shear rate. In particular: yield stress is the force applied per unit area to initiate the flow, and 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. An image showing the local stress in a vane rheometer is shown in Figure 13.

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 in each material 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. Additionally, the more similar the size of the rocks in a concrete suspension, the harder it is to get the concrete to flow. In this case, the concrete may actually jam when poured through a narrow opening, thus causing delays in construction. Clearly, to optimize the flow properties of concrete and other suspensions, one needs

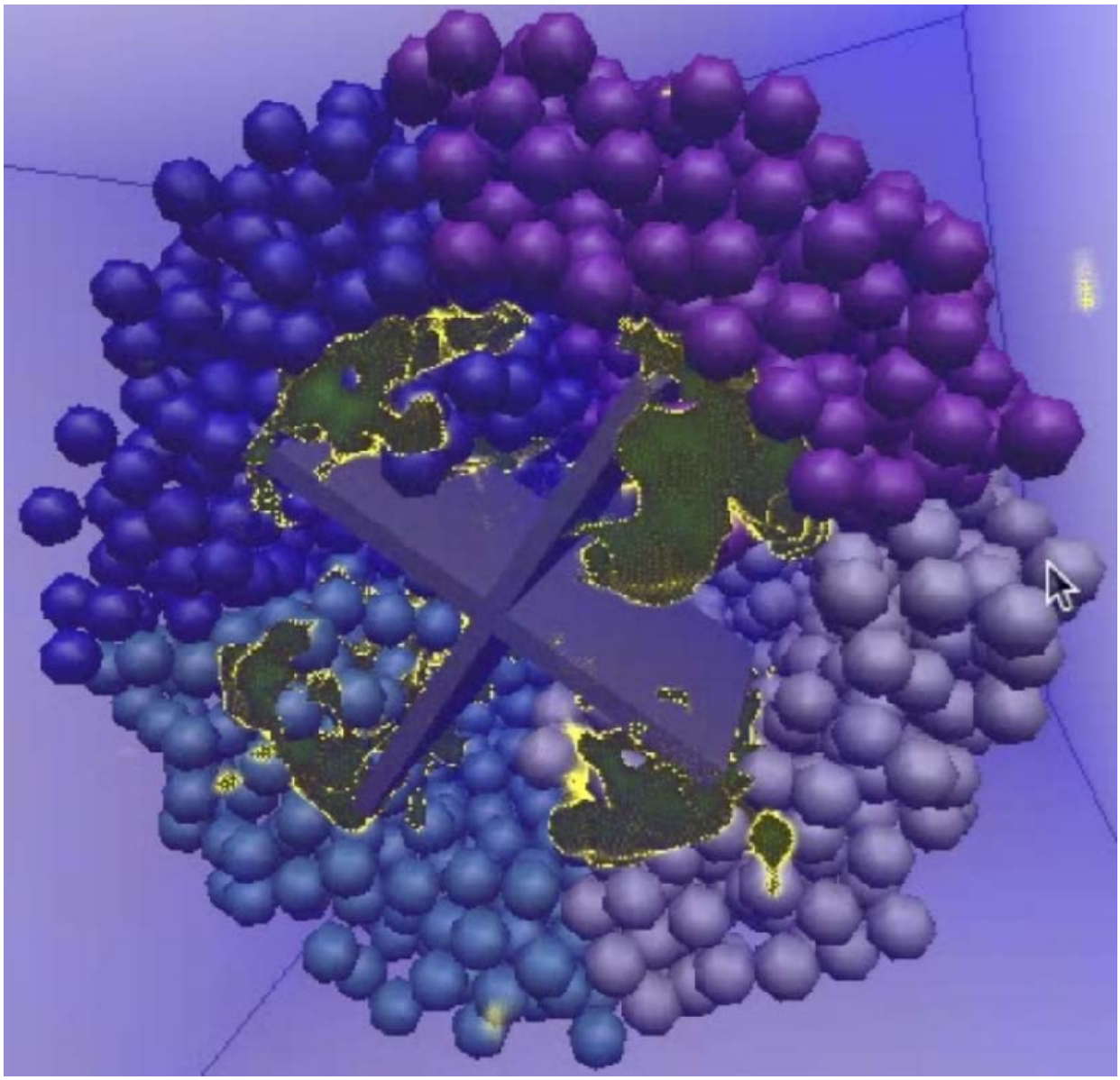

Figure 14. *A snapshot of a vane rheometer simulation displayed with a volume visualization of the magnitude of the local stress within the system. As in* Figure 13*, the suspended spheres are color coded by the octant they started in. Only 4 of the 8 octants are shown here in order to see details around the vanes. For the added volume visualization, stress is color coded from yellow (low stress), to green (high stress), with stresses below a set threshold not shown. The blades of the rheometer are rotating clockwise.*

to understand the relationship between flow and properties of the fluid's constituents.

Our current focus is on enabling the use of vane rheometers for measuring the rheological properties of fresh concrete, something that is not currently possible. While different "concrete rheometer" measurements can be found to correlate, they usually do not agree well in actual measurements in fundamental units. A vane geometry combined with a strongly random suspension will result in complex local stress and strain/strain rate fields. Simulations will enable us to map out these fields in 3D, and bring insight into the vane design process. There is no expectation that current vanes are optimized for precise measurement (or mixers for best mixing practice), and the results from simulations can be used to optimize vane design. We are also using simulations in the design process for new standard reference materials (SRMs) which will be used for calibrating rheometers. This year we completed NIST SRM 2492 – Cement Paste.

QDPD. Modeling and predicting the flow of suspensions such as concrete represents a great scientific challenge since these are complex disordered systems with a variety of components that can interact in many different ways. Indeed, accounting for the size and

shape variation of the solid components of the suspension (cement particles, sand, or rocks) poses many computational challenges. A representative system may entail keeping track of up to 100,000 solids 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 neighboring aggregates, which requires keeping track of the location, orientation and shortest distance between neighboring solids. Clearly, modeling such systems necessitates large scale simulations at a fundamental level to accurately predict its properties. We have adopted and developed some novel approaches, originally based on cellular automata methods, which can successfully take into account many of the features of a suspension. Our original code, QDPD, 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 [1], which stands for Quaternian-based Dissipative Particle Dynamics (DPD), uses modified versions of the recently developed DPD 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 the DPD and SPH techniques, other forces are computed in these systems to better account for the interaction between the inclusions (the large particles) in the suspensions. These additional forces 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.

From the original serial version of this simulator we have enhanced QDPD to utilize the power of large parallel machines, regularly using 500+ processors, and, for large production runs, using 32 thousand processors. QDPD remains under constant development to improve its capabilities as well as to improve its parallel performance.

Argonne National Laboratory's DOE Leadership Computing Facility. During the 2011 calendar year we have had access to the 164,000 processor IBM Blue Gene/P supercomputer Intrepid, having been awarded 25 million CPU-hours of compute time on this machine from the DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE). This access has enabled us to perform several very large simulations of a four-blade vane rheometer. We have been awarded a second year of compute time, for 2012, on Intrepid through our peer-reviewed INCITE proposal.

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

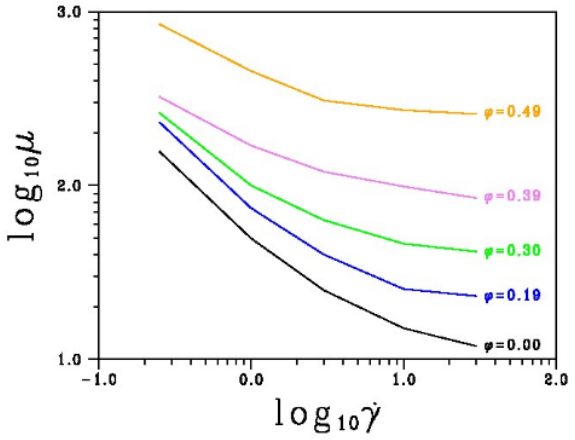

Figure 15. *The visosity of a suspension, comprised of a proposed standard reference material (SRM 2492) + 1 mm diameter glass beads, is shown for various volume fractions from 0.00 % (i.e., pure fluid matrix) to 49%.*

Over the last few years our simulations have provided fundamental insights into mechanisms that control the onset of flow in suspensions that can be linked to macroscopic properties such as yield stress and viscosity. We have developed a novel way of describing the interparticle stress fields and their spatial correlations. Though 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 have 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 as a consequence of temperature effects.

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

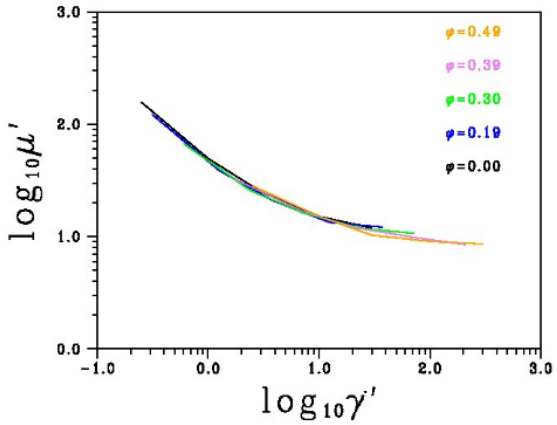

Figure 16. *The curves in Figure 15 collapse onto the 0% volume fraction curve using the same function to collapse each curve to the 'universal curve' for this matrix fluid.*

Our studies have enabled us to discover that, given the properties of the matrix non-Newtonian fluid in a dense suspension, such as a mortar or concrete, we can predict the rheological properties of those dense suspensions. In Figure 15 the visosity of a suspension, comprised of a proposed standard reference material (SRM 2492) of + 1 mm diameter glass beads, is shown for various volume fractions from 0.00 % (i.e., pure fluid matrix) to 49 %. Figure 16 shows these plots collapse onto the 0 % volume fraction curve using the same function to collapse each curve to the "universal curve" for this matrix fluid.

Finally, while the main thrust of our research focuses on predicting the rheological (flow) properties of cement based materials such as concrete, an improved general understanding of rheological properties derived from this research should have a broad impact. Suspensions are utilized in wide variety of technological processes and, as our study is largely parametric in nature, results will be transferable to other suspensions of interest such as nanoparticle systems. Understanding mechanisms for the dispersion or agglomeration of such systems remains a challenge in many industries ranging from pharmaceuticals to coatings.

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

Segmentation and Tracking of Breast Cancer Cells

The ability of cells to migrate varies widely during the development and life of multicellular organisms. Cell- and organ-specific regulation of the migratory behavior of cells is critical. In normal epithelia, such as breast epithelium, cell migration is restricted, but epithelial cells that are transformed into tumor cells acquire mutations that allow them to migrate into the surrounding connective tissue (invasive tumor) and then to distant sites to establish metastatic disease [1]. Investigating the migratory behavior of epithelial and tumor cells may enable biologists to find ways to control migration of tumor cells and reduce metastasis.

We have developed new techniques to automatically identify and track individual cells within images of a breast cancer cell line in order to study cell migration and metastasis. Within each image observable cell characteristics vary widely, ranging from very bright completely bounded cells to barely visible cells with few to no apparent boundaries. A set of different segmentation algorithms are used in series to identify each cell type. Normally cell segmentation and tracking are performed as two separate steps. However, in this work they are done simultaneously so that predictions can be made about where cell boundaries lie on an image at each time step. A new method for background subtraction is described and a new method of selective dilation is used to segment the barely visible cells. Initial results are encouraging.

Adele Peskin

Cell migration can be studied by visualizing cell responses through the capture of time-lapse images for long periods of time. Quantitative analysis of these images is performed by tracking the position of individual cells, a labor-intensive process which can only be done manually for a few selected cells. Images from the cell line in this study, MCF10CA1a [2], do not lend themselves to well known automated segmentation and tracking methods. The goal of this work is to automate these processes in order to better understand the cell migration in this cell line.

The difficulties in processing these images are several-fold. The individual cells move at varying speeds, sometimes quite rapidly, making them hard to track from image to image over time. The morphologies of the cells themselves vary greatly over a single image. As shown in Figure 17, a typical image of these cells contains cells that are bright with dark edges that are straightforward to segment, along with cells that are barely visible at times, so that their apparent shape changes over the course of a few minutes.

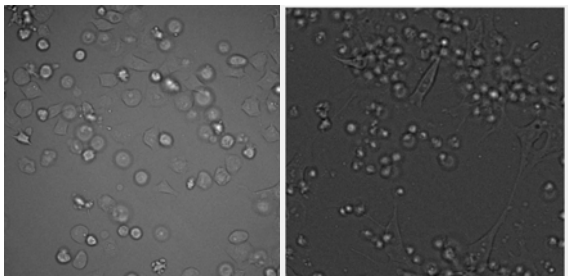

Figure 17. *An early image in a time series and a later image.*

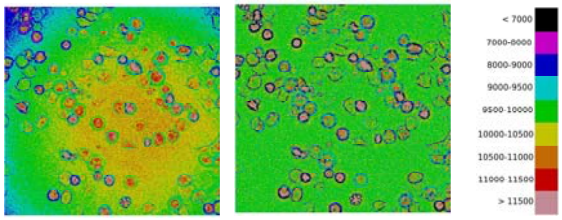

Figure 18. *Sample image color-coded before and after background removal. The color table at the right shows pixel intensities before background removal.*

We have developed segmentation techniques to identify individual cells and track them from image to image at early growth times. The steps involve background removal, predicting cell size and location based on the previous image in time, and then defining the new location and shape. Background removal in a timed series is often accomplished by examining the whole series to find examples of each part of the background when it is free of cells [3]. However, to process in real time it is important to be able to remove background noise for each individual image. For each image, a mean value is found for the image as a whole, and all pixels with intensity higher than three standard deviations above the mean (where cells are located) are temporarily replaced by the mean value to smooth out the image. Then the background value for each individual pixel is determined by the average value in a small neighborhood of that pixel. Figure 18 shows an image at the start of growth, color-coded by pixel intensity, before and after background removal.

Figure 19 shows sections of an image containing a variety of cell morphologies. The dark cell boundaries and brighter cell areas are easily captured by looking for clusters of pixel intensities significantly above and below the mean value of the image. The larger pixel clusters that represent cell boundaries and cell bodies are distinguished from much smaller background clusters by a new method of selective dilation that diffuses only the larger clusters to slightly larger shapes to sepa-

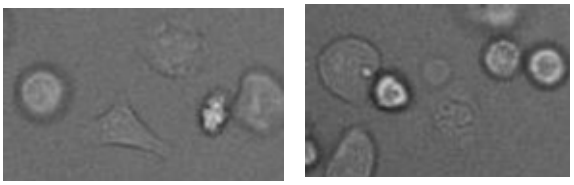

Figure 19. *Sub-sections of the image in Figure 2, showing different cell morphologies.*

rate them. To segment the barely visible regions, clusters of pixels are defined whose intensities in very localized regions have higher than average standard deviations. These clusters are matched with the predicted locations of cells from past time steps. The software keeps track of cells that are actively moving and their current velocities in past time steps, as well as the size and shapes of each cell. Cell velocities are used to predict cell locations at the next step. To enhance the high standard deviation clusters, the new technique of selective dilation is also applied. The total number of cells in an image can only vary from time step to time step if cells move into or out of the field of view at the images boundaries, or if cells divide. It is also important to keep track of cells that die, but remain in the field of view. Dead cells have characteristic morphologies and in general no longer move or change shape. Recognition of dead cells is important because there is no need to track their shape changes and behaviors.

The details of the segmentation and cell tracking, which are performed simultaneously, are given in [4]. For short periods of time, we are able to track every cell in our test set of images. Cell divisions are identified during the cell tracking, which is an important feature. Figure 20 shows some example images and their corresponding segmentation/tracking.

Future work will include larger scale tests and comparisons with manually collected data. We are developing a more general model so that we can segment and track cell lines with large masses of cells with individual cells whose boundaries go into and out of the field of vision of the microscope over time.

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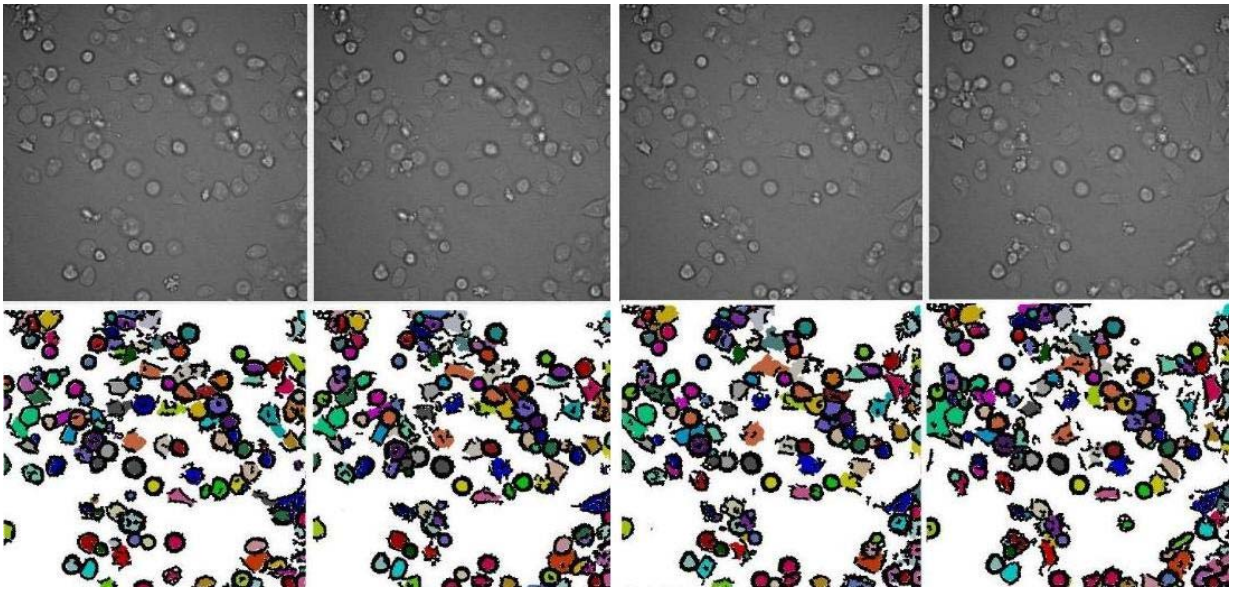

Figure 20. *Images and resulting masks at 0, 10, 20, and 30 minutes.*

Single Photon Up-conversion and Quantum Information Science

Photons play an important role in quantum information science. Information can be stored in their quantum states (e.g., polarization), and their mobility enables these states to be transported over long distances. As a result, reliable generation and detection of single photons are important enablers of quantum information science and engineering. Photons with wavelengths in the near infrared (NIR) are ideal for long-distance communication since they suffer the least loss in optical fiber. Unfortunately, commercially available detectors are very unreliable at these wavelengths.

To address this problem, the ITL quantum communication research team has developed novel single photon detectors in the NIR range and significantly improved their performance in recent years. These detectors are based on so-called up-conversion technology, in which the photon's wavelength is converted to one where detectors are efficient, without changing essential properties, such as the quantum state in which information is encoded.

Such detectors have wide application in both quantum information and in metrology. Using the up-conversion detectors the team has performed several otherwise difficult or impossible quantum optical measurements. The team is working with US industry to commercialize the technology via the NIST Small Business Innovative Research (SBIR) program.

Xiao Tang

Upconversion[12] is a process by which two optical fields combine in a nonlinear medium to generate a third field at a frequency equal to the sum of the two inputs. As well as energy conservation, this process requires momentum conservation, placing a condition on the phase velocities of the three beams. Recently, it has been shown that quasi-phase-matching, a process in which a grating in the nonlinear medium is used to compensate for wave vector mismatch between the sum frequency beam and the two input beams, can enable highly efficient upconversion, with near unity conversion efficiencies achieved in periodically poled $LiNbO_3$ (PPLN) waveguides. Because upconversion can, in principle, be used to transduce one photon at a given wavelength to a photon at another wavelength, one could imagine using it to couple different quantum systems at different energies. This kind of hybrid quantum-information scheme enables the use of photons for efficient transmission of quantum information over large distances, and robust, stationary quantum systems such as trapped atoms or ions, atomic ensembles, or spins in quantum dots for manipulation and storage. Another important application of quantum transduction is the frequency upconversion of telecommunications-band photons (e.g., a wavelength of 1310 nm) to the visible part of the spectrum (e.g., 850 nm) for detection with commercially available low-noise silicon avalanche photo diode (Si-APD) detectors, for example, as part of a quantum information protocol. While photons at 1310 nm are ideal for long-distance transmission over optical fibers, photon detectors are extremely inefficient at that wavelength.

A few years ago, the ITL quantum communication research team adapted this technology to develop up-conversion detectors at NIST. In 2007, the research team successfully demonstrated their use in a fiber-based high speed quantum cryptographic key distribution (QKD) system. Since then, the devices have been significantly improved. For example, during the past year, the detection noise level, or so called dark count rate (the detector records events even if there is no signal input), has been significantly reduced by an order of magnitude [1]. As another example, the team developed a multi-wavelength pumping scheme that increases the system data rate beyond the barrier set by the performance limitations of the Si-APD detectors [2]. In addition, using our up-conversion detectors, the team performed several otherwise difficult or impossible quantum optical measurements. These include: the characterization of semiconductor quantum dots; the measurement of higher (second-, third- and fourth) orders of photon temporal correlation; and optical sampling at the single photon level using a pulsed up-conversion technique. These results demonstrate that our up-conversion technique enables advanced quantum optics research with applications in future quantum computing and quantum communications systems.

In quantum information science, individual photons can be used as information carriers. Therefore, the study and development of single photon sources has become a key research area and opportunity. Semiconductor quantum dots can emit photons one at a time and have high potential as practical single photon sources. In 2010, the team conducted a joint experiment in collaboration with NIST colleagues in the Center for Nanoscale Science and Technology (CNST). The up-conversion detectors were used to detect single photons at 1310 nm from a semiconductor quantum dot. Because of the high sensitivity and low dark count rate, our up-conversion detector is able to measure the quantum dot exciton lifetime with a much higher accuracy than by using commercial indium gallium arsenide (InGaAs)-based detectors typically used at such frequencies. A photon correlation measurement is a good

[12] Part of this introduction is taken from [3].

way to characterize a source and to determine whether or not it is emitting single photons. By using the up-conversion detectors, the team performed a second order intensity correlation measurement for the photons emitted from the quantum dot and demonstrated for the first time that the converted photons preserve their quantum characteristics during frequency conversion. In FY2011, this important conclusion was reported in *Nature Photonics* [3].

To further prove this result, the ITL team, in collaboration with researchers in CNST and the NIST Physical Measurement Laboratory (PML), conducted higher (2^{nd}, 3^{rd} and 4^{th}) order correlation measurements for photons from an attenuated pseudo thermal source (similar to a lamp) and a coherent source (attenuated laser) in the NIR region. Use of ITL's detectors proved critical, since otherwise it would be very difficult or nearly impossible to measure such higher-order correlations due to the lack of suitable commercial detectors for photons in the NIR region. Our results, published in Optics Express [4], nicely match with theoretical predictions. Figure 21 shows the fourth order correlation of photons from the pseudo thermal source.

The integration of two disparate quantum systems requires that the photons from the two systems must have same wavelength and same spectral linewidth (so called indistinguishable). As described above, up-conversion provides the capability to convert or adjust the photon's wavelength. The question then arises, "is it possible to adjust the linewidth?" To answer this question, the ITL team has collaborated with CNST and demonstrated an optical sampling process at the single photon power level to accomplish this [5]. Frequency up-conversion devices can be operated with a pulsed pump. When a pump pulse width is narrower than the signal pulse, in general, it can be viewed as a gate for optical sampling. In this process, the photon wavelength is transduced and the amplitude profile of the photon wave packet is simultaneously modulated by the pump pulse shape. The amplitude modulation can be used to select the coherent part of the single photon wave packet (or change of the linewidth) which enables us to make two independent photons perfectly indistinguishable. This allows a better integration of two disparate quantum systems, which is essential for future quantum networks and long distance quantum communications.

Currently, the ITL quantum communication research team is exploring new areas of quantum research by using their up-conversion technique, as well as working with US industries for its commercialization through the NIST SBIR program.

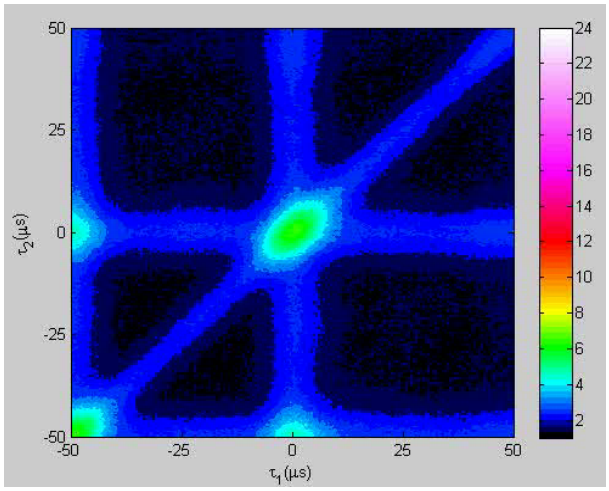

Figure 21. *Frame from a movie showing the measured fourth-order photon correlation function for a pseudo-thermal source. The function has four-dimensions. In addition to the x and y dimensions we use color as the third dimension, and present it in a movie showing time as the fourth dimension. To view the movie, go to* http://www.nist.gov/itl/quantum/quantum.cfm

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Participants

Lijun Ma, Oliver Slattery, Barry Hershman, Alan Mink, Xiao Tang (ACMD); Martin J. Stevens, Joshua C. Bienfang (PML); Matthew T. Rakher, Marcelo Davanço, and Kartik Srinivasan (CNST).

Community and Cluster Detection: Alternative Measures for Network Structure

Detecting community structure in large graphs is one of the fundamental challenges in network science. A "community" is loosely defined as a subset of nodes which are highly connected to each other, but less connected to other nodes in the graph. Identifying such groups can be useful in understanding graph structure, as well as its dynamic characteristics, such as evolution and synchronization. In various application contexts, community detection can classify persons or objects with unifying characteristics. Some examples include identifying groups in social networks, determining graph layouts for visualization, and modeling the spreading of infectious diseases. In this project we are assessing the performance of the many community detection algorithms that have been proposed. In the course of this work we have uncovered a novel framework for describing the fundamental structure of such networks.

Roldan Pozo

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

The underlying question remains: how well do these approaches work in practice? So far, there has been limited work in verifying and validating the results on a wide array of application domains. The results of current state-of-the-art algorithms work well in some situations, such as when vertices clearly belong to one (and only) community, but the real world is not so ideal. More complicated approaches allow for overlapping communities, but fundamental problems remain.

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 resulting network. That is, given a degree threshold, we create a subgraph consisting of only nodes with that less than or equal to that degree value. This subgraph is largely fragmented into disconnected components, which can be useful in finding small, isolated fringe groups amidst the noise of large-order hubs.

Figure 23, for example, shows the shows the non-trivial connected components of a web network (http://math.nist.gov/) by restricting it to a subgraph of nodes with (in/out) degree 15 or less. It reveals various structures: e.g. ladders, star, and cluster patterns representing tightly coupled webpages. These form the nucleus of isolated communities, and by varying the degree parameter we can direct the size and granularity of groups revealed. This information can be used to augment a conventional algorithm to better identify small or rural 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 see a small fragmented graph of either isolated nodes, or individual pairs of nodes. As we increase this value, we include more nodes in the subgraph, increasing the number of communities. However, some of these communities also increase in

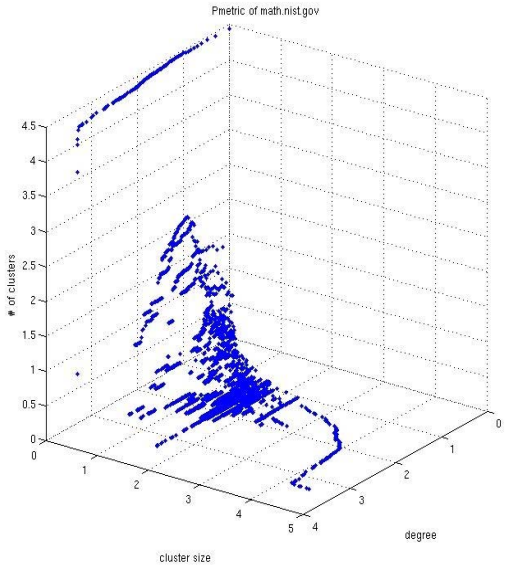

Figure 22. *P-Metric of the math.nist.gov web graph, showing cluster size distribution as the degree threshold varies from 0 to the maximum degree of the graph. The "wall" on the left illustrates the large number of leaf nodes and described the "bushiness" of the graph; the "hill" in the middle reveals the medium-sized clusters (10-100) which form good candidates for coarsening; the "hook" on the right reveals the formation and growth of the giant component.*

size and merge with others, thus providing a contraction effect. For connected networks, as the threshold is increased to the maximum degree, we are left with a single component: the complete network graph. Thus, as one turns the degree-threshold parameter, the number of components (communities) starts out small, grows, and eventually shrinks to number of connected components in the original graph.

A more detailed analysis not only includes the component count at a given degree value, but also the size distribution of these components. The Profile Metric (or P-Metric) of a graph is the frequency distribution of component sizes of a degree-induced subgraph as the threshold value varies between 0 and the maximum degree of the graph; see Figure 22. This not only reveals several properties (such as the degree distribution, and the formation and growth of the giant component) but also provides a visual thumbprint of the graph structure, which is different from conventional community detection results. This measurement can be used to identify clusters for graph coarsening, or to reveal differences between "real" and "random" graphs. We are currently investigating these ideas to develop hybrid metrics which better describe the complex nature of these graphs.

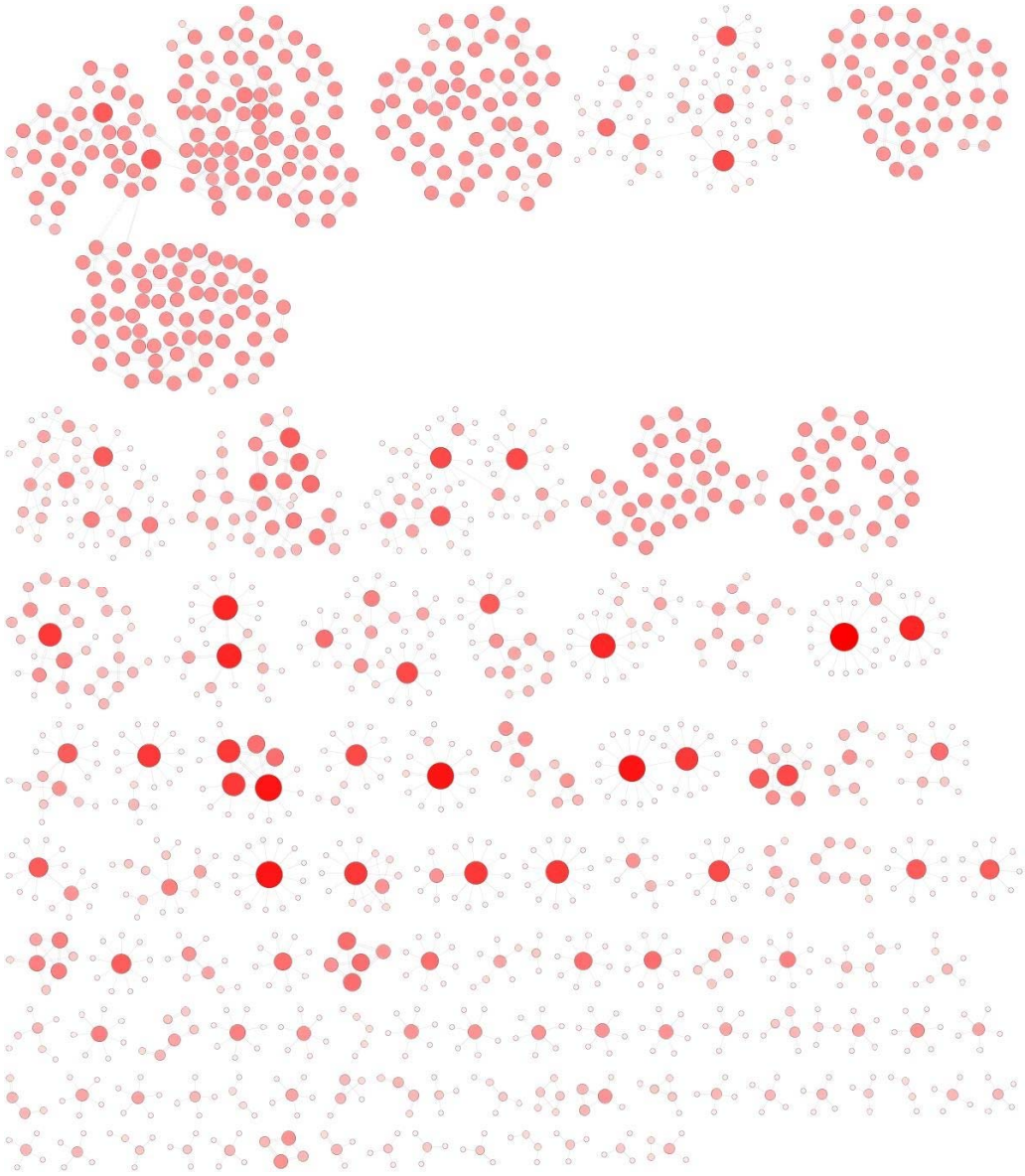

Figure 23. *Non-trivial components of the math.nist.gov web graph, restricted to nodes with combined degree less than or equal to 15, classifying 1,380 pages into 101 groups. These form meaningful "communities" which can be useful in reducing the original graph to a coarsened version.*

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 to critical measurement science applications.

Unsuspected Nonuniqueness in Solving Parabolic Equations Backward in Time

Alfred Carasso

See feature article, page 29.

Molecular Movies: Imaging Femtosecond Motion during Electrochemical Transitions

Bradley Alpert
Joel Ullom et al. (NIST PML)
Chris 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 release, transport, and transfer in engineered nanostructures. This project, chosen in 2010 for a NIST Innovations in Measurement Science 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 the NIST Quantum Electronics and Photonics 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

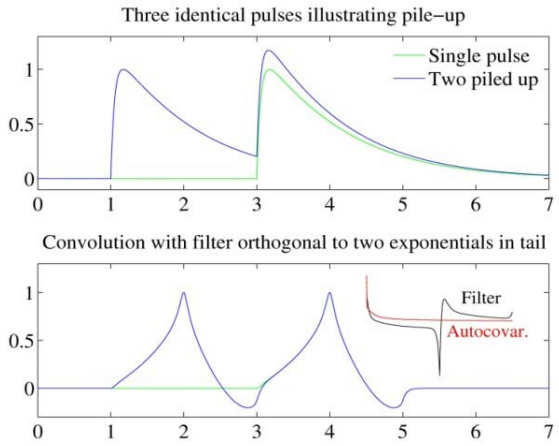

Figure 24. *Pulses illustrating pile-up.*

- 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 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.

This year progress occurred in the following areas:

1. Alpert proposed a method for computing filters in the time domain, rather than the frequency domain, eliminating processing artifacts of the discrete Fourier transform, which are significant in this application. The motivation for the change,

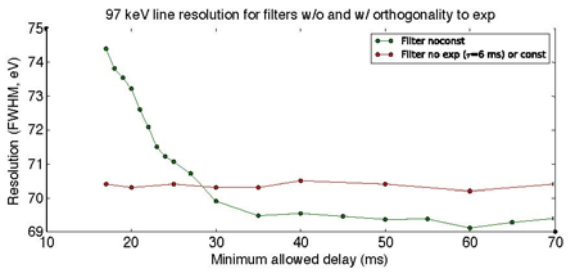

Figure 25. *97 keV line resolution.*

however, was to obtain a flexibility that allows imposition of filtering constraints. In particular, orthogonality to exponentials of one or more time constants enables a measured pulse energy to be insensitive to prior pulses. Initial tests of the new filters, at relatively low pulse rates, provided encouraging results [1]. Higher-rate experiments are being developed.

2. A filtering method recently proposed by other researchers, which is intended for inline processing and trades some resolution for simplicity and ability to handle high pulse rates, was analyzed [2].
3. A computational tool was developed that should enable rapid construction of filters, "on the fly," for particular pulse arrival times. The tool provides fast application to a vector of the inverse of a covariance matrix for stationary noise whose covariance can be expressed as a short linear combination of exponentials. The potential here is the elimination of any signal-to-noise penalty associated with the method [1] mentioned above.

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.

Two scenarios, one with pile-up, are shown in Figure 24 (top). From the pulse shape and noise autocovariance, a filter orthogonal to exponentials of two slow decays is computed (inset, separate vertical scales). Convolving the filter with the signal yields peaks of essentially constant height (bottom), nearly eliminating pile-up dependence.

Energy resolution (i.e., uncertainty) for the 97 keV gamma-ray emission line of 153 Gd is shown in Figure 25 as a function of the minimum pulse separation time, for two different filters. The first filter (green) is orthogonal to constants, while the second (red) is orthogonal to both constants and decaying exponentials with 6 ms time constant. The added constraint removes sensitivity to nearby pulses, while incurring some penalty in signal-to-noise ratio.

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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 some 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, have received considerable attention from mathematicians in recent years, 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 improved recoveries.

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 Chen are conducting extensive 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 may be 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.

Applied Hierarchical Control

Anthony Kearsley

Optimal control problems constitute an interesting case of PDE-based optimization problems. Instances of these types of problems abound in applications, especially those in measurement science. Efficient numerical methods for the solution of these problems have been the subject of significant recent research [1], but recently specialized numerical methods are being developed for application-specific problems.

Motivated by specific scientific and engineering applications, such as those arising in calibrating and optimizing instrument performance, we investigate a means of formulating a class of optimal control problems in which desired behavior of solutions or "targets" can be partitioned into categories of increasing relative importance.

There is no unique mathematical formulation of these types of problems; indeed different formulations can generate completely different "optima" or solutions. In one formulation, the problem is posed as the minimization of a weighted sum of the deviations from the targets with weights corresponding to an established priority among the targets (see [7]). Another formulation, sometimes referred to as goal programming, insists that a set of preferred targets be satisfied to within certain tolerances and the others be reduced as much as possible within these constraints (see [5]). Both of these approaches involve the choice of a set of weights or tolerances for which there may be little theoretical guidance.

An instance of this problem occurs, for example, in calibrating a MALDI/TOF mass-spectrometer when one knows the total amount of compound present in a sample, suggesting one minimizes a least squares or distance regression function while simultaneously maximizing signal to noise. Motivated by this application, and others, we seek to formulate this problem as a collection of nested optimization problems in which the solutions of the inner problems are determined using the variables in the outer problems as parameters. This approach is based on the work of von Stackelberg [3] in an economic context, requiring that the deviations from the least important targets, called the "follower" targets, be decreased only after the deviations from the most important targets, called the "leader" targets, satisfy prescribed bounds. This type of optimal control problem has been termed hierarchical control [2]. One way of formulating this type of problem is in terms of nested optimization structure in which, in an "inner minimization," the follower targets are minimized subject to fixed values of certain of the control variables, and then an "outer minimization" is performed over the remaining control variables to obtain optimal leader target satisfaction [3]. The accuracy on the follower targets is therefore determined by, and is subordinate to, the optimization over the leader targets. In the case of MALDI/TOF calibration, matching known experimental parameters would be a primary objective and maximizing signal to noise, a secondary or "follower" objective.

Recently we have derived optimality conditions for a linear differential equation [8] and are very close to extending our results to a more general reaction diffusion equation [9]. This work constitutes significant steps towards the ultimate goal of robustly and reproducibly optimizing instrument performance for multiple objectives (e.g., matching output while simultaneously maximizing signal to noise).

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Denoising Helium Ion Microscope Nanoscale Imagery

Alfred Carasso
Andras Vladar (NIST PML)

Helium Ion Microscope (HIM) images are particularly rich in surface morphological detail, but are generally quite noisy. A major challenge is to denoise these images while preserving delicate surface information. A NIST-invented technology, based on smoothing HIM images $g(x, y)$ by applying a fractional diffusion equation,

$$w_t = -(\Delta)^{\beta} w, \quad t > 0, w(.,0) = g(x,y),$$

with fixed β such that $0.1 \le \beta \le 0.2$, has been found very useful. In that method, $\|\nabla g\|_1$, the L^1 norm of the gradient of the noisy HIM image, is first evaluated. A value of λ, with $0 < \lambda < 1$ is then prescribed, and the forward solution of the diffusion equation is terminated at the earliest time $t^{\dagger}$ where

$$\|\nabla w(.,t)\|_1 \le \lambda \|\nabla g\|_1$$

FFT algorithms are used to solve the fractional diffusion equation. By visually monitoring the evolution up to time $t^{\dagger}$, a user can decide whether too much or too little smoothing has occurred. One can then backtrack to an earlier image, or restart the procedure with a new value of λ. Values of $\lambda \approx 0.3$ have been found useful for many HIM images at NIST.

Considerable work has been published on other denoising methods. One of the best-known is the total variation (TV) method, which assumes the true noiseless image to be of bounded variation and defines the TV denoised image by means of

$$g^{\mathrm{tv}}(x,y) = \mathrm{Arg\,min}_{u \in BV(R^2)} \{ \|\nabla u\|_1 + \frac{\omega}{2} \|u - g\|_2^2 \}.$$

The minimization needed to produce g^{tv} can best be accomplished by one of two methods: applying the Split Bregman iteration, or computing the long time steady-state solution to the nonlinear Marquina-Osher second order parabolic equation, with the noisy image $g(x, y)$ as initial data. Here, in contrast to the fractional diffusion method, there is no a-priori user control on the gradient of g^{tv}, and consequently,

$$\|\nabla g^{\mathrm{tv}}\|_1 << \|\nabla g\|_1$$

typically. This characteristic feature of TV denoising has been found detrimental in NIST applications to HIM imagery. Indeed, as noted below, the fundamental reason why TV denoising is not helpful is because HIM and SEM images are not of bounded variation.

Lipschitz exponent analysis. Many natural images $f(x,y)$ are not smoothly differentiable functions of x and y, but involve non-differentiable localized fine structures and texture, in addition to edges. The L^1 Lipschitz exponent α, where $0 < \alpha \le 1$ is a mathematical index that can be used to estimate image fine structure content. Images that are of bounded variation or smoother have α=1. The value of α decreases with increasing fine structure. A patented NIST-developed methodology, based on FFT algorithms, can be used to evaluate image Lipschitz exponents. Typical SEM or HIM images have Lipschitz exponents $\alpha < 0.6$, and are not of bounded variation. TV denoising forces $g^{\mathrm{tv}}(x,y) \in \mathrm{BV}(R^2)$, which often leads to smoothing out of texture and/or elimination of localized fine scale information. A typical example is shown in Figure 1 and confirmed in Table 1. The fractional diffusion image maintains fidelity to the surface morphology of the sample, as is evident from the jagged edges and foreground surface texture. These important elements are not well-recovered in the TV image. Fractional diffusion reduces $\|\nabla g\|_1$ by a prescribed factor of 3, while conserving $\|g\|_1$, leading to a denoised Lip $\alpha = 0.451$. In contrast TV denoising falsely reduces $\|g\|_1$ by 16%, reduces $\|\nabla g\|_1$ by a factor of 7 or more, and leads to a significantly higher denoised Lip $\alpha = 0.751$.

Quantitative validation of fractional diffusion denoising. A research project of considerable interest to the NIST Mechanical Metrology Division involves artificially generated SEM and HIM nanoscale images, obtained by using a sophisticated computer program developed in PML. This program can generate physically realistic degraded images that mimic very precisely the characteristics of modern nanoscale instrumentation. The amount and type of noise can be controlled, as well as the amount and type of blur. Because the true image is known, such realistic degraded imagery can be used to evaluate the performance of

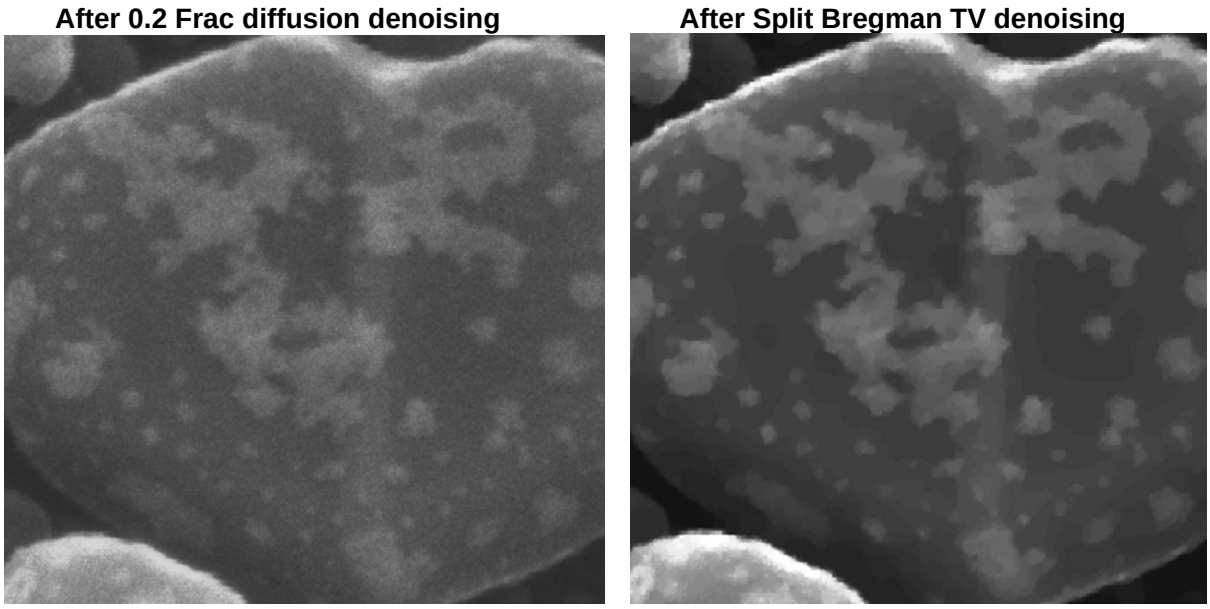

Figure 26. *TV denoising retains less fidelity to surface morphology than does fractional diffusion denoising, leading to a higher Lipschitz exponent.*

Table 1.

Image g(x, y)	$\|g\|_1$	$\|\nabla g\|_1$	Lip α
Noisy HIM original (600 nm)	88	25000	0.231
After Frac diffusion ($\beta = 0.2$, $t^\dagger = 0.1$)	88	8500	0.451
After Split Bregman TV ($\omega = 0.025$)	74	3400	0.751

various image processing methodologies. Fractional diffusion denoising was applied to five artificially generated SEM and HIM images, with increasing levels of noise-induced degradations. Excellent results were found when comparing the denoised images with the true images, with noise being reduced by quite significant amounts ranging from 35 to 46 percent.

Equivalent short time smoothing using other evolution equations. An obvious advantage of the fractional diffusion method is the ability to terminate the process at the exit time $t^\dagger$, the earliest time at which $\|\nabla g\|_1$ has been reduced by the prescribed amount. A natural question is whether similar useful denoising can be obtained with more standard evolution equations, by exiting at the same prescribed value of $\|\nabla g\|_1$. Two natural candidates are the linear isotropic heat conduction equation, and the nonlinear anisotropic Marquina-Osher equation. This topic is currently being explored.

Uncertainty Quantification in Scientific Computing

Andrew Dienstfrey
Ronald Boisvert

http://www.nist.gov/itl/math/ifip-woco-10.cfm

ACMD hosted the Working Conference on Uncertainty Quantification in Scientific Computing in Boulder, CO on August 1-4, 2011. The 76 participants representing 10 countries were a unique mix of mathematicians, statisticians, computer scientists, application scientists and managers who gathered together to consider the role of metrology in mathematical modeling and computer simulation. Such techniques and tools increasingly are playing critical roles as adjuncts to, or replacements for, direct physical measurement in both product design and societal decision making.

The program was divided into four theme areas: (1) Uncertainty Quantification Need: Risk, Policy and Decision Making, (2) Uncertainty Quantification Theory, (3) Uncertainty Quantification Tools, and (4) Uncertainty Quantification Practice. Keynote addresses

were delivered by Pasky Pascual of the US Environmental Protection Agency, Michael Goldstein of Durham University (UK), William Kahan of the University of California at Berkeley, Scott Ferson of Applied Biomathematics, and Maurice Cox of the National Physical Laboratory (UK). A panel discussion featured Sandy Landsberg of the DOE Office of Science, Larry Winter, former Deputy Director of the National Center for Atmospheric Research, and Charles Romine of NIST. Antonio Possolo, Chief of ITL's Statistical Engineering Division, and Mark Cunningham of the US Nuclear Regulatory Commission, were also notable plenary speakers.

The participants represented a wide variety of applications, including cosmology, weather/climate modeling, remote sensing/atmospheric chemistry, hydrology, nuclear energy/safety, fluid dynamics, engineering mechanics, manufacturing processes, medicine, toxicology, and computer security.

The meeting was organized by Andrew Dienstfrey and Ronald Boisvert of ACMD as part of ITL's Virtual Measurements Program. It was co-sponsored by the International Federation for Information Processing (IFIP) Working Group 2.5 on Numerical Software. The proceedings, currently under development, will be published by Springer.

ITL Program: *Virtual Measurement Systems*

Virtual Measurements in Quantum Chemistry

Raghu Kacker
Rüdiger Kessel
Russell Johnson (NIST MML)
Karl Irikura (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 determining reliable uncertainties in virtual measurements is being recognized. This project is focused on developing and applying methods for quantifying the uncertainty associated with a virtual measurement in quantum chemistry. The benefits accrue to research and development of chemical processes, materials development, and drug discovery.

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 computa-computational predictions to bring them closer to the true measured 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* [1], which is an international standard. The uncertainties for scaling factors lead to the corresponding uncertainties for virtual predictions.

Our 2005 paper on uncertainties in the scaling factors for *ab initio* vibrational frequencies [2] has been cited 132 times. This indicates that scientific community has started paying attention to uncertainties in the outputs of computational models.

Recently, the *Journal of Chemical Physics* received a critique of our 2009 paper "Uncertainties in scaling factors for ab initio vibrational zero-point energies" and of another paper like ours. Our response, appearing in the *Journal of Chemical Physics* [3], points out that the problem addressed in the critique is different than the problem which we addressed. An independent response submitted to the same journal reached the same conclusion.

In 2010 we had reported scaling factors and uncertainties separately for low and high vibrational anharmonic frequencies. Anharmonic frequencies are calculated from higher order models and require considerably more computational effort. However, our continuing investigations indicate that the scaling factors are not substantially improved relative to lower order harmonic vibrational frequencies. This leads to questions about the benefits of higher order anharmonic frequencies.

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[2] 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.

[3] R.D. Johnson III, K.K. Irikura, R. Kacker, and R. Kessel, Response to "Comment on 'Uncertainty in scaling factors for ab initio vibrational zero-point energies' and 'Calibration sets and the accuracy of vibrational scaling factors: A case study with the X3LYP hybrid functional,'" *Journal of Chemical Physics* **134** (2011), article 167102.

ITL Program: *Virtual Measurement Systems*

Bubble Motion and Size Variation during Thermal Migration with Phase Change

Asha Nurse
Geoffrey McFadden
Sam Coriell (NIST MML)

If a temperature gradient is applied to a liquid containing gas bubbles, the bubbles can occasionally be observed to migrate in the direction of higher temperatures; this effect can even overcome the usual buoyancy forces on the bubble. The source of such bubble motion is often the so-called *Marangoni force* that arises due to the temperature dependence of the gas-liquid surface energy. A thermally-induced variation of surface energy tangential to the interface gives rise to lateral stresses that drag fluid from the hotter regions to colder regions; the resulting flow tends to translate the drop into hotter regions.

The general study of surface effects such as the Marangoni force is important in many materials processing applications, where a parent phase is transformed into a daughter phase. If the parent and daughter phases are both fluids, then the effects of fluid flow in general, and Marangoni flow in particular, can have an important effect on the quality of the processed material. Steve Hardy, a NIST material scientist, conducted a series of experiments studying the motion of an air bubble in silicone oil under carefully controlled thermal conditions [1]. By comparing with theoretical predictions of bubble velocity versus temperature gradient, he was able to measure the temperature dependence of the surface energy, which is a quantity of fundamental interest in this field.

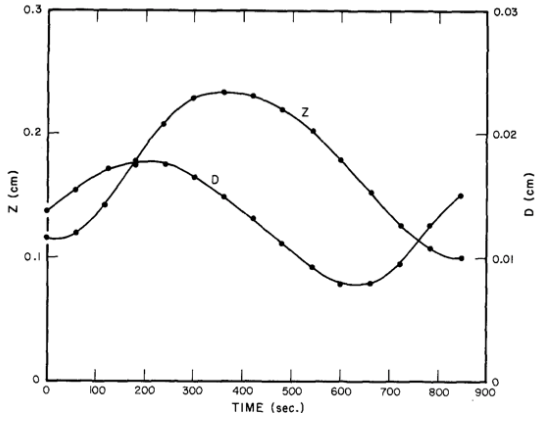

Figure 27. *The vertical position Z(t) of an air bubble and diameter D(t) in silicone oil with a vertical temperature gradient of about 110 K/cm plotted as a function of time t. (From S. Hardy [1]).*

To interpret his experiments Hardy used the theory of drop migration developed by Young, Goldstein, and Block in 1959 [2]. They obtained an expression for the steady velocity of a fluid drop contained in an immiscible liquid with a vertical temperature gradient. The velocity depends on the drop radius, the applied temperature gradient, the gravitational acceleration, and various material properties, and represents the interplay of the Marangoni force and the buoyancy force on the bubble. In particular they predict the possibility of stationary drops when these forces exactly balance; in that case there is a linear relation between drop radius and the applied temperature gradient.

In many cases Hardy observed that the bubble did not translate at a uniform rate, but instead moved up and down on a vertical trajectory while the radius of the drop also oscillated periodically in time; an example is shown in Figure 27. His measurements were made at the limits of the motion where the bubble reverses direction, and at these points he applied the corresponding results of Young et al. for the stationary bubble. Hardy's explanation for the observed oscillatory behavior was based on the exchange of air between the bubble and the liquid. The solubility of air in the liquid phase depends on temperature, and the liquid may be super-saturated with air in its hotter regions and under-saturated in the colder regions. In hot regions the diffusion of gas from the liquid into the bubble causes the radius to increase, and also causes the buoyancy force to increase so that the bubble rises. In the cooler region the opposite occurs, leading to the oscillatory behavior.

We have extended the theory of Young et al. to consider the case of a drop that can grow or shrink in time, and move with a non-uniform velocity. In our preliminary work the drop is assumed to be the vapor phase of the corresponding liquid. The change in phase as the drop grows or translates can give rise to a density-driven flow through the interface as well as local heating due to the latent heat release at the interface; these effects are absent in the treatment of Young et al. By solving the coupled Navier-Stokes equation and heat equation for the two-phase system in a quasi-static limit we derive first order nonlinear ordinary differential equations for the time dependence of the bubble radius and the position of the center of the bubble. In certain limits we recover the results of Young et al., but in other regimes we obtain more complicated predictions. In particular, our equations permit a stationary steady state whose stability can be studied by a linear analysis in terms of normal modes. Under some conditions we find an oscillatory instability whose evolution to finite amplitude leads to transient behavior similar to that observed by Hardy. We also find that the effects of latent heat can overwhelm the Marangoni force, leading to motion in which the velocity is predicted to be a balance between latent heat release and buoyancy. This

work was presented at the 2011 Annual Meeting of the APS Division of Fluid Dynamics [3].

[1] S.C. Hardy, The Motion of Bubbles in a Vertical Temperature Gradient, *Journal of Colloid and Interface Science* **69** (1979), pp. 157-162.

[2] N.O. Young, J.S. Goldstein, and M.I. Block, The Motion of Bubbles in a Vertical Temperature Gradient, *Journal of Fluid Mechanics* **6** (1959), pp. 350-356.

[3] A. Nurse, G. McFadden, and S. Coriell, Bubble Motion and Size Variation during Thermal Migration with Phase Change, 64th Annual Meeting of the APS Division of Fluid Dynamics, Baltimore, MD, November 20-22, 2011.

Shape and Stability of Rotating Toroidal Drops

Asha Nurse
Geoffrey McFadden
Sam Coriell (NIST MML)

Recently it has been shown that cells can self-assemble into microtissues, a process relevant to tissue engineering. The forces that drive such assembly are an area of intense current interest. In [1] this process was studied for tissue assembly on a patterned substrate consisting of multiple wells that each contains a conical post, which leads the cell to acquire a toroidal geometry as the tissue accommodates the post. Surface forces that would otherwise promote a spherical shape tend to cause the toroid to contract inwards, and are balanced by the contact forces on the post. In some instances the toroidal shapes are observed to develop a type of fluting instability in the azimuthal direction, reminiscent of the capillary-driven Rayleigh instability of a cylindrical column of fluid. In the present project we examine such instabilities in a simpler setting in which the restoring forces provided by the post are replaced by the centrifugal forces experienced by a rotating fluid drop, which tends to fling the fluid outwards. We derive the shapes of axisymmetric toroidal drops that minimize an appropriate energy functional depending on surface energy and rotational energy, and determine their stability by examining the second variation of the energy functional.

The shape and stability of rotating spheroidal drops was studied by the blind experimenter J.A.F. Plateau in the 19th century [2]. Plateau was interested in the analogous problem that arises for rotating, self-gravitating celestial bodies, and realized that small scale experiments were possible by replacing the gravitational force by the force of surface tension, which also tends to consolidate the fluid. He observed that if the rotational forces are strong enough spheroidal drops elongate at the equator and contract at the poles, eventually leading to a pinch-off at the axis of rotation to form toroidal shapes. The spheroidal problem was studied theoretically by Brown and Scriven [3], who performed finite element computations of the deformed shapes based on variational principles, and by Chandrasekhar [4] who included the effects of fluid flow inside the drop by using a method of moments.

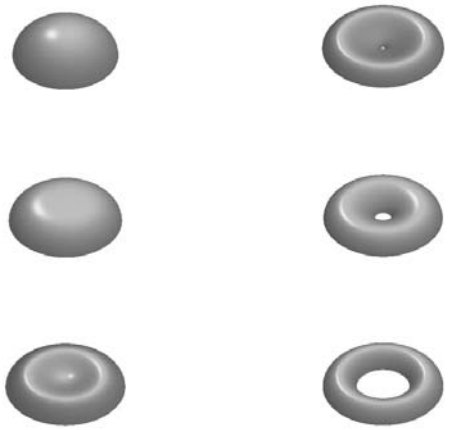

Figure 28. *Axisymmetric liquid drops for various rotation rates; only the upper half of the shapes are shown. On the left are three oblate spheroidal shapes that develop a pronounced dimple on the axis of symmetry as the rotation rate increases. On the right are toroidal shapes that branch from the spheroidal family with further changes in the rotational rate.*

We have extended the previous work by examining the transition from spheroidal to toroidal axisymmetric rotating drops, as illustrated in Figure 28. We have computed numerical solutions for the shapes in terms of an angle-arclength formulation, which involves the numerical solution of a two-point boundary value problem for nonlinear ordinary differential equations. These ODEs are the Euler-Lagrange equations for the energy functional, which includes both kinetic and potential energies from the rotation and capillarity. The stability of these solutions is then obtained by a diagonalization of the associated second variation, which is solved as an eigenvalue problem for the system of ODEs. Our angle-arclength formulation allows us to examine a larger range of parameters than Brown and Scriven, who were limited to single-valued spheroidal shapes by their use of a spherical coordinate system. Our findings include an additional instability to 5-lobed shapes with increasing rotation rate for the spheroidal solutions. We have also found numerous instabilities on the toroidal solution branch for both axisymmetric and non-axisymmetric perturbations. In addition we find a new solution branch of prolate spheroids in the case of a lighter drop (bubble) in a heavier fluid medium. In this case, the shapes become elongated at the poles and contract along the equator, in contrast to the oblate shapes that result from rotation of a heavier drop within a lighter fluid.

[1] J. Youssef, A. K. Nurse, L. B. Freund, and J. R. Morgana, Quantification of the Forces Driving Self-assembly of Three-dimensional Microtissues, *Proceedings of the National Academy of Sciences* **108** (2011), pp. 6993–6998.

[2] J. A. F. Plateau, Experimental and Theoretical Researches on the Figures of Equilibrium of a Liquid Mass Withdrawn from the Action of Gravity, *Annual Report of the Board of Regents of the Smithsonian Institution* (1863), pp. 270-285, Washington, D.C.

[3] R. A. Brown and L. E. Scriven, The Shape and Stability of Rotating Liquid Drops, *Proceedings of the Royal Society of London A* **371** (1980), pp. 331-357.

[4] S. Chandrasekhar, The stability of a rotating liquid drop, *Proceedings of the Royal Society of London A* **286** (1965), pp. 1-26.

Boundary Slip Effect on the Stability of Spiral Poiseuille Flow

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P. Aaron Lott (Lawrence Livermore National Lab)

Advances in micro-fabrication techniques have provided significant understanding into the behavior of fluids at small scales. Small-scale experiments, with flow driven by pressure gradients, drainage, shear, or an electric field have reported a breakdown of the no- slip boundary condition, with observed slip lengths as large as microns. In addition, numerical studies of fluids are often performed with no-slip boundary conditions, and the effects of introducing slip as a model of surface roughness is of current interest.

We consider the effect boundary slip has on the stability of spiral Poiseuille flow, which is an annular flow with an applied pressure gradient. This flow provides a good test-bed for stability studies, as it combines the effects of axial pressure gradients and centripetal acceleration associated with curved boundaries. We find that under certain conditions slip has a significant effect on the linear stability of the flow. Numerical results indicate that linear stability is sensitive to the ratio between the inner and outer cylinder radii, as well as the slip length. Changes in these parameters cause the flow to be stabilized or destabilized in reference to a flow where no-slip conditions are applied; this change in stability is indicated by change in critical Taylor number. The dependence of stability on radius ratio becomes more complicated as the Reynolds number is increased; in particular, the flow becomes destabilized by small ratios, stabilized by mid-range ratios and de-stabilized again for large ratios. We have computed estimates of the critical radius ratios where slip has no effect on the stability of the flow. The results have been submitted for publication [1].

[1] D.L. Cotrell, P.A. Lott and G.B. McFadden, Boundary Slip Effects on the Stability of Spiral Poiseuille Flow, submitted.

A Multicomponent and Multiphase Model of Reactive Wetting

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

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. These effects result 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 free surfaces and contact angles.

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. To alleviate this effect we introduce 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 in the dynamical description of the motion.

The mechanisms of reactive wetting thus involve the interplay of fluid flow, heat and mass transport, capillary phenomena, and phase transformations. We have recently developed a mathematical model of reactive wetting in an isothermal, three-component, four-phase system. To treat free surfaces and contact lines in the problem, a diffuse interface, or phase field, model is used, which involves the introduction of additional order parameters that track the local phase at each point and incorporate the effects of capillarity and interfacial adsorption of solute. A manuscript describing the work has been completed, and is currently under internal review prior to submission for publication.

[1] W. Villanueva, W.J. Boettinger, G.B. McFadden, and J.A. Warren, A Multicomponent and Multiphase Model of Reactive Wetting, submitted.

Measurement of the Flow Stress of Carbon Steel for High-Speed Machining Simulations

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Richard Rhorer (NIST EL)
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Debasis Basak (Orbital Sciences Corporation)

In a high-speed machining operation on a carbon steel such as AISI 1045, a small region (see Figure 29) of thickness on the order of magnitude of 10 µm is deformed plastically in the primary shear zone at a strain rate of the order of magnitude of 10,000 s^{-1}, to a true strain on the order of 100%, on a time interval on the order of 10 microseconds. Subsequently, the material is subjected to additional large plastic strain in the secondary shear zone, for a time that is typically less than 1 millisecond. During this very short cutting time, the work material is sheared so rapidly that it undergoes an increase in temperature of the order of magnitude of 1000 ºC (see Figure 30). Thus, plastic working by rapid shear in these two thin material regions induces a heating rate on the order of magnitude of one million degrees Celsius per second. Under such extreme dynamic loading conditions, there is insufficient time for thermally-activated processes that take place on significantly longer time scales to cause significant changes in the material's microstructure. On the other hand, unique non-equilibrium superheated microstructural states can be present during high-speed machining operations. As a result, the material flow stress in a high-speed machining process can differ significantly from that which is measured experimentally under equilibrium high-temperature conditions. This presents unique difficulties for both experimental measurement and constitutive response modeling of the flow stress in these materials for use in finite-element simulations of high-speed machining processes. The NIST Pulse-Heated Kolsky Bar Laboratory has been developed to obtain improved constitutive response data under conditions of rapid heating for application to machining studies, as well as for other applications.

Following our discovery using the NIST Kolsky Bar that AISI 1075 steel exhibits a nonequilibrium phase transition under conditions of rapid heating and very short time at high temperature [1], we reviewed our experimental data on AISI 1045 steel. The AISI 1045 was also found to exhibit a nonequilibrium phase transformation at high strain rate, which is similar to the one we had observed to take place in AISI 1075 steel [2]. An interesting feature of both of these data sets is that the material has a stiffer response to compressive loading when it has been preheated using pulse-heating to a testing temperature that is below the

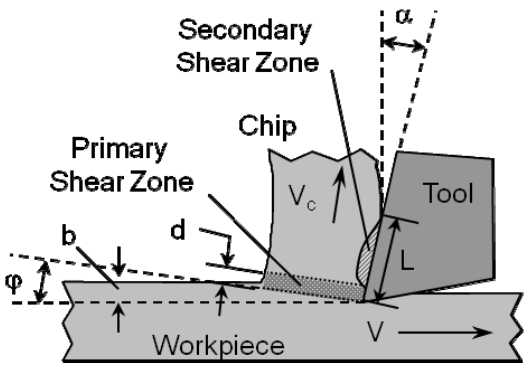

Figure 29. *Schematic drawing of two-dimensional orthogonal cutting operation, showing primary and secondary shear zones.*

eutectoid temperature, than it does when it has been preheated using a slower heating method. On the other hand, in both cases, when the material has been pulse-heated to a temperature that exceeds the eutectoid temperature prior to compressive loading on the Kolsky bar, it is shown to exhibit a significant loss of strength. A consequence of this behavior is that fixed-parameter constitutive models, such as the well-known Johnson-Cook model, which is frequently used in finite-element simulations of high-strain-rate deformation processes, cannot be used to describe this constitutive response behavior. This may help to explain, at least in part, why sophisticated, state of the art finite-element software gives poor temperature predictions in computer simulations of high-speed machining processes on carbon steels of interest in manufacturing, such as AISI 1045.

[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 & Technology* **15** (2011), pp. 1–20.

[2] T.J. Burns, S.P. Mates, R.L. Rhorer, E.P. Whitenton, D. Basak, Effect on Flow Stress of a Rapid Phase Transition in AISI 1045 Steel, in *Proceedings of the ASME*

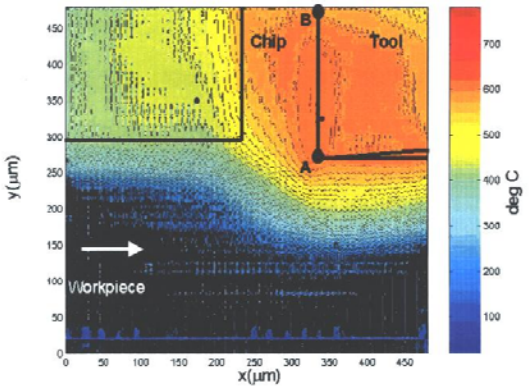

Figure 30. *False-color thermal image of high-speed, steady-state orthogonal machining of AISI 1045 steel; taken from [3].*

2011 International Manufacturing Science and Engineering Conference, Corvallis, Oregon, June 13-17, 2011.

[3] M.A. Davies, H. Yoon, T.L. Schmitz, T.J. Burns, and M.D. Kennedy, Calibrated Thermal Microscopy of the Tool-chip Interface in Machining, *Machining Science & Technology* **7** (2003), pp. 166-190.

Modeling the Temperature on the Tool-Chip Interface during High-Speed Machining

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Richard Rhorer (NIST EL)
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Debasis Basak (Orbital Sciences Corp.)

During high-speed machining of many materials, very high temperatures are generated along the tool-chip interface. In a simplified planar orthogonal cutting model that is still widely used in the literature (see Figure 31), the workpiece material enters a thin cutting region called the primary shear zone at temperature θ_0, where it is deformed by rapid plastic shearing, and is heated to a much higher temperature, θ_s. The bulk of the heat generated in the primary shear zone is rapidly convected away from the workpiece, along with the chip of removed material is that is being formed. Some of this heat is also conducted into the tool and into the workpiece material. The material continues to deform and rapidly increase in temperature as it moves up the face of the tool, under conditions of large frictional forces, in a region called the secondary shear zone. Experimental measurements indicate that the maximum temperature, θ_m, occurs along the interface between the chip and the tool, near the region where the chip begins to curl away and lose contact with the tool. There is also a large transfer of heat away from this secondary deformation zone, mainly by convection along with the chip, but also by conduction. This high temperature environment can cause rapid tool wear. Thus, there is considerable interest in obtaining an estimate of the peak temperature, θ_m, under realistic cutting conditions.

Peak temperature predictions using state of the art finite-element (FEM) software have been found to underestimate the temperature in orthogonal cutting of AISI 1045 steel by as much as 33%. There are two likely reasons for this poor predictive capability. The first is that the forces used in the simulations, which are computed using the workpiece material flow stress constitutive model that is used in the FEM software, are not modeled accurately. The second is that the models used to simulate the friction along the tool-chip interface are inadequate. Our current work [1] involves

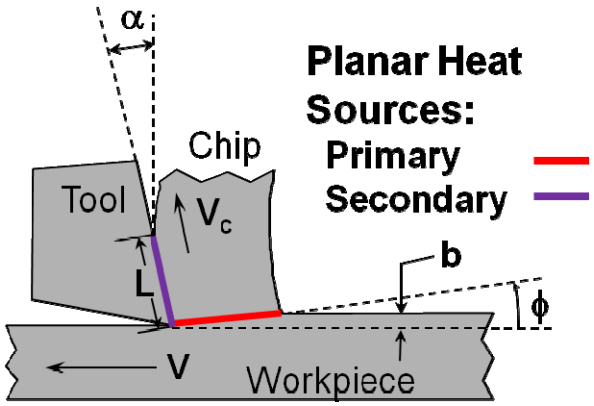

Figure 31. *Schematic drawing of orthogonal cutting process. The first region of large heat generation during high-speed machining is in the primary shear zone, indicated in red, and the second region of large heat generation is in the secondary shear zone along the tool- material contact region of length L, indicated in purple.*

using experimental measurements, obtained using the NIST Kolsky bar, of the stress strain response of AISI 1045 steel, along with a friction model that is more sophisticated than the usual Coulomb sliding friction model that is used in the FEM software, to achieve improved peak temperature predictions of some experimentally measured orthogonal cutting tests. These predictions are obtained using a two-dimensional singularly-perturbed convection-diffusion model for the temperature distribution that is based on a number of cutting temperature models in the machining literature.

[1] 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, submitted.

Simulation of Bioregulatory Networks Involved in Cell Cycle Control

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S. Kim (National Institutes of Health)
Kurt Kohn (National Institutes of Health)
A. Luna (NIH and Boston University)

G. McFadden is a co-advisor to Sohyoung Kim, a post-doctoral fellow, and Augustin Luna, a graduate student from Boston University, who are both doing research at the National Institutes of Health (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 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 by Sohyoung Kim 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 proteins will operate together under various conditions. To address those questions a mathematical model has been developed [1] to investigate the interactions of these three proteins by numerical simulations. The modeling work has suggested experimental investigations of the role of Mdmx in the cell cycle that are currently being performed by Dr. Kim at the Laboratory for Molecular Pharmacology at the NIH National Cancer Institute.

Recent work by Augustin Luna includes the development of models for 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. This work is modeling the effects of SIRT1 on the mammalian circadian clock cycle. It is known that the time of day that cancer treatments are administered affects drug efficacy, and circadian rhythms are also known to affect DNA damage response. SIRT1 is known to play a role in the DNA damage sensor that triggers the cellular response to genotoxic stress. In this work existing models for the circadian clock are being modified to include the specific effects of SIRT1 on the interaction between the DNA damage response and the circadian cycle in cells. A poster describing this work was presented at a recent international conference on systems biology [2]. G. McFadden is serving on A. Luna's Ph.D. thesis 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).

[2] A. Luna, G. McFadden, M. Aladjem, and K. Kohn, A Computational Mammalian Circadian Clock Model with Connections to the DNA Damage Response, 12th International Conference on Systems Biology, Heidelberg, Germany, August 28 - September 1, 2011.

Mathematical Optimization of Procedures for Cryoprotectant Equilibration

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Stabilization of viable cells by cryopreservation is important in several areas, including cell-based therapy, tissue engineering and transplantation medicine. Cryopreservation nearly universally depends on the equilibration of cells and tissues with high concentrations of permeating chemicals known as cryoprotective agents, or CPAs. Despite their protective properties, CPAs can cause damage as a result of osmotically-driven cell volume changes, as well as chemical toxicity. In this study, we have used previously published data to determine a toxicity cost function, a quantity that represents the cumulative damage caused by toxicity. We then used this cost function to define and numerically solve the optimal control problem for CPA equilibration, using human oocytes as representative cell type with high clinical relevance. The resulting toxicity-optimal procedures are predicted to yield significantly less toxicity than conventional stepwise procedures. In particular, our results show that toxicity is minimized during CPA addition by inducing the cell to swell to its maximum tolerable volume and then loading it with CPA while in the swollen state. This counterintuitive result is considerably different from the conventional stepwise strategy, which involves exposure to successively higher CPA concentrations in order to avoid excessive shrinkage. The procedures identified in the present study have the potential to significantly reduce damage due to toxicity. A manuscript describing this work is currently under review.

[1] J. Benson, A. J. Kearsley, and A. Z. Higgins, Mathematical Optimization of Procedures for Cryoprotectant Equilibriation Using a Toxicity Cost Function, *Cryobiology*, accepted.

A Standard Candle for Extragalactic Metrology

Bert W. Rust

Type Ia supernova are so luminous at peak brightness, with lightcurves so uniform and regular, that they promise to be excellent standard candles for measuring distances to their parent galaxies. To use them for this purpose, it will be necessary to calibrate their luminosities by observing detailed light curves of several supernovae in nearby galaxies whose distances can be reliably estimated by more conventional methods. These distances can then be used to give good estimates of the absolute luminosities of the supernovae, which can then be compared to the observed luminosities of more distant supernovae to get estimates of their distances.

It has long been known [1] that the late time decline of the light curve is powered by the nuclear decay chain $^{56}\text{Ni} \rightarrow {}^{56}\text{Co} \rightarrow {}^{56}\text{Fe}$, with the two decay rates accelerated by a common factor, presumably because the decays take place in the interiors of white dwarf stars. The deposition and subsequent decay of the ^{56}Ni can be modeled by

$$W(t) \rightarrow {}^{56}\text{Ni} \xrightarrow{k_1} {}^{56}\text{Co} \xrightarrow{k_2} {}^{56}\text{Fe}$$

where $W(t)$ is a three-parameter Weibull probability density function, i.e.,

$$W(t) \equiv W(t;\alpha_1,\alpha_2,\alpha_3) = \frac{\alpha_2}{\alpha_3}\left(\frac{t-\alpha_1}{\alpha_3}\right)^{(\alpha_3-1)} \exp\left[-\left(\frac{t-\alpha_1}{\alpha_3}\right)^{\alpha_2}\right]$$

with adjustable parameters, α_1, the time that ^{56}Ni deposition begins, α_2, a shape parameter, and α_3, a scale parameter. The decay rates are well modeled by

$$k_1 = \frac{1}{8.764\alpha_4}, \quad k_2 = \frac{1}{111.42\alpha_4}, \quad 0 < \alpha_4 \le 1,$$

where 8.764 d and 111.42 d are the terrestrial half-lives of ^{56}Ni and ^{56}Co, respectively, and the adjustable parameter α_4 specifies the amount by which these half-lives are shortened by the ambient temperature and density in the white dwarf. If $N_1(t)$, $N_2(t)$, and $N_3(t)$ are the relative abundances of ^{56}Ni, ^{56}Co, and ^{56}Fe, then

$$\frac{dN_1}{dt} = W(t) - k_1 N_1, \qquad N_1(\alpha_1) = 0,$$

$$\frac{dN_2}{dt} = k_1 N_1 - k_2 N_2, \quad N_2(\alpha_1) = 0,$$

$$\frac{dN_3}{dt} = k_2 N_2, \quad N_3(\alpha_1) = 0,$$

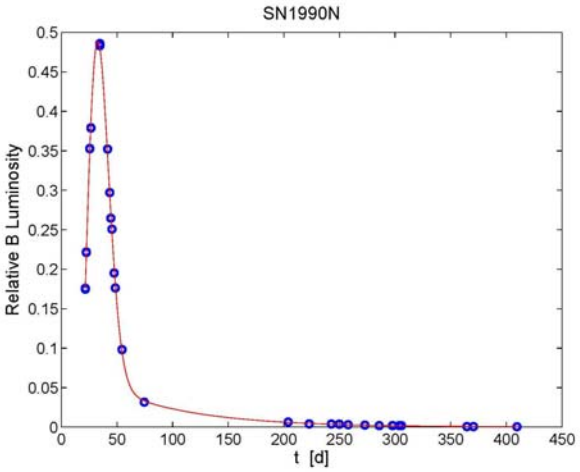

Figure 32. *The light curve of SN1990N in relative luminosity units. The time variable is measured in Julian Day units. The discrete data points are the observed luminosities and the smooth curve is the model fit.*

Assuming that the ratio of the energy releases from the ^{56}Ni and ^{56}Co decays is the same as that observed in a terrestrial setting, i.e., 3.67 MeV / 1.71 MeV = 2.146, the observed luminosity can be modeled by

$$L(t) = C_1 W(t) + C_2\left[k_1 N_1(t) + 2.146 k_2 N_2(t)\right],$$

where C_1 and C_2 are adjustable parameters which convert fluxes into relative luminosities. Thus the model has six free parameters, four nonlinear and two linear. Figure 32 shows the result when it is fitted to the observations for supernova SN1990N. The fit explains 99.91% of the total variance in the measurements!

The ratio of the estimates $\hat{C}_1$ and $\hat{C}_2$ and their standard uncertainties, i.e.,

$$\frac{\hat{C}_1 \pm \sigma(\hat{C}_1)}{\hat{C}_2 \pm \sigma(\hat{C}_2)} = 5.0156 \pm 0.228,$$

provides a means to estimate the energy per nucleon produced by the ^{56}Ni deposition process:

$E(^{56}\text{Ni depos.})/\text{nucleon} = 8.577 \pm .390\text{MeV}$.

Since the binding energy per nucleon for the ^{56}Ni nucleus, 8.790 MeV, lies well inside the 1σ interval, the above results are consistent with the hypothesis that the deposition of ^{56}Ni is accomplished by the fusion of 56 protons.

[1] B.W. Rust, M. Leventhal and S.L. McCall, Evidence for a radioactive decay hypothesis for supernova luminosity, *Nature* **262** (1976) pp. 118-120.

Unfolding Optical Spectrum Measurements

Bert W. Rust
Dianne P. O'Leary
Stephen W. Brown (NIST PML)

We have begun a consulting effort with Steven W. Brown of the NIST Optical Technology Division (685) on correcting optical spectrum measurements for scattered light in a spectrometer. Figure 34 shows (in cyan) the spectrum measured for a lamp used as a calibration source. The black curve is a crude first approximation to the corrected spectrum. The gaps in the black curve represent wavelength intervals in which the correction process gave negative values, a physical impossibility. The object of the current effort is to compute statistical confidence interval bounds for the corrected spectrum, to compare them with first approximations like the one shown in the Figure, and to develop alternate methods for computing the corrected spectra.

In order to do a proper job of unfolding the measured spectra, it is necessary to determine an instrument response function. As a start toward this objective we have been given 54 measured line spread functions (LSF) corresponding to 54 distinct non-equally-spaced wavelengths λ_L in the range 220.0000–859.9250 nm. For each of these wavelengths, the corresponding LSF is measured at 1024 equally-spaced wavelengths λ in the range 198.9388–873.9835 nm. The 54 measured 1024-vectors are plotted in Figure 33. This 1024 × 54 matrix must be expanded, by interpolation, into a 1024 × 1024 matrix **A**. This means that we must find, on average, about 19 new functions in each gap between every pair of measured ones. The resulting matrix **A** can then be used in a discrete approximation to an integral equation

$$f(\lambda) = \int_{220.0000}^{859.920} \mathbf{A}(\lambda, \lambda_L) x(\lambda_L)\, d\lambda_L + \varepsilon(\lambda), \qquad 198.9388 \le \lambda \le 873.9835,$$

where $f(\lambda)$ is a measured spectrum to be corrected, $\varepsilon(\lambda)$ is the measurement error in $f(\lambda)$, $x(\lambda_L)$ is the unknown corrected spectrum, and $\mathbf{A}(\lambda,\lambda_L)$ is the instrument response function.

Let the discretized integral equation be written

$$f = \mathbf{A}x + \varepsilon,$$

where **A** is the required 1024 ×1024 matrix and ε is an unknown random 1024-vector satisfying

$$\varepsilon \approx N(0, S^2),$$

where S^2 is the positive definite covariance matrix for the measurement errors. We are currently in the process of retrieving estimates of this matrix for all five of the calibration sources in the study. These matrices are

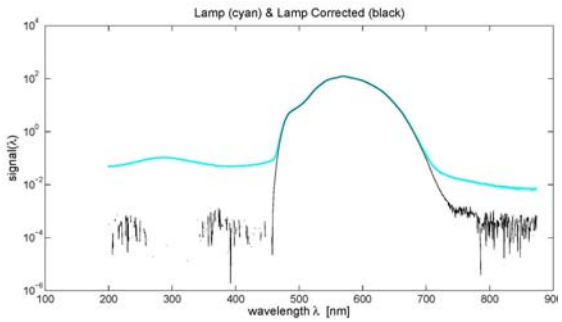

Figure 34. *The spectrum measured for a lamp used as a calibration source (cyan) and a crude first approximation to the corrected spectrum (black).*

vitally important for computing estimates $\hat{x}$ of the corrected spectra and in computing confidence intervals for those estimates. Those confidence intervals will be computed using the BRAKET-LS algorithm. We have already tested that procedure using a very crude first approximation to S^2. To compute a complete set of 1024 upper and lower bounds required over 40 hours on the Sun server "entity." So it will not be practical to compute confidence intervals for every measured spectrum, but it is important to compute them for all of the calibration sources.

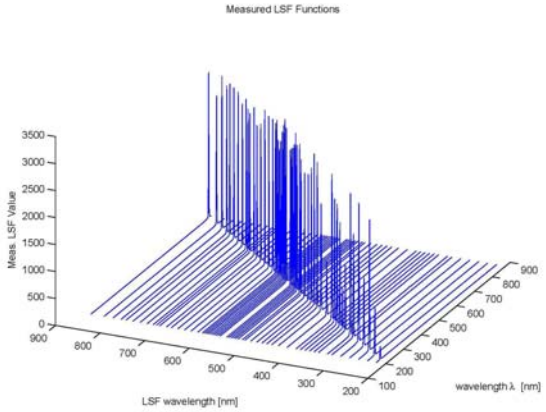

Figure 33. *The measured LSF functions.*

Variable Projection for Nonlinear Least Squares Problems

Dianne P. O'Leary
Bert Rust

Fitting a model to measured data provides the most basic tool in science and engineering, essential to discovering and analyzing patterns and causality. Software that accomplishes this task should be both efficient and robust, providing reliable estimates of the model's parameters in a reasonable amount of time.

Yet data fitting problems are often quite challenging numerically. In fitting exponential models, for example, small changes in the data can make large changes in the optimal parameters. Equally serious is the fact that data fitting problems are most often nonconvex, so a set of parameters can be optimal among nearby sets of parameters without being globally optimal, and software can be fooled into accepting a suboptimal solution.

We focus in this work on fitting nonlinear models in a (weighted) least squares sense. Most nonlinear models have some parameters – perhaps quite a few – 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

$$y(t) \approx c_1 e^{\alpha_1 t} + c_2 e^{\alpha_2 t} \equiv \eta(\boldsymbol{\alpha}, \mathbf{c}, t). \qquad (1)$$

The parameters $\mathbf{c} = [c_1, c_2]^T$ appear linearly, so for every choice of nonlinear parameters $\boldsymbol{\alpha} = [\alpha_1, \alpha_2]^T$, optimal values for c can be found by solving a linear least-squares problem, a rather simple computational task. How can this be used to our advantage? Consider the nonlinear least-squares problem

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

where the ith component of the vector $\mathbf{y}$ is the observed value $y(t_i)$, and the ith component of the vector $\boldsymbol{\eta}$ is the model prediction at t_i ($i = 1, \ldots, m$). Then the solution to (2) is the same as the solution to

$$\min_{\boldsymbol{\alpha}} \left\| \mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\alpha}, \mathbf{c}(\boldsymbol{\alpha})) \right\|_2^2, \qquad (3)$$

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

This simple observation was made and exploited in 1973 by Gene Golub and Victor Pereyra [1]. They called (2) a separable least squares problem and proposed solving it using the variable projection algorithm (3). In 1974, Fred Krogh [2] discussed some implementation issues and noted that this approach solved problems for which the standard nonlinear least squares algorithm failed. The variable projection algorithm was implemented in a very widely-used software module called `varpro`, written in 1977 in Fortran by John Bolstad [3], using ideas of Linda Kaufman [4] to speed up the computation of derivatives. This code is also distinguished as being the first least squares code produced by the numerical analysis community that included computation of the covariance matrix, which provides the foundation for the statistical analysis of the estimate. The history and wide range of applications of `varpro` are summarized in [5]. The beauty of variable projection is that it reduces the number of parameters in the minimization problem, thus improving efficiency and possibly reducing the number of local minimizers. Convergence to the globally optimal solution is therefore more likely. Implementation of the idea is rather complicated, though, since the Jacobian matrix for (3) must be derived from that for (2).

Inevitably, the 1977 `varpro` program is showing its age. In particular, the thousand-line program relies on 1970s technology for overcoming the limitations of static storage allocation, and it uses an outdated implementation of a minimization algorithm. The purpose of our work is to provide a 21st century sample implementation of the variable projection method (in Matlab) that allows a more general formulation (with constraints on the parameters), more clearly identifies its key ingredients so that improvements can be made, computes the Jacobian matrix more accurately, and makes future implementations in other languages easy. Our Matlab implementation contains over 400 lines of comments for fewer than 160 lines of code [6]. It also has the advantage that it returns extensive statistical diagnostics that are extremely important not only for validating the model, but also in changing the model when it is shown to be inadequate.

[1] G. H. Golub and V. Pereyra, The Differentiation of Pseudoinverses and Nonlinear Least Squares Problems whose Variables Separate. *SIAM Journal on Numerical Analysis* **10** (1973), pp. 413–432.

[2] Fred T. Krogh, Efficient Implementation of a Variable Projection Algorithm for Nonlinear Least Squares Problems. *Communications of the ACM* **17** (March 1974), pp. 167–169.

[3] John Bolstad, VARPRO computer program, January 1977. Computer Science Department, Serra House, Stanford University.

[4] L. Kaufman, A variable projection method for solving separable nonlinear least squares problems. *BIT Numerical Mathematics* **15** (1975), pp. 49–57.

[5] G. H. Golub and V. Pereyra, Separable nonlinear least squares: The variable projection method and its applications. *Inverse Problems* **19** (2003), pp. 1–26.

[6] D. P. O'Leary and B. W. Rust, Variable Projection for Nonlinear Least Squares, submitted.

Shape Analysis

Javier Bernal
Charles Hagwood (NIST ITL)
John Elliott (NIST MML)
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.

Work is currently under way for the development of a framework based on differential geometry for formulating mathematical representations of shape and for performing calculus with these representations. In this framework shapes will be treated as points in a differential manifold with a Riemannian metric and tools for computing geodesic distances between points will be readily available.

[1] C. Hagwood, J. Bernal, M. Halter, and J. Elliott, Evaluation of Segmentation Algorithms on Cell Populations Using CDF Curves, *IEEE Transactions on Medical Imaging*, accepted.

Neural Networks

Javier Bernal

A backpropagation algorithm is being implemented for training neural networks to be used 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 partition-partitioning data into classes.

During the training with the backpropagation algorithm the average squared error between the network's output and a target value is minimized for each point or pattern (in d-dimensional space) in the training set. 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.

Since learning in a neural network is equivalent to minimizing an error function of several variables (weights in the network), the Conjugate Gradient Method (CGM) has been implemented. Two tasks remain to be completed:

i. Implementation of a “model trust region” method for correcting the situation in which the error function is not quadratic enough around the current weights for the CGM to work, a situation that occurs when the Hessian of the error function is not positive definite or when the current weights are not close enough to the optimal solution.

ii. Implementation of a probabilistic heuristic (e. g., simulated annealing) for correcting the situation in which the CGM gets stuck at a local minimum that is not a global optimum.

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.

Rheology of Dense Suspensions

John Hagedorn
Steven Satterfield
Marc Olano
Judith Terrill
Nicos Martys, Edward Garboczi (NIST EL)
Pascal Hebraud (CNRS/ESPCI, France)

See feature article, page 34.

Segmentation and Tracking of Breast Cancer Cells

Adele Peskin
D.J. Hoeppner (National Institutes of Health)
C.H. Stuelten (National Institutes of Health)

See feature article, page 38.

Body Area Network Visualization and Analysis

John Hagedorn
Judith Terrill
Kamran Sayrafian-Pour (NIST ITL)
Wen-Bin Yang (NIST ITL)
Kamya Yekeh Yazdandoost (University of Oulu)
Attaphongse Taparugssanagorn (University of Oulu)
Matti Hämäläinen (University of Oulu, Finland)
Jari Iinatti (University of Oulu, Finland)

See feature article, page 32.

ITL Program: *Pervasive Information Technology*

Modeling, Visualization of Cement Paste Hydration and Microstructure Development

William George
Steven Satterfield
Judith Terrill
Jean-Loup Traore
Jeffrey Bullard (NIST EL)
Edward Garboczi (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 hydration process that transforms the paste from a fluid suspension into a hardened solid involves complex chemical and microstructural changes. Understanding and predicting the rates of these changes is a longstanding goal. Computational modeling of the hydration of cement is challenging because it involves a large number of coupled nonlinear rate equations that must be solved in a highly irregular three-dimensional spatial domain. To address these challenges we are applying a new computational model called HydratiCA, which has several advantages. HydratiCA 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 cementious systems.

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 is important both for validation and to understand the results. Over the course of the simulation time, a series of data volumes is produced at the time values of interest.

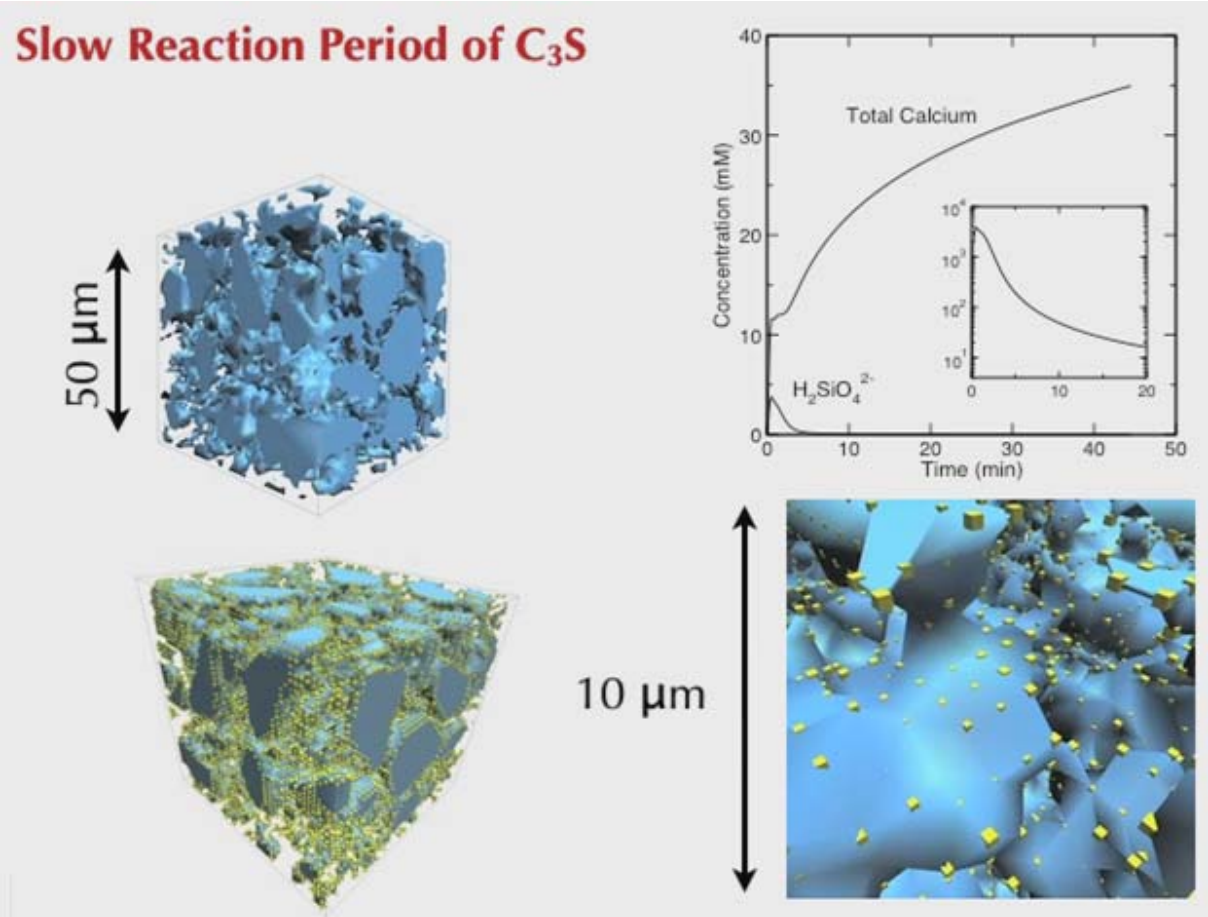

Figure 35. *This is a visualization of a simulation of the hydration of tricalcium silicate (C_3S) in water. The blue particles are C_3S, a soluble mineral which is the majority component of Portland cement concrete. The yellow glyphs indicate areas where the primary hydration product phase, calcium silicate gel, nucleates and grows on the C_3S particle surfaces. The graph shows the time dependence of the concentration of calcium and silicate ions in solution, illustrating the level of quantitative detail that can be extracted from the simulations.*

Our paper describing the modeling [1] was selected as one of the top 10 highlights of the journal *Modeling and Simulation in Materials Science and Engineering* for 2010[13].

This year we implemented the creation and coalescence of void space in the simulation. Cement hydration reactions conserve mass, but generally result in reduced volume of condensed matter (liquid or solid). The computational domain has a fixed volume throughout the simulation, so it is necessary to handle the reduction in total condensed volume as a simulation proceeds. We modified the program to create a bubble object in the largest open pore space and then grow the size of the bubble with time. We contributed to a paper on using supercomputers [2] as well as a keynote presentation at a major international cement chemistry meeting [3]. We also completed a computational and quantitative visualization study of the C_3S-gypsum system [4] (see Figure 35). In the coming year, we plan to use quantitative visualization to study new cases.

[1] 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, *Modelling and Simulation in Materials Science and Engineering* **18** (2) (March 2010), article 025007 (16 pages).

[2] 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* **33** (1) (Jan. 2011), pp. 24-29.

[3] J. W. Bullard, N. S. Martys, J.-L. Traore, W. L. George, S. G. Satterfield, Computer Models as Guides Through Material Design Space, International Congress on the Chemistry of Cement, Madrid, Spain, July 3-8, 2011.

[4] L. Valentini, J. W. Bullard, G. Artioli, J. Traore, J.E. Terrill, Role of Sulfate Incorporation into C-S-H during Cement Hydration: Results from Numerical Modeling of the System, C_3S-gypsum, submitted.

[13] http://iopscience.iop.org/0965-0393/page/Highlights%20of%202010

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 objects of study in widely diverse scientific disciplines and the depiction of surfaces and interactions with surfaces are important tasks in scientific visualization. In this context, we often (indeed, typically) work with surface models that are approximations of the true surfaces that they represent. When the representations of surfaces 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. In this project we have developed quantitative 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 with the simple idea of 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 this distance error over the surface. Surface area and volume errors are much simpler to assess. For surface area, we simply 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 of the underlying surface.

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 way) to emulate an experimental situation, and in that vein we added various levels of noise to the gridded data sets. We note that these methods can be applied to any surface type and any polygonization.

For each surface and each polygonization 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. For example, Figure 36 shows a scatterplot of our normalized mean distance error metric versus the number of triangles for each of four polygonization schemes for our tests of elliptic paraboloids. This plot also shows the curves that we have fit to the data.

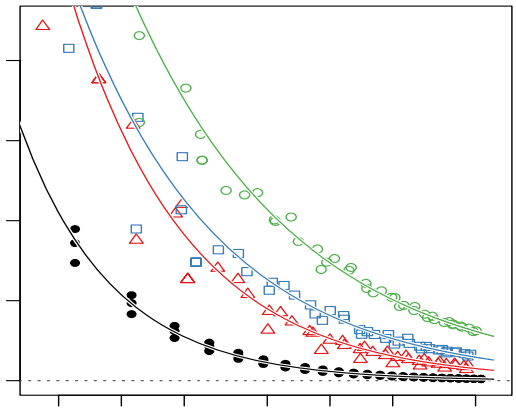

Figure 36. *Scatterplot of normalized mean distance error versus number of triangles for all polygonizations of the elliptic paraboloids. Data for each of the four polygonization schemes has been fitted and the resulting lines plotted.*

Unlike the other statistics, the surface area error metric does not appear to tend to zero as the number of triangles increase for isosurface polygonizations 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 mathematical 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 measure and 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, J. Terrill, Measuring Errors in Polygonal Representations of Surfaces, submitted.

ITL Program: *Virtual Measurement Systems*

Processing Large Phantom Image Sets

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

A large number of image sets of artificial lungs with tumors ("phantoms") are available from the FDA to serve as ground truth for the assessment of measurements of lung tumor properties [1]. Anthropomorphic phantom data can be set up and scanned repeatedly across many different sites to compare imaging equipment and tumor volume measurements. Figure 38 shows the FDA phantom lung, into which sets of phantom tumors consisting of materials of known density are placed, and a sample resulting slice of CT data. CT scans of the data yield spots of predictable pixels intensities, corresponding to the density of the tumors that are inserted. In order to use the CT data for volumetric comparisons, the exact locations of tumors in each data set are needed. These can be extracted manually, but this is an extremely time consuming job. We are creating a processing tool to extract the location of each tumor in these sets, and then calculate a tumor volume, based on our biweight volumetric measurement algorithm [2].

The main challenge of extracting the tumors in the lung data is to separate them from the lung walls and from surrounding blood vessels, both of which have similar densities, and so resulting CT data will contain pixel intensities in the same range. We currently have an algorithm that will isolate most of the tumors from these sets. An example is shown in Figure 37. The algorithm involves separating the inside from the

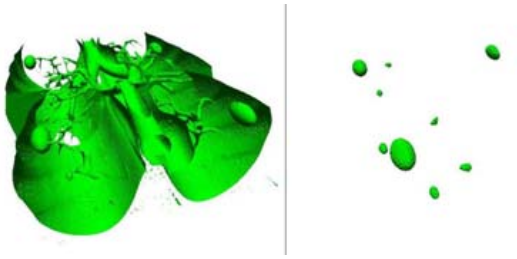

Figure 37. *A sample lung data set, shown with an iso-surface of -100 Hounsfield units, to display the lung tumors, lung walls, and sections of blood vessels. To the right the corresponding extracted tumors are displayed at the same locations.*

outside of the lung in each slice of data, finding clusters of pixels with intensities in the range of the tumor, and then eroding and dilating to separate the tumors from surrounding structures. Resulting pixel clusters are then chosen as tumors according to their geometry and their size.

Currently we are working on improving our algorithm to process the thousands of data sets available from the FDA efficiently. This work includes improving our location of the lung wall, more accurate tumor geometry selection, and removal of pieces of blood vessels from the tumors according to the pixel distributions inside the pixel clusters that represent the blood vessels.

This work will also provide the foundation for a more generalized problem of locating lung tumors in clinical data, a much harder problem. In clinical data, the tumor geometries are unknown, and blood vessels attachments can be more complicated, as are the ways in which clinical tumors attach to the lung wall. Small tumors are the most challenging, often not providing enough pixel data to detect a peak in a histogram of the pixel distribution in the area of the tumor. However, automated location of tumors in large sets of clinical

Figure 38. *FDA lung phantom (left), and sample CT slice containing a phantom tumor (right).*

data would be a powerful tool in disease detection and in monitoring tumor growth over time.

[1] https://wiki.nci.nih.gov/display/CIP/Phantom+FDA

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

Visualizing Fire and the Resulting Deformation of Structures

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Greg Rami
Dennis Backhaus
Marc Olano
Kevin Harrison
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 in order 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 (finite element heat transfer analysis) calculates how heat computed by FDS diffuses into structural members. A third program (finite element analysis) takes the output of the second code and computes how the structure deforms over time due to combined effects of thermal and mechanical loads. After specifying a scenario, we run the three simulations followed by our software to automatically create the geometry of the building, our software to specify crack patterns in windows, and our software (based upon the Bullet Physic Engine) for the dynamics of the shards in breaking glass windows. Then, we link the fire, thermal, structural data, and any window dynamics with a separate real-time visualization capability that can be run on the desktop and in the NIST 3D immersive environment. This enables interactive measurement and analysis of the resulting data.

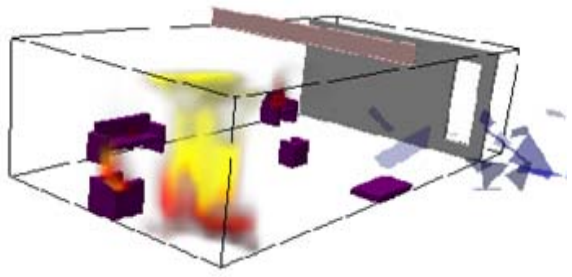

Figure 39. *Single frame showing glass window breaking in Fire-Structure simulation.*

This year we wrote a 3D room navigator that works by clicking on rooms in a displayed map. This enables real-time visualization and analysis in multi-story multi-room buildings. We enhanced our software to create the dynamics of broken glass shards; see Figure 39. We developed a tool to automate the layout of a building (floors, rooms) and included the capability to specify beam types. We completed the automation of the process to create a demo, and added enhanced analysis tools. In the coming year, we will be studying new building structures.

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

James S. Sims
John Kelso
Garnett W. Bryant (NIST PML)

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

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 (Qds), are one of the most intensely studied nanotechnology paradigms. Nanoparticles are typically 1 nm to 10 nm in size, with 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 the bulk and from 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.

In a joint project with the NIST Physical Measurement Lab we are developing computationally efficient large scale simulations of such nanostructures, and we are also developing immersive visualization techniques and tools to enable analysis of highly com-

plex computational results of this type. The electrical and optical properties of semiconductor nanocrystals and quantum dots are studied. In the most complex structures this entails modeling structures with on the order of a million atoms. Highly parallel computational and visualization platforms are critical for obtaining the computational speeds necessary for a systematic, comprehensive study. Often it is easy to define the simple subsystems that make up a complex, heterogeneous nanosystem [1]. However, it may be difficult to explicitly define the entire structure. A novel feature of the code being developed is the ability to link together heterogeneous nanostructures.

This year the work was focused on modulating and controlling the optical properties of self-assembled quantum dots using external strain [2], and using electric fields [3]. Calculations were carried out on NIST's 4,404-processor Linux cluster.

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 have been considered. The dependence of the dot's electronic states and optical transitions on the coupling to bending modes of the oscillator has been studied. The dependence on applied stress can be understood as a competition between the internal and external stress that can affect the local strain at the dot. 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.

Future work will add the effect of external magnetic fields into the tight-binding diagonalization tool and to expand the atomic orbital basis to include the effect of d orbitals.

[1] G.W. Bryant and W. Jaskolski, Electronic Properties of Quantum-dot Molecules, *Physica E* **17** (2003), pp. 40-41.

[2] 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**, article 067404 (2010).

[3] G.W. Bryant, N. Malkova, J. Sims, M. Zielinski, W. Jaskolski, and J. Aizpurua, Controlling the Optics of Quantum Dots with Nanomechanical Strain, *Physical Review B: Condensed Matter and Materials Physics*, accepted.

3D in Web Pages

Sandy Ressler
Halley Coplin
John Hagedorn
Kamran Sayrafian (ITL)

http://www.nist.gov/itl/math/hpcvg/3dweb.cfm

It is now possible to embed 3D computer graphics into web pages such that the 3D graphics are "first class citizens." A recent effort led by Fraunhoffer-Gesellschaft and the Web3D Consortium has produced a set of tools, called X3DOM [1], for "3D declarative markup" that works with most modern web browsers. The result is the ability to put 3D graphics, generated using a variety of techniques, seamlessly into web pages. This 3D markup can be queried and manipulated in exactly the same way as document elements, such as paragraphs, headings, and fonts can be manipulated for textual components of a page. For example, one can query all "spheres" and change their color or scale.

Seeking to move the technology in the standards arena, Sandy Ressler is participating in the W3C Declarative 3D Community Working Group. In addition, he has produced some exemplars that demonstrate the practicality of these techniques, and has developed some software [2] to ease integration of 3D models with web pages.

Another example of the value of declarative 3D is the work of SURF student Halley Coplin. In this collaboration with Kamran Sayrafian and John Hagedorn, we introduced motion to the humans in the "Modeling RF Propagation within the Human Body" project [3]. This resulted in successfully animating the human geometry (surface only, not organs); see Figure 40.

Figure 40. *Single Frame in an animation sequence of a human.*

Viewers to the web site [4] can see the animations live on the web page and customize various aspects of the animation.

In the coming year we anticipate enhancing the graphics of the DLMF project [5] via X3DOM. A number of functional controls (direction of animation, surface selection, navigation type) have already been implemented. This approach has the potential to open up DLMF graphics to more compute platforms (e.g., Linux) than currently exist [6].

[1] Fraunhofer, http://www.x3dom.org/.

[2] S. Ressler, Integrating jQuery with the 3D Descriptive Markup of X3DOM, NISTIR 7827, October 2011.

[3] K. Sayrafian, http://www.nist.gov/healthcare/emerging/rfpropagation.cfm, 2011.

[4] H. Coplin, S. Ressler, J. Hagedorn, RF Propagation Body, http://math.nist.gov/~SRessler/RF/walk50.xhtml

[5] Digital Library of Mathematical Functions. 2011. National Institute of Standards and Technology, http://dlmf.nist.gov/.

[6] S. Ressler, http://math.nist.gov/~SRessler/x3dom/dlmf/AIanim.xhtml

Information Visualization

Sandy Ressler

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

Information Visualization (InfoVis) is a type of visualization that focuses on non-physical data. For example the results of a search, the configuration of a network, and stock market prices are all the type of data that can be visualized using InfoVis techniques. Scientific visualization generally represents physical entities such as maps, weather, medical organs and data associated directly with physical objects. Our work in InfoVis has focused on a particular experiment concerning congestion control of networks and the resources consumed by a simulation of a cloud computing scenario [1].

Figure 41, produced by Ressler, is a single frame of an animation that displays how six different variables representing resources used in the cloud computing simulation are consumed [2]. The *x* axis represents 100 clusters, and the *y* axis represents 1000 nodes in those clusters, for each variable.

In observing the animations the researchers a) were able to confirm that the simulation was functioning as expected ,and b) observed some unknown phephenomenon concerning resource utilization was also present posing questions for future research. The animations were produced using a collection of R scripts [3] developed for this project.

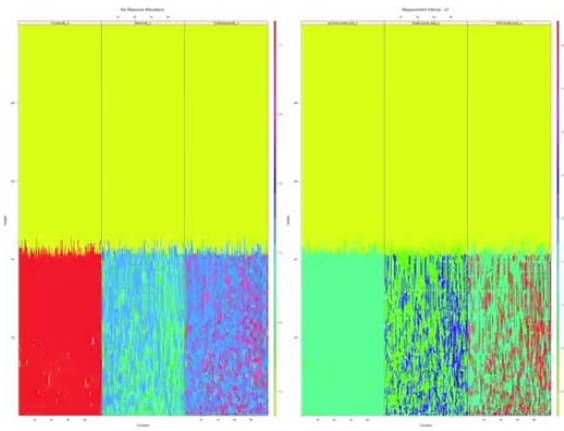

Figure 41. *Single frame of an animation displaying how six variables representing resources used in the cloud computing simulation are consumed. The x axis represents 100 clusters, and the Y axis 1000 nodes in those clusters, for each variable.*

In addition the project has also produced a simple hand computed demonstration of a visualization of the Common Vulnerability Scoring System (V2) [4,5]. Computing vulnerabilities are given a score based on the criteria of the CVSS-V2 specification. We plan on developing additional visualizations of computing security data in the forthcoming year.

In the coming year we anticipate performing several more visualizations focused on the cloud computing simulation project that is ongoing. Subsequent to this a collection of tools will be assembled with the goal of enabling the production of InfoVis simpler and faster in order to have impact on the research problems being addressed.

[1] K. Mills, J. Filliben, D. Cho, E. Schwartz and D. Genin, Study of Proposed Internet Congestion Control Mechanisms, NIST Special Publication 500-282, May 2010, 534 pages.

[2] S. Ressler, Visualizing Cloud Computing Simulations, http://math.nist.gov/~SRessler/cloudviz.html

[3] R Development Core Team (2003). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.

[4] S. Ressler, http://math.nist.gov/~SRessler/nvdvis/nvd_cvssv2.html

[5] P. Mell, K. Scarfone, and S. Romanosky, CVSS A Complete Guide to the Common Vulnerability Scoring System Version 2.0, June 2007, http://www.first.org/cvss/cvss-guide.html

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.

hp-Adaptive Finite Element Methods

William F. Mitchell
Marjorie McClain

See feature article, page 27.

OOF: Finite Element Analysis of Material Microstructures

Stephen A. Langer
Valerie R. Coffman
Andrew C.E. Reid (NIST MML)
Günay Doğan (Theiss Research)

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, academia, and government laboratories and as a teaching tool in universities. Including all available versions, OOF2 was downloaded 1,314 times this year, a 20% decrease from last year. The on-line version, available at Purdue's nanoHUB site for computational materials science[14], was run by 183 users (up 30% from last year) from 10 countries.

The major milestone in OOF development during FY11 was the February release of version 2.1.0, which allowed for the solution of time dependent problems and included more robust nonlinear solvers, as well as a large number of improved features and bug fixes. Four subsequent bug-fix releases brought the version number up to 2.1.5. A complete description of the new features of version 2.1.0 is available online[15].

The new, more flexible nonlinear solvers were used by a highly nonlinear elastic constitutive model, which demonstrated the facility and correctness of the OOF extension scheme; this work was presented at FEMTEC 2011, a finite-element modeling conference which represents a new audience for the OOF software.

Other work during FY11 concentrated on three topics: surface properties (Andrew Reid), image segmentation (Günay Doğan), and three dimensions (Steve Langer and Valerie Coffman).

Surface properties in OOF2 assign material characteristics to the boundary between two materials in a microstructure, in contrast to bulk properties, which determine the behavior of a single material away from the boundaries. It was discovered that the existing surface property infrastructure did not make effective use of the main solver routines, so a new surface property scheme was constructed which would be better integrated with the bulk solvers. In the process, a bug was identified in the automatically generated surface boundary conditions, which are used to tie together field values across an interface, and also used to implement periodic boundary conditions. This necessitated a review of some of the boundary condition code, and the construction of a new class of boundary conditions for the out-of-plane parts of the fields. Implementation of surface properties then proceeded, and has reached the point where surface-specific constant-flux contributions can be correctly represented.

Image segmentation is the problem of identifying distinct regions or objects in a given image. This is the first step for microstructure analysis with OOF. During FY11 a powerful class of segmentation models was implemented, applicable to a wealth of images in material science as well as other domains, particularly those of interest to the NIST Innovations in Measurement Science Project on Shape Metrology, which was initiated this year. The underlying principle of the approach is energy minimization. Shapes, such as curves or surfaces, are assigned energies which are minimized when the shapes are aligned with boundaries in the image. The algorithm works by iteratively deforming specified

[14] http://nanoHUB.org/

[15] http://www.ctcms.nist.gov/oof/oof2/new_in_21.html

initial shapes until an energy minimum is obtained. The infrastructure to do this in two dimensions is now complete, including algorithms for shape optimization, topological changes (to adjust the number of curves when finding an unknown number objects), and handling image boundaries. A significant portion of the development effort went into making the method efficient for large images, using adaptivity to save CPU time while preserving accuracy, efficient linear algebra to take advantage of the special structure of the problem, Newton-type descent methods to reduce the number iterations needed, and a separate algorithm to get good starting points in certain cases.

Progress on the three dimensional code, OOF3D, was slowed somewhat by the July departure of Valerie Coffman, who had been leading the effort. At that point, OOF3D could perform all of the steps required to perform a complete calculation in a minimal fashion. It lacked a working test suite, though, and was therefore not ready for release. Since then efforts have concentrated on the test suite, with several long diversions to fix bugs or add features necessary to make the program easy to use. An initial alpha release of OOF3D is expected in FY12.

In addition to the above topics, a significant effort was spent on user support, such as regression testing of OOF2 releases on many operating systems, including OS X, NetBSD and a number of Linux distributions. This task has been simplified by the availability of mature virtualization tools.

[1] A. Reid, Object-Oriented Finite Element Materials Modeling at NIST, *3rd International Conference on Computational Methods in Engineering and Science (FEMTEC 2011)*, Stateline, NV, May 9, 2011.

Micromagnetic Modeling

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

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. ACMD 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 2011 alone, the software was downloaded more than 5,000 times, and use of OOMMF was acknowledged in 129 peer-reviewed journal articles. OOMMF has become an invaluable tool in the magnetics research community.

Key new developments in OOMMF over the last year include:

- Implemented 1D periodic boundary conditions, including development of techniques to improve accuracy and accelerate convergence of the infinite sums needed to compute long-range magnetostatic fields. These methods work well when the computational cells are nearly cubes, but are not accurate for cells with large aspect ratios.
- Implemented two preconditioners for the conjugate-gradient solver, improving computation speed of simulations with highly non-uniform edges by a factor of ten.
- Continued development on measurement, analysis, and improvement of the performance of multi-threaded computations on non-uniform memory access (NUMA) architectures. Major issues include effective propagation of task requests to and wake-up latency of worker threads.

Ongoing work includes extension of periodic boundary condition support to two dimensions, refinement of asymptotic approximations to improve accuracy for cells with large aspect ratio, and implementation of enhanced task dispatching techniques in multi-threaded operations.

OOMMF is part of a larger activity, the Micromagnetic Modeling Activity Group (muMAG), 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. ACMD 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. A solver that computes spin momentum transfer is based on one of two competing equations. A standard problem must be stated in terms that solvers based on either equation can be directed to solve. While translating the proposed problem into these terms, it became apparent that extending the problem into a sequence of problems would enhance its usefulness. Each problem in the sequence prescribes a different value for the degree of non-adiabaticity, ξ. Solving the problem for small values of ξ achieves the goal of the original proposed problem, while larger values of ξ illustrate where the two competing equations diverge in their predictions. Testing of the proposed problem also revealed the importance of an explicit description of the boundary conditions to impose where current enters and leaves the magnetic material.

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." This work involves development of methods for modeling polycrystalline materials with magnetically thick grain boundaries.

In collaboration with the University of Konstanz we continue to use OOMMF to study magnetic structures in nanowires. Recent work has examined a novel pseudo-periodic domain structure of counter-rotating axial domains which may explain certain experimental findings of long period domain structures. The ACMD micromagnetic project produced one journal paper [2] and one conference presentation [3] 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] G. S. Abo, Y. K. Hong, B. C. Choi, M. J. Donahue, et al., Micromagnetic Computer Simulated Scaling Effect of S-shaped Permalloy Nano-element on Operating Fields for AND or OR Logic, *IEEE Transactions on Magnetics*, to appear.

[3] M. Donahue, Parallelizing a Micromagnetic Program for Multi-processor Non-uniform Memory Access Computers, *Conference on Magnetism and Magnetic Materials*, Atlanta, GA, Nov. 15, 2010.

Parallel Adaptive Refinement and Multigrid Finite Element Methods

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Marjorie A. McClain
James Benson
Eite Tiesinga (NIST PML)
Thomas Hanna (NIST PML)
John Villarrubia (NIST PML)
Pavel Solin (University of Nevada, Reno)

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 automatically 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 are useful for many NIST laboratory programs, including those in material design, semiconductor device simulation, and the quantum physics of matter.

This year the effort was primarily focused on a study of the performance of several proposed *hp*-adaptive strategies; see page 27. But the development and application of PHAML continue to be of prime importance. For example, as multicore computers begin to dominate the market, additional models of parallelism need to be implemented in scientific software. During the past year we have added OpenMP directives to PHAML to implement a shared memory model. Not only is this appropriate for a multicore computer, but it can be combined with the previously implemented MPI message passing model to form a hybrid MPI/OpenMP model that uses shared memory parallelism on the multicore nodes of a cluster and message passing between the nodes.

A number of collaborative efforts to apply PHAML took place during this year:

- In collaboration with Prof. Pavel Solin of the University of Nevada at Reno, PHAML has been added to FEMhub[16]. FEMhub provides a unified Python interface on top of open source finite element packages. PHAML is the second FEM package in FEMhub, after Prof. Solin's own finite element software.

[16] http://FEMhub.org/

- In collaboration with Eite Tiesinga and Tom Hanna of the NIST Physical Measurement Laboratory (PML), PHAML is being used to calculate the bound states, scattering properties, and dynamics of two dipolar molecules held in a cylindrically symmetric trap. We have studied in detail the two-body energy spectrum, and shown for the first time that the trap may be used to actively control the strength of the interactions.
- We began a new collaboration with John Villarrubia of NIST PML to apply PHAML to the modeling of scanning electron microscope images of samples that contain a mixture of conducting and insulating regions. Villarrubia has a code that models electron scattering in materials, secondary electron production, and detection. This code will be coupled with PHAML which will perform the finite element analysis to determine the electric fields that affect the image.
- James Benson is using PHAML to solve a coupled system of advection diffusion equations to model the fluid and concentration fields in a two domain system. One domain corresponds to the exterior region surrounding a tissue and the other domain is the interior of the tissue.

Future work will continue to enhance PHAML with additional capabilities, robustness and efficiency, implement and study some recently proposed *hp*-adaptive strategies, and extend PHAML to solve 3D problems, which is needed for both the work with Villarrubia and a new application with Tiesinga involving the collision of one atom and a di-atomic molecule.

[1] W.F. Mitchell and M.A. McClain, A Survey of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations, in *Recent Advances in Computational and Applied Mathematics* (T.E. Simos, ed.), Springer, 2011, pp. 227-258.

[2] W.F. Mitchell and M.A. McClain, A Comparison of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations, submitted.

[3] W.F. Mitchell and M.A. McClain, A Comparison of *hp*-Adaptive Strategies for Elliptic Partial Differential Equations (long version), NISTIR 7824, 2011.

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

[5] T.M. Hanna, E. Tiesinga, W.F. Mitchell and P.S. Julienne, Resonant Control of Polar Molecules in an Optical Lattice, arXiv:1111.0227v1, 2011.

[6] W.F. Mitchell and M.A. McClain, Performance of *hp*-Adaptive Finite Element Methods, SIAM Conference on Computational Science and Engineering, Reno, NV, February 2011.

[7] T.M. Hanna, E. Tiesinga, W.F. Mitchell and P.S. Julienne, Bound States of Interacting Polar Molecules in an Optical Lattice, 42nd Annual DAMOP Meeting, Atlanta, GA, June 2011.

[8] W.F. Mitchell and M.A. McClain, Comparison of *hp*-Adaptive Finite Element Strategies, Foundations of Computational Mathematics, Budapest, July 2011.

Finite Differences Using Voronoi Cells

Javier Bernal
Nicos Martys (NIST EL)

A finite difference scheme based on Voronoi cells is being developed for numerical modeling of the diffusion operator on arbitrary unstructured grids. For the purpose of computing Laplace interpolants associated with Voronoi neighbors, programs will be implemented for computing volumes of Voronoi cells, areas of Voronoi facets, and distances between neighbors in 3-d Voronoi diagrams, as well as areas of Voronoi cells, lengths of Voronoi faces, and distances between Voronoi neighbors in 2-d Voronoi diagrams.

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.

Digital Library of Mathematical Functions

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

http://dlmf.nist.gov/

Nearly half a century ago, in 1964, NBS published the immensely influential *Handbook of Mathematical Functions*, edited by Milton Abramowitz and Irene Stegun. Known simply as *A&S*, it can be found on the reference shelf of physicists, other scientists, engineers, and applied mathematicians all over the world. This has made it the best-selling NIST/NBS publication of all time. The trend of citations to *A&S* until recently has actually been *increasing*. These attributes are due in large part to the care with which it was produced by a carefully assembled team of subject area specialists who produced a largely error-free compendium of the most important formulas for mathematical special functions according to their use in research and scientific applications. In short, *A&S* became the standard reference for the properties of the special functions.

It is a testament to the universality of mathematics that an old standard can have such vital force today. But mathematics and ways of applying mathematics have not stood still, and for many years there have been calls for a new standard. Creating this new standard was the purpose of the DLMF Project. Conceived, funded, and led by NIST, the project was initiated in 1997, and after long years of effort it released the online Digital Library of Mathematical Functions and its print companion, published by Cambridge University Press, in May 2010. The DLMF Project adopted the *A&S* method of production, with over 50 carefully selected and highly qualified contributors from 10 different countries, but strengthened and expanded it in several significant ways: (a) every formula has a link to a proof, (b) every chapter was reviewed by a referee unknown to the author, (c) twice the number of formulas and many more graphs are included, (d) preferred notations are clearly stated and related to alternative notations, and (e) brief accounts of illustrative scientific applications are included. The online website provides: (a) links to software rather than voluminous numerical tables, (b) links to reviews and full texts of references, (c) internal links to the DLMF definition of each symbol in every displayed equation, (d) a way to download formulas for use by document processors, (e) interactive visualization of functions of two variables, and (f) an innovative math search engine.

NIST is committed to maintain, update, and expand the mathematical content. A continuing need is to collect suggestions and reports of errors from users, investigate them, and respond to them by making changes on the website, and eventually in a reprinting of the Cambridge edition. This process led to Release 1.0.1 on June 27, 2011, that included several text clarifications, additions to the bibliography, and 8 corrections to five equations (of the nearly 10,000 in the DLMF), two tables, and one figure. The second and third releases on July 1 and August 29 identified several minor improvements affecting display on the website, and added a few more text clarifications and bibliographic citations; no errors in equations, tables, or figures were needed. In the future it is anticipated that chapters will be added, or existing chapters expanded, in a substantial second edition.

NIST is also committed to building upon the expertise it developed to improve the dissemination of mathematical material on the web in ways that enable its more effective use by researchers and practitioners. For example, the processor developed at NIST for generating high-quality web display of mathematics encoded in LaTeX is the vehicle for the eventual inclusion of mathematical meaning, a capability that will allow formulas to be cut-and-pasted into computer algebra systems for use in subsequent symbolic processing. As a second example, an early prototype of a web service to produce standard reference tables for user-specified arguments and parameters, and to user-specified accuracy, has been constructed. This kind of table is unprecedented because the accuracy is guaran-

teed, not just estimated. These activities are being carried out in collaboration with other research groups, for example at Jacobs University in Germany and the University of Antwerp. Research collaborations in graphical visualization of functions and further development of the search capability are also in progress.

Mathematical Knowledge Management

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Heinrich Stamerjohanns (Jacobs University, Germany)

Our activity in Mathematical Knowledge Management (MKM) began in earnest with the Digital Library of Mathematical Functions (DLMF) project. Tools developed there soon found application outside. And, as often happens in science, those outside experiences bring benefits back to original project.

Here, we primarily refer to LaTeXML [1], a tool developed in ACMD to convert DLMF's source documents from LaTeX into flexible XML formats. Naturally, the Web was a target, but supporting MathML improved usability, re-usability and accessibility. Additionally, rich XML formats accommodate a variety of enrichments, helping the user find relations between the mathematical functions and concepts.

Interest in LaTeXML sprang up; a project [2] was begun at Jacobs University to convert the material in Cornell's preprint archive (arXiv)[17] from TeX to XML. Not only would it be available on the web, but it would serve as a test corpus for other MKM research such as mathematical search and semantic inference. The half-million-article arXiv is a strenuous test: the science may be first-rate, but the markup quality is highly variable. The planetary [3] project was then initiated to create Semantic Mathematical Wikis that would allow convenient and familiar authoring using LaTeX, and yet provide all the benefits of semantic representation of mathematics in terms of reuse, search and discovery of mathematical relationships.

These projects have helped focus and drive development of LaTeXML. The arXiv project improved the robustness and coverage of the software. The dynamic environment of Wikis spurred the creation of a 'Daemon' process [4] which converts document fragments on the fly.

The real challenge, however, is ongoing work involving the generation of Content MathML, or semantic representation, of the mathematics. Always a goal, and further prodded by the planetary project, inferring the semantics of ambiguous markup is not necessarily always possible, short of full human intelligence (or AI?). Nevertheless, much can be inferred or clarified by augmenting the documents or, at least, recording and representing the ambiguities for later analysis. How such inferences are best done, on the one hand, and how to represent ambiguities, on the other, are continuing work [5]. Much infrastructural work within LaTeXML has been carried out to support such conversions and the interconnected parallel representations needed to make use of them.

All of these developments eventually lead back to DLMF. Truly reusable mathematics based on content MathML will allow importing to other software such as computer algebra or graphics systems; perhaps even automated validation. Capabilities such as the planetary system could be used for mathematics-aware social media related to DLMF. Further, these enhancements along with others such as Scalable Vector Graphics generation from embedded graphical material and work towards supporting the ePub format will further improve the accessibility and portability of the DLMF.

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

[3] M. Kohlhase, et al., The Planetary System: Web 3.0 & Active Documents for STEM, in *Proceedings of the 2011 International Conference on Computational Science* (M. Sato, S. Matsuoka, P.M. Sloot, G.D. van Albada and J. Dongarra, eds.), Volume 4, pp. 598-607.

[4] D. Ginev, H. Stammerjohanns, B. Miller, and M. Kohlhase, The LaTeXML Daemon: Editable Math on the Collaborative Web, *Lecture Notes in Computer Science* **6824** (2011), pp. 292-294.

[5] D. Ginev, The Structure of Mathematical Expressions, Master's Thesis, Jacobs University, 2011.

[17] http://arXiv.org/

DLMF Standard Reference Tables on Demand

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Marjorie McClain
Daniel Lozier
Chris Schanzle
Annie Cuyt (University of Antwerp)
Stefan Becuwe (University of Antwerp)
Franky Backeljauw (University of Antwerp)

Published tables have long been used to supply numerical values of elementary and special functions for numerical exploration, software validation, program debugging, algorithm construction, and graphics production. For example, the original special function procedures in Mathematica were validated by comparison with the 1964 NBS *Handbook of Mathematical Functions*. More recently, a communication was received from Microsoft seeking assistance with the validation of functions in its own numerical library, which is under development.

The goal of our project is to develop a website at NIST that provides 21st century tools to escape the severe limitations of many previously published tables: low precision, sparsity of arguments and parameters, lack of coverage of complex variables, and inability to accommodate alternate function definitions. Our site will allow users to specify (within reasonable limits) these attributes, and it will return values with an accuracy certification.

The first phase of the project, computing tables of high precision function values at real inputs assumed to be exact, is well underway. We first searched for reliable reference software, that is, software that establishes an error bound, preferably *a priori*, along with each function value. Such a package has been developed by a group at the University of Antwerp under the leadership of Prof. Dr. Annie Cuyt [1]. Their software package, which uses continued fractions as the main tool, covers a substantial subset of the functions included in the DLMF. After discussions at a NIST meeting in October 2010, we decided to collaborate with Dr. Cuyt's group and developed an action plan. The NIST team worked on the front end user interface and the web software for the system, while Cuyt's group refined the software for the computational engine. In December 2011 the two groups met again at NIST to integrate the various parts for a preliminary system with a small number of functions. During the two week meeting a selected group of testers at NIST and the University of Antwerp were given access to the system to provide feedback. Over the next few months more functions will be included, and additional modifications and testing will be conducted before the site is expanded into a prototype that will be released for wider testing.

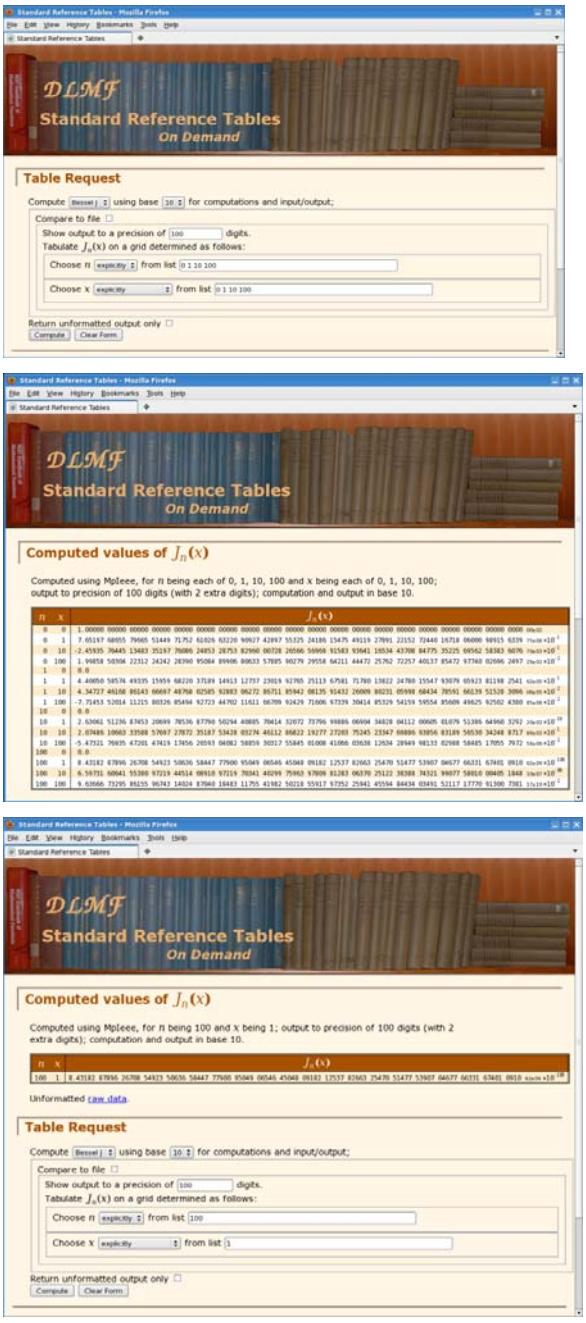

Figure 42. *Prototype of DLMF Standards Reference Tables.*

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ITL Program: *Virtual Measurement Systems*

Visualization of Complex Functions Data

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During the development of the NIST Digital Library of Mathematical Functions (DLMF), a considerable effort was invested in creating accurate user-friendly visualizations to help users understand the behavior of complex functions. We have continued to improve these visualizations by developing better computational grids and redesigning the computation and movement of cutting planes used in interactive 3D visualizations. However, we would also like to increase accessibility to the interactive 3D visualizations. The current 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. While several viewers are available for Windows and Mac platforms, we have not found an acceptable Linux viewer that easily handles all the custom features implemented in our visualizations. Also, we must continually test the visualizations to catch anomalies that arise when the plugin, browser, or operating system is updated. We are addressing the accessibility problem in two ways: constructing a DLMF PDF file with embedded graphics, and adding the appropriate software code and modifications to our graphics files to allow users to see our visualizations on a web page without the use of a plugin.

Creation and testing of the enhanced DLMF PDF file with embedded graphics has been completed. With a common PDF reader users can rotate 3D function surfaces, use the zoom feature, and explore other built-in options. We were concerned that the embedded graphics would greatly increase the size of the PDF file, but were relieved to find that it increased by only 10 MB from about 25 MB to 35 MB. The other concern was that the embedding process would have to be redone every time the DLMF database and PDF file were regenerated. Fortunately, we found a package that would embed the graphics files directly into the DLMF LaTeX source files before PDF conversion.

We are also attacking the accessibility problem from another direction by determining the modifications needed to view our files in a WebGL environ-environment. HTML5 contains WebGL attributes that allow users to view interactive graphics inside a web page without the need of a special plugin. Our X3D graphics files can be integrated with HTML5 via the

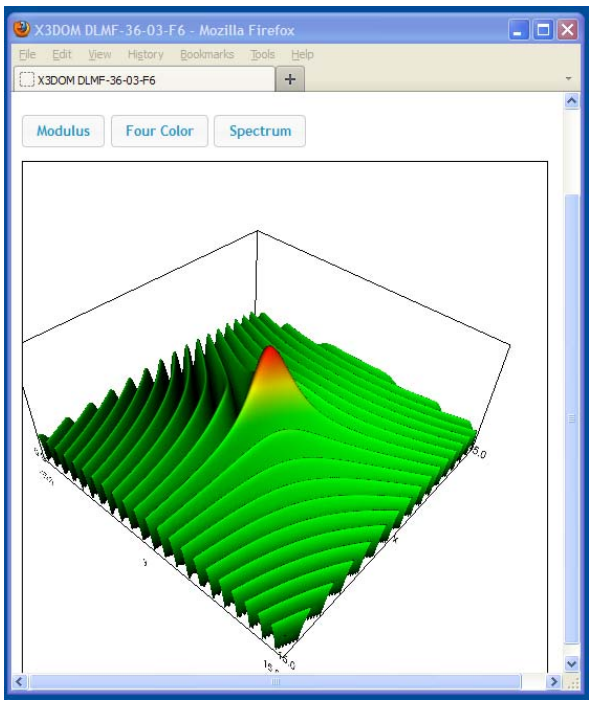

Figure 43. *Modulus of elliptic umbilic canonical integral function* $|\Psi^{(E)}(x,y,0)|$ *displayed in HTML5 using X3DOM.*

X3DOM open source framework. We have successfully displayed simplified versions of some of our files in HTML5 browsers. An example is shown in Figure 43. The latest versions of several browsers now support WebGL, but for a while we will still need to provide files that are viewable with VRML/X3D plugins.

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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.

Single Photon Upconversion and Quantum Information Science

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See feature article, page 40.

ITL Program: *Quantum Information*

Quantum Computing Benchmarks

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Quantum computing is still in its infancy. There are many experimental efforts involving a diverse collection of physical systems and engineering platforms for implementing the basic tasks, but it is still not possible to routinely implement even two-quantum-bit (qubit) quantum computations. To compare the different platforms in a standardized way, we are involved in developing and implementing benchmark procedures to evaluate the quality of basic quantum computing operations. In previous years, we developed a standard method for determining an error per gate (EPG) for one-qubit computations that is being implemented on an increasing number of platforms, ranging from nuclear magnetic resonance (NMR) spectrometers to ion traps. This year we participated in a new implementation of this benchmark in an ion trap where the qubits are manipulated with microwaves instead of laser light. This implementation successfully demonstrated EPGs below the critical value of 0.0001, which is believed to be necessary for practical scalable quantum computing.

An important question is how to standardize such benchmarks for more than one qubit. We developed a technique that can do this by requiring the experimenter to implement random sequences of so-called Clifford unitary operators. By specifying the family of operators rather than the specific elementary steps required to implement them, the benchmark can be realized on any platform, independent of the details of the underlying physics. The family of operators is well-defined for any number n of qubits, and implementing a random such operator typically requires of the order of n^2 elementary steps. As a result, the ability to implement them is already a demonstration of the power of a platform.

Our benchmarks are not intended to diagnose the causes for imperfections in gates. Their main purpose is to compare different computing platforms at different stages of their development. Nevertheless, it would be helpful if some diagnostics were available. For this purpose, we modified the Clifford-unitary-based benchmark so that individual operations to be characterized can be inserted between steps. This makes it possible to determine an EPG for such operations.

The two benchmarking ideas of the above paragraphs were implemented in an ion trap developed by the NIST Ion Storage group. This ion trap is a testbed for many of the technologies needed to scale up ion-trap quantum computing. In particular, it includes multiple trapping zones where the ions can be manipulated, and it realizes a sympathetic cooling strategy whereby the qubit-ions are cooled by an ion of a different atomic species. The benchmark was realized with two qubit-ions and implemented up to six random Clifford unitaries in sequence. A key two-qubit operation, the phase gate, was characterized and shown to have an EPG of

about 0.07. While this is far from sufficient for scalable quantum computing, and other experiments have indicated lower EPGs in restricted settings, the experiment shows that our proposed two-qubit benchmark is feasible and able to characterize individual gates.

The relationship between the benchmark EPG and the actual error behavior of underlying operations is understood only in highly idealized situations. However, these benchmarks provide useful, standardized methods for comparing quantum computing platforms. We are developing guidelines for ensuring that the EPG computed from the benchmarks is meaningful. The guidelines include suggestions for consistency checks that should be performed. Further theoretical work is required to investigate the relationship between benchmark EPGs and the physical error behavior in practical settings.

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[2] J.P. Gaebler et al., Randomized Benchmarking of Two-Qubit Gates, in progress.

ITL Program: *Quantum Information*

Quantum State Estimation Theory and Applications

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Warren Grice (Oak Ridge National Laboratory)
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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 focused on collaborations with two experimental groups using quantum state estimation.

The first of these is an experiment to prepare squeezed light for quantum information processing applications. The creation of high quality squeezed light is helpful for quantum enhanced interferometry, optical quantum computation, and other technologies. However, these technologies are limited by the quality of squeezed light, which is often contaminated with photons in pulses that overlap the primary squeezed pulse and whose mode structure is not suitable for some intended applications. Experimentalists in our team engineered a nonlinear crystal and laser pumping strategy to produce highly pure squeezed light, and ACMD members helped to design a measurement and analysis strategy to demonstrate the experiment's success in avoiding contaminating photons and matching the desired pulse shapes. We showed world record overlap of two entangled, squeezed pulses and published the results in *Optics Express*.

The second experiment is the DARPA-funded collaboration with JILA, "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 2011 we prepared an entangled state of quantum microwaves and verified the entanglement with preliminary measurements, which will be presented at the American Physical Society's March Meeting in 2012. We are developing methods to calibrate the measurements and fully quantify the amount of entanglement.

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ITL Program: *Quantum Information*

Quantum State Tomography using Compressed Sensing

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Quantum state tomography is a family of techniques for estimating the state of a quantum system. Tomography provides a full characterization of the state, including all effects due to noise and decoherence. This makes it a useful tool in experiments involving quantum-enhanced metrology and quantum computation. However, tomography of large quantum systems is very resource-intensive: for a system of n qubits, standard methods of tomography require measuring 4^n different observables.

Recently it was shown that tomography can be done using far fewer measurements, using compressed sensing techniques, provided that the state is low-rank or pure — a condition that is satisfied in most experiments [1]. In particular, if the state has rank r, then it is sufficient to measure only $O(2^n\ r\ \mathrm{poly}(n))$ Pauli observables, in order to completely characterize the state. Furthermore, given the measurement data, one can compute the density matrix easily, by solving a trace-minimization convex program. This approach is known as compressed tomography.

In the last year, the first tight error bounds were determined for compressed tomography [2]. These quantify how the error in the estimated density matrix depends on errors in the measurement data. They also give the first useful bounds on the sample complexity of compressed tomography. (Sample complexity describes how many copies of the unknown state are required.) These results are obtained from a new analysis of compressed tomography using the restricted isometry property (RIP) [2,3].

Roughly speaking, a mapping satisfies RIP if it approximately preserves the geometry (as measured by the 2-norm) of the set of low-rank matrices. In [2], it is shown that the random Pauli sampling operator satisfies RIP with high probability. This is quite surprising, because the sampling operator embeds a nonlinear manifold (the set of all low-rank matrices) into a linear space, with only a slight increase in the dimension. The proof of this claim is highly nontrivial: it uses Dudley's inequality for bounding the supremum of a Gaussian process, and bounds on covering numbers using entropy duality. Then, once RIP is established, the results of [3] imply error bounds for compressed tomography.

These error bounds complete our understanding of the practical resource requirements for compressed tomography. It was known before that compressed tomography uses fewer measurement settings and less classical postprocessing than standard tomography. The new error bounds show that compressed tomography has roughly the same sample complexity as standard tomography (up to log factors). Thus, there is no "hidden cost" in the sample complexity. In fact, this sample complexity is nearly optimal, in the sense that no scheme for pure-state tomography using Pauli measurements can do better (up to log factors) [4].

The next major step in this project will be an experimental demonstration of compressed tomography, likely using ion traps. To this end, it will be useful to develop faster algorithms for solving the trace-minimization convex program. The algorithm in [1], singular value thresholding (SVT), can reconstruct the density matrix for about 8 qubits on a laptop computer. It may be possible to handle more qubits, using parallel versions of the algorithm, or alternative optimization techniques such as gradient descent on the Grassmannian manifold. Also, it will be interesting to construct estimators that combine the compressed sensing approach with traditional maximum-likelihood estimation (MLE), e.g., trace-norm-regularized MLE. Finally, one might hope to adapt compressed sensing techniques to continuous-variable systems, e.g., optical homodyne tomography.

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ITL Program: *Quantum Information*

Quantum Computing Theory

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Adam Meier
Mike Mullan
Yanbao Zhang
Bryan Eastin (Northrop Grumman)
Emilio Cobanera (Indiana University)
Gerardo Ortiz (Indiana University)

Our theoretical work on quantum computing and information progressed in four main areas this year. We developed and implemented a new and statistically rigorous method for analyzing demonstrations of nonclassicality in experiments, we formalized a method of optimizing phase interrogations for atomic clocks and

initiated a program to test the method on simulations, we determined and analyzed a new method for "magic state" distillation, and we contributed to the theory of duality for quantum lattice models relevant to condensed matter studies.

Our work on quantum lattice dualities is still preliminary. Our main contribution so far is to help establish new dualities involving so-called Hopf-algebraic one-dimensional lattice models. A hope is that such models may illuminate condensed matter systems of interest, though a more likely outcome is that they provide small examples for testing future analog quantum simulators such as those based on atoms in optical lattices.

Magic-state distillation is a strategy envisioned for use in future fault-tolerant quantum computers, where it is required for universal computing. The distillation process improves initially noisy special states to the point where they are almost noise-free. The standard magic state distillation routines are based on a seven and a five quantum bit (qubit) error-correcting code. We investigated the use of a four qubit error-detecting code and found that it leads to a distillation routine requiring fewer resources per iteration. However, the distilled states improve less in comparison. We determined the exact behavior of the routine in combination with other routines and found that for a given reduction in noise, its use can reduce resources required by up to a factor of about 10. This should help reduce the large overheads for noise reduction in proposed methods for fault-tolerant quantum computing.

Quantum methods for phase measurements used in modern atomic frequency standards and clocks promise to improve their precision over the shot-noise limit. The most advanced clocks being experimentally tested at NIST have the potential for using such methods, but the methods need to be modified from the theoretical ones to work in the presence of classical phase noise in the reference oscillators ("flywheels") used. We have adapted semidefinite programming techniques from quantum query complexity to this problem and are currently testing them on simulated clocks. So far we have established that gains over conventional and theoretical quantum methods are possible in one clock interrogation step. In order to demonstrate this, we showed that the continuous phase estimation problem can be efficiently discretized for the purpose of semidefinite programming. Work in progress involves adapting our techniques to the situation where sequential interrogations are used to monitor frequency and phase. The main task is to implement a flexible simulator where we can choose the relevant noise model and keep track of the accumulated phase from previous interrogations.

The best-known proof that quantum non-locality is not consistent with classical, local-realistic expectations is based on the quantum violation of Bell-inequalities for two-party measurement outcomes that are satisfied by local realism. There still has not been a completely loop-hole free demonstration of such violation. The main obstacle is the difficulty of setting up an experiment with sufficiently low photon loss and large separation between the two parties making the measurements. Loop-hole-free demonstrations are also needed to enable many quantum information protocols. In the past, the (conditional) success of Bell-inequality experiments was quantified by the number of standard-deviations of violation of the inequality. We formally verified that this measure of success is not statistically justifiable, can lead to excessive confidence in violation, and cannot be compared between independent experiments. We remedied this situation by showing how a statistically rigorous p-value for violation of local realism can be computed for any experiment, independent of any particular Bell-inequality or the experimental setup. Our method is efficient and can be used "on-the-fly" to optimize experiments to enable more efficient protocols. We developed and released software that implements our method.

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ITL Program: *Quantum Information*

Quantum Algorithms for Quantum Field Theories

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John Preskill (Caltech)

Quantum field theory has wide-ranging applications in both high-energy and condensed-matter physics. In particular, it reconciles quantum mechanics with special relativity and provides the most fundamental theory of physics to be tested by experiment: the so-called Standard Model of particle physics.

The question of whether quantum field theories can be efficiently simulated by quantum computers was first posed by Feynman three decades ago when he introduced the notion of quantum computers. Since then, efficient quantum algorithms have been developed to simulate the dynamics of quantum lattice models and quantum systems with a fixed number of particles, but the question about quantum field theories has remained open.

We have developed a fast quantum algorithm for simulating relativistic particle scattering in a well-known quantum field theory called phi-fourth theory. While simpler than the standard model, which encompasses all physical processes except those involving gravity, phi-fourth theory illustrates the essential challenges of simulating quantum field theories.

The two most essential challenges in simulating quantum field theories on a quantum computer are discretization and state preparation. The discretization problem arises because, in principle, a quantum field has infinitely many degrees of freedom, even within finite volume. Thus, an exact description of the quantum state of the field requires infinitely many qubits. The obvious approach to this challenge is to discretize space onto a lattice. We show that this approach works, although it is nontrivial due to a uniquely quantum field-theoretic effect called renormalization. The state preparation problem is to design efficient quantum circuits that construct qubit representations of physically realistic initial states for the simulation. We achieve this by developing a new generalization of a widely-used quantum algorithmic technique called adiabatic state preparation.

Upon successful construction of a large-scale quantum computer, a fast quantum algorithm for simulating quantum field theories will be useful in simulating processes from nuclear, particle, astronomical, and condensed-matter physics. Furthermore, the question of whether quantum field theories can be efficiently simulated by a quantum computer bears on the fundamental computational power of the universe. If quantum computers cannot efficiently simulate the Standard Model, this raises the possibility of quantum field computers exponentially more powerful than "ordinary" quantum computers. Conversely, if the methods introduced in this work can be extended to efficiently simulate the full Standard Model, this would definitively eliminate the possibility of such exponential speedups.

[1] S.P. Jordan, K.S.M. Lee and J. Preskill, Quantum Algorithms for Quantum Field Theories, arXiv:1111.3633, submitted.

ITL Program: *Quantum Information*

Post-Quantum Cryptography

Stephen Jordan
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Ray Perlner (NIST ITL)
Daniel Smith (NIST ITL)

In 1994, Peter Shor discovered a polynomial-time quantum algorithm for factoring integers and computing discrete logarithms. This has far-reaching consequences for cryptography: if large-scale quantum computers are built, they would break essentially all of the public-key cryptosystems currently used for internet commerce, including RSA and elliptic curve cryptosystems. For this reason, we are beginning to study alternative cryptosystems that would be secure against quantum attacks.

There are three main classes of cryptosystems that have been proposed to replace RSA: lattice-based (such as NTRU), code-based (such as McEliece), and multivariate (such as HFE and its variants). However, there are significant open questions regarding these proposals. For instance, many practical lattice-based cryptosystems use special classes of lattices, such as cyclic or ideal lattices, whose security is not as well-understood (compared to the case of general lattices). Indeed, ideal lattices have a surprisingly powerful algebraic structure, which is a topic of current research, and which enables tasks such as fully homomorphic encryption. On the other hand, code-based cryptosystems tend to have large key sizes, which would have a significant impact on the broader public-key infrastructure. To deploy these cryptosystems on a large scale, one will need better strategies for mitigating this impact. Finally, there have been successful attacks against some multivariate cryptosystems, and it is an interesting open problem to understand what algebraic features are sufficient to ensure the security of such schemes.

There are also major open questions relating to quantum computation. First, what kinds of problems can be solved efficiently on a quantum computer? It is known that there are various ways in which quantum computers can achieve speed-ups over classical computers: for instance, using the quantum Fourier transform to solve certain algebraic problems involving hidden subgroups and hidden shifts; or using adiabatic evolution and quantum "tunneling" to solve certain combinatorial optimization problems. In particular, Shor's algorithm is an example of the first strategy. In fact there are many other quantum algorithms that solve algebraic problems, and it is important to understand whether these algorithms are cryptographically relevant.

In addition, we are monitoring ongoing developments in experimental quantum computation, in order to predict when (or whether) quantum computers will pose a significant threat to RSA and other cryptosystems currently in use. There are several different approaches to building large-scale quantum computers, including ion traps, adiabatic quantum computation, superconducting circuits, and topological anyons. The rate at which these technologies mature and scale up will determine when it becomes necessary to deploy new "quantum-resistant" cryptosystems.

Finally, there is an interesting possibility that ideas from quantum information may lead to novel cryptographic protocols. Quantum key distribution is one

well-known example, and we are considering others, including schemes for encrypted quantum computation based on braid groups, and implementations of secure hardware using non-orthogonal quantum states.

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.

Community and Cluster Detection: Alternative Measures for Network Structure

Roldan Pozo

See feature article, page 42.

ITL Program: *Complex Systems*

Algorithms to Approximate Multivariate Network Reliability

Isabel Beichl
Elizabeth Moseman
Francis Sullivan (IDA Center for Computing Sciences)

In estimating the reliability of a real-world network, one difficult but common problem is that of dealing with network connections of varying robustness. Some links might be easily broken while others are much less likely to fail. The situation to avoid in designing and maintaining a network is a set of weak links whose failure causes the whole network to collapse. A first step in attacking this problem is to devise algorithms to estimate the reliability of a multi-variate network—one in which every edge can have a different probability of failure.

We think of the network as a graph $G = (V,E)$ with V, the nodes, and E, the edges, connecting some of the nodes. We are also given a vector $\boldsymbol{p} = (p_e)_{e \in E}$ indexed by the edges, e, where p_e is the probability that edge, e, is connected. There is a naive way to compute the probability of connection of such a multivariate network, namely, for each sample allow an existing edge to be connected with probability p_e, for all e, and then determine if the resulting graph is connected. The percentage of times the resulting graph is connected will give an estimate of the reliability. However the variance of this simple "vanilla" method of Bernoulli trials is large, especially if the p_e are small.

We give two new probabilistic methods based on sequential importance sampling to approximate the reliability of the network. The strength of these algorithms is that they only look at local changes in the graph to make their estimates and have significantly lower variance than Bernoulli trials.

The first of our new methods uses the formulation of reliability as a variation on computing the Tutte polynomial. In computing the Tutte polynomial for a graph, one builds a tree where at each node of the tree, one edge of the graph is examined. Since our edges have associated probabilities, p_e, this gives us a way to select a path from the root of the tree of the Tutte polynomial to one of its leaves.

The probability at each tree node to remove the edge e in the resulting subgraph is $1\text{-}p_e$ unless removing it would disconnect the graph. In that case, leave it in with probability one. The resulting subgraph is guaranteed to be connected. We are using importance sampling so that we choose with some probability q and then divide by that probability, (p_e if the edge is left in and $1\text{-}p_e$ if it is removed). We have proved that in this algorithm all probabilities cancel except for the edges that would have caused a disconnection. The product of probabilities remaining gives an unbiased estimate of the reliability. A remarkable feature of this method is that, although the result itself is independent of the order in which the edges are chosen, the variance does, in fact, depend on order of selection. The optimal order is increasing probability p_e.

The second new method is somewhat similar, except that the decision to remove an edge is made probabilistically over the set of all currently removable edges. This results in a different importance function

with different cancellations and different variance behavior. If the p_e are close to one, the second method has larger variance than the first. For small p_e, the situation is reversed. In this case, the first method tends to behave like the "vanilla" method while the second method does better.

ITL Program: *Complex Systems*

New Importance Functions and Efficient Algorithms for Network Reliability

Isabel Beichl
David G. Harris (National Security Agency)
Francis Sullivan (IDA Center for Computing Sciences)

We can think of a network as a graph, that is, a set of vertices V, and a set of edges, E, that connect two of the vertices. A graph is connected if there is a sequence of edges between any two vertices in V. The reliability polynomial of a graph gives the probability that a graph is connected as a function of the probability that each edge is connected. The coefficients of the reliability polynomial, c_k, are the number of connected subgraphs of size k. The coefficients give more information about the network than the reliability alone. Computing the reliability polynomial is #P complete and so it is important to find probabilistic methods to approximate the coefficients. Sequential importance sampling (SIS) is a Monte Carlo method based on a statistical technique, importance sampling, which can often be used to reduce variance.

Algorithms based on sequential importance sampling (SIS) were proposed to estimate a graph's reliability polynomial. We develop a new SIS algorithm that uses a new importance function based on the number of spanning trees to sample among the connected spanning subgraphs. The new method chooses a spanning tree at random and adds edges back until the original graph is recovered. The determinant of a certain matrix (the Laplacian) is known to give the number of spanning trees of a graph. This determinant is calculated at each stage of the importance sampling in order to give an importance function and in order to estimate the reliability coefficients. The complexity is controlled because each subgraph is built on previous subgraphs by adding only one edge, resulting in only rank one updates to the Laplacian matrix. This algorithm improves on existing algorithms in that it has lower complexity $\sim O(E^2)$ as opposed to $O(E\ V^3)$, and the new importance function does indeed reduce variance. Lower variance implies that each sample drawn is more efficient and that far fewer random samples need to be drawn, thus improving the state of the art from theoretical algorithms to practical computation.

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ITL Program: *Complex Systems*

Affiliation Networks

Brian D. Cloteaux
James Shook

Many networks can be naturally represented as relationships between entities and the groups (or affiliations) to which the entities belong. A network that records these relationships between the entities and the affiliations to which they belong is called an affiliation network. An example of a network and its associated affiliation network is shown in Figure 44.

To understand what an affiliation network is, we can consider collaboration networks. A collaboration networks records authors who have worked together on papers. Thus it is typically a simple graph where the nodes are authors and the edges represent a coauthoring relationship. We can represent the same information using an affiliation network having a set of authors and a set of papers produced by those authors. If an author has written a paper, then there is a link between author and paper. We notice that we can still extract the information about co-authorships by examining the coauthors on all the papers that an author has produced. This operation of extracting a simple (or one-mode) network from an affiliation network is called a projection.

A recent upsurge in affiliations research has followed from two observations. This first is that there are a large number of real-world networks that have a natural bipartite structure inherent in them. Affiliation networks are a natural way to capture this structure. Additionally, it has been shown that several desirable properties for models, seen in real-world networks, can be explained and captured by examining the changes to the affiliations associated with the networks. These properties include power-law distribution, small world properties, clustering, densification, and a shrinking diameter. It appears that understanding the affiliations associated with certain networks are necessary to be able to accurately model how those networks will evolve.

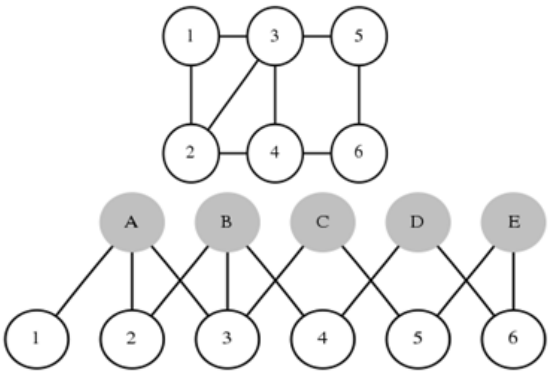

Figure 44. *A graph (top) and its associated affiliation network (bottom).*

B. Cloteaux and J. Shook are investigating methods to increase the accuracy of modeling using affiliation networks. Their approach uses probabilistic projections of the affiliation networks. A probabilistic projection is a projection where each edge has some probability of being included in the one-mode graph. The purpose behind using a probabilistic approach is to capture the idea that simply sharing an affiliation does not always translate into forming a relationship for entities in many real-world networks. The goal of this project is to create more realistic network models while preserving the advantages of creating these models using an affiliation approach.

ITL Program: *Complex Systems*

Degree-Based Modeling

Brian D. Cloteaux

During the past decade, there have been a number of papers devoted to describing the relationships between entities in a system using networks with power-law distributed degree sequences. In a network, the number of edges connected to a node is called the degree of the node and the set of all the degrees in a graph is called its degree distribution. For a degree sequence to be power-law distributed means that the probability that a node has k adjacent edges is $P(k) \sim k^{\alpha}$ for some $\alpha > 1$. This distribution in a graph produces a few nodes with very high degree (often called hub nodes) and a large number of low degree nodes. The importance of networks, especially those having power law distributions, for modeling applications lies in the number of areas in which they are found. These networks have been shown to arise naturally in systems of both biological and social interactions. They also appear in many engineered systems such as the power grid, the Internet, and software components. Thus, realistic models of these types of interactions need to reflect their power-law distribution.

A usual first step in the creation of a model of a real-world complex network is to construct a graph with a given degree sequence. A problem rising from the random modeling of graphs is to generate a degree sequence from some given probability distribution. Specifically, the problem is assuring that the generated sequence can be realized by some graph. One approach, originally suggested by Mihail and Vishnoi [3], is to find the closest graphical sequence to a non-graphical integer sequence using a measure they call *discrepancy*. The discrepancy δ between two sequences, a and b, is given by the formula

$$\Delta(a,b) = \sum_{i=1}^{n} |a_i - b_i|$$

While Mihail and Vishnoi did show an algorithm for this problem that is polynomial, their algorithm is far from optimal. B. Cloteaux has developed an algorithm [1], that runs in near-optimal time (linear time), for the determination of the closest graphical degree sequence in terms of discrepancy to a given non-graphical degree sequence. This result has been submitted to a journal, and a software implementation of the algorithm has been released [2].

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ITL Program: *Complex Systems*

Scaling of Congestion in Small World Networks

Iraj Saniee (Alcatel-Lucent Bell Labs)
Gabriel H. Tucci (Alcatel-Lucent Bell Labs)

A remarkable and widely discussed phenomenon associated with networks in many applications is the small world property. It is observed in many such networks, man-made or natural, that the typical distance between the nodes is surprisingly small. More formally, as a function of the number of nodes, N, the average distance between a node pair typically scales at or below $O(\log(N))$. In this work, we study the load characteristics of small world networks. Assuming one unit of demand between each node pair, we quantify as a function of N, how the maximal nodal load scales, independently of how each unit of demand may be

routed. In other words, we are interested in the smallest of such maximal nodal loads as a function of routing, which we refer to as congestion that the network could experience.

We have shown that in planar small-world networks congestion is almost quadratic in N, which is as high as it can get, specifically $O(N^2/\log(N))$. In contrast, for some non-planar small-world networks, congestion may be almost linear in N, namely $O(N^{1+e})$ for arbitrarily small e. Since congestion in a network with N nodes cannot have scaling order less than $O(N)$ or more than $O(N^2)$, we conclude that the small world property alone is not sufficient to predict the level of congestion a priori and additional characteristics may be needed to explain congestion features of complex networks.

Additionally, we investigate what happens to congestion when we change the link metric that prescribes routing. That is, for a network with edge weight $\{d_e\}_{e \in E}$ we change the metric by a factor $0 \le w_e \le \infty$ thus assigning each edge e a new weight $w_e d_e$. We explore the extent to which this change in the metric can change congestion in the network. We prove that if we allow the weights to get arbitrarily small or large, i.e., when for some edges, we approach zero and for some others we approach infinity, then considerable changes in congestion can occur. On the other hand, if we require the weights to be bounded away from zero and infinity, i.e. when $0 < k \le w_e \le K < \infty$ for all edges e, then congestion cannot change significantly. These observations quantify the degree to which remetrization in a small world network may be helpful in affecting congestion.

This work was performed at Alcatel-Lucent Bell Labs under a grant from NIST.

[1] Iraj Saniee and Gabriel H. Tucci, Scaling of Congestion in Small World Networks, submitted.

ITL Program: *Complex Systems*

Bootstrap Percolation on Random Geometric Graphs

Milan Bradonjić (Alcatel-Lucent Bell Labs)
Iraj Saniee (Alcatel-Lucent Bell Labs)

Some crystals or lattices studied in physics and chemistry can be modeled as consisting of atoms occupying sites with specified probabilities. The lattice as a whole would then exhibit certain macroscopic properties, such as (ferro)magnetism, only when a sufficient number of neighboring sites of each atom are also similarly occupied. In computer memory arrays each functional memory unit can be considered as an occupied site, and a minimum percentage of functioning units are needed in the vicinity of each memory unit in order to maintain the array with proper functioning. In adoption of new technology or emergence of cultural fads, an individual is positively influenced when a sufficient number of its close friends have also done so.

All three examples cited above may be modeled via a formal process called "bootstrap percolation," which is a dynamic process that evolves similar to a cellular automaton. Unlike cellular automata, however, this process can be defined on arbitrary graphs and starts with random initial conditions. Vertices are either active or inactive. Once activated, a vertex remains active forever. Each vertex is initially active with a (given) probability p. Subsequently and at each (discrete) time step, a vertex becomes active if θ of its nearest neighbors are active, for a fixed value of $\theta = 1, 2, 3 \ldots$ As time evolves, a fraction Φ of all the vertices are activated. The emergence of macroscopic properties of interest typically involve Φ to be at or close to 1.

Many diffusion processes of interest have a *physical contact* element. A link in an *ad hoc* wireless network, a sensor network, or an epidemiological graph connotes physical proximity within a certain locality. Study of diffusion of virus spread in *ad hoc* wireless, sensor or epidemiological graphs requires this notion of neighborhood for accurate estimation of likelihood of full percolation. This is in contrast to models with long-range reach where physical proximity plays little, if any, role. The natural random model for such phenomena is the random geometric graph. In this work, we focus on bootstrap percolation on random geometric graphs, a topic that has not been investigated, to the best of our knowledge. We derive tight bounds on the critical threshold, p_c, such that for all $p > p_c$ full percolation takes place. We conclude with simulations that compare numerical thresholds with those obtained analytically.

This work was performed at Alcatel-Lucent Bell Labs under a grant from NIST.

[1] Milan Bradonjić and Iraj Saniee, Bootstrap Percolation on Random Geometric Graphs, submitted.

ITL Program: *Complex Systems*

Cross-layer Network Optimization for Diverse QoS Requirements

Vladimir Marbukh

Aggregate utility maximization as a goal for balancing competing user-level requirements was proposed in [1]. A distributed, price-based network utility maximization (NUM) framework for achieving this goal in a case when users express their utilities in terms of the end-to-end network bandwidth was developed in [2].

This framework assumes that elastic users respond to resource congestion prices represented by Lagrange multipliers associated with the capacity constraints. Later, NUM was extended to cross-layer optimization of wire-line as well as wireless networks [3,4]. These and other extensions retain the basic assumption of [2] that user utilities are expressed in terms of the end-to-end bandwidth.

However, typically it is more natural for users to quantify their preferences in terms of the high-level quality of service (QoS) parameters rather than low-level parameters such as end-to-end bandwidth, packet loss, etc. In [5] we suggest that the distributed, pricing-based framework [2,3,4] can be extended to this more general case by assuming that the user utilities are functions of both network and user level parameters, and the goal is to maximize the aggregate utility which is the sum of the individual user utilities. Replacing capacity constraints with constraints on the feasible QoS parameters may allow direct pricing of the QoS parameters in terms of the Lagrange multipliers associated with the QoS parameter constraints.

To demonstrate flexibility of the proposed framework we consider two instances of QoS-sensitive utility maximization [5]. The first is end-to-end bandwidth allocation subject to the worst-case scenario end-to-end delay. The allocation is based on generalized processor sharing (GPS) [6,7]. The second is end-to-end bandwidth allocation subject to the average end-to-end packet delay. This optimization framework relies on M/G/1 conservation laws for each link and assumes statistical independence of the queues on different links [8]. Both assume users sensitive to average transmission rate and end-to-end packet delays, which explicitly enter the user utility functions.

The first instance is inherently simpler than the second since the worst-case scenario delay for GPS-controlled traffic is only determined by GPS parameters and does not depend on the packet-level traffic structure. The second instance yields an explicit solution for the QoS-sensitive traffic scheduling in a case of user utilities being linear with respect to the average end-to-end delays. The proposed cross-layer optimization increases the aggregate utility as compared to the conventional NUM by taking advantage of the heterogeneity of user QoS requirements. Possible extensions include optimization of non-linear user level utilities with respect to the average end-to-end delays. Generally, this optimization yields dynamic priority scheduling. A distributed user-level utility maximization should be based on direct pricing of QoS requirements, which includes numerous research issues.

In our future work we plan to apply the proposed optimization technique to investigate architectural and methodological challenges of designing intelligent distributed systems capable of managing information assurance and security (IAS) related risks. We expect that system architecture should include sufficient intelligence enabling the system to assess and inform users on the IAS related risks, so that users would be able to select the acceptable level of risk according to their individual preferences. We intend to employ the relevant decision theory frameworks developed and successfully applied in economics and finance for IAS related risk assessment and management.

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ITL Program: *Complex Systems*

Analysis of a Distributed Protocol for an Access Network with Multiple Users

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 and ensure some fairness in the allocation of bandwidth. It was shown by Frank Kelly and later 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 an algorithm for solving the optimization problem. As the need for system robustness has grown amidst cyber security 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 proposed a protocol [1] 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 unconstrained use of this protocol. In previous work on example networks with a single source and destination, e.g., [2], we showed that maximum utility could be achieved with an allocation of traffic that minimizes mean route cost. There we analyzed in detail the dynamics of the prices of constituent links that make up the routes.

We have extended this 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 consists of a link connecting to its nearest neighbor followed by a direct route to the destination. Building on the analysis of a simple two-link network with a time constant route allocation, we examined the tradeoff between path diversity and utility in two situations. The first occurs when the capacities of all the direct links are equal to the same constant, with nearest neighbor links all having equal capacity (in general different from that of the direct links). By examining how utility varies with the route allocation entropy we identified conditions where the aggregate (or average) utility could be increased by increasing the amount of traffic on the indirect routes. Such off-loading of traffic can occur up to a critical value of the route allocation that depends on the link capacities. In the second case, the capacities of links are chosen to vary depending on the source the link is connected to. As in the previous case, each source has a critical value that determines the limit to which traffic can be transferred from direct to indirect routes. Here, that value differs for each source because it depends on the ratio of the capacities of the links attached to the source. Thus for some sources, individual source utility could benefit from offloading while the aggregate utility decreases, and the opposite could be true for other sources.

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ITL Program: *Complex Systems*

Methods that Streamline Search for Failure Scenarios in Large-Scale Systems

Fern Y. Hunt
Christopher Dabrowski (NIST ITL)
Katherine Morrison (University of Nebraska–Lincoln)

In recent years, the advent of large scale distributed systems such as computing grids and commercial cloud systems has made mass computing services available to populations of users on demand. These systems are dynamic, heterogeneous and—due to the interactions of its 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 key system parameters can lead to large differences in performance (see references in [1]). By large scale simulation we mean the discrete event simulations that simulate in detail the various stages encountered by an individual task over time. While the large scale simulations used in these studies are more practical than operational testbeds, computational expense rises dramatically with model size and number of tasks. This is a critical roadblock to extensive investigation of dynamical behavior in large scale systems.

To address this situation, we introduced in earlier work [2], 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 system parameters [2].

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 and were obtained with a substantial reduction in computational cost (hours vs. weeks of simulation). 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 ultimately control of these systems will depend on the ability to discover these scenarios quickly and perhaps in real time. This is the motivation of the work that is described in [1,2,3].

One approach is based on analyzing the underlying graph of the Markov chain. By efficiently identifying cut sets in the graph, system failure scenarios can be very rapidly identified. The method has been applied to grid systems, cloud systems, and to large energy systems as well. A second approach is based on the spectral properties of the Markov Chain. Our contribution here is two-fold. First, in the context of grid computing, we have developed a method for quickly generating the time course of a key variable of the system, the proportion of tasks completed for arbitrary system parameters,

Second, we can measure 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 simulation; however, the correlation is not perfect. In a small number of cases, elevated values occurred without any sign of a decrease in system performance.

Nevertheless, we believe that these methodologies offer a promising first step toward the development ofscalable and efficient complex system monitoring and prediction. The use of Markov chains to approximate the dynamics of a variety of systems is well known. However, most of the applications involve the use of time homogeneous systems that reach steady state. The grid and cloud computing systems discussed here 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 that appeared this year are [2] and [3]. The graph theory method is described in [1].

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ITL Program: *Complex Systems*

Advanced Combinatorial Testing for Systems

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Combinatorial testing (CT) is an approach to detect combinatorial interaction faults, which may cause a complex software based system to fail when some particular values of certain parameters combine with some particular values of certain other parameters. Many critical system failures in recent times have been traced to interaction faults in the underlying software. CT is a versatile and broadly applicable methodology for ensuring trustworthy software in business, industrial, medical, scientific, and transport systems. It is often difficult or impossible to characterize all possible combinatorial interactions, let alone test them. CT is based on the observation that most interaction faults involve only a few parameters. Several studies of actual faults show that most faults involved a single parameter, a smaller proportion of faults resulted from interactions between values of two parameters, and progressively fewer interaction faults involved 3, 4, 5, and 6 parameters. So far, a fault involving more than six parameters has not been seen. Most combinatorial testing has until recently been limited to pair-wise (2-way) testing in which all interactions involving two parameters are detected. A reason is that efficient test methods and tools to detect higher order interaction faults have so far not been available. The goal of this project is to advance the technology from pair-wise to higher order (strength) testing and to demonstrate successful applications of high strength combinatorial testing.

We have made major revisions to the NIST/UTA software tool ACTS for generating high strength combinatorial test suites with constraints, distributed 950 copies of ACTS worldwide, and approved redistribution within companies. We estimate the number of users of ACTS tool to be several thousand. We continue to provide consulting services upon request. Major ACTS Improvements made in 2011:

1. *Base-Choice Testing.* This feature allows the user to designate a base value for each parameter.
2. *Test Output Specification.* This feature allows the user to specify the expected output behavior for each test case.
3. *New Interface for Constraint Support.* This new interface allows the user to free-type constraints. Significant validation support has also been added in the backend to ensure the legality of constraints before users enter into the test generation stage.
4. *API Interface.* This feature allows the user to access the features of ACTS in a programmatic manner.
5. *Various Other Improvements.* Better error handling, additional export formats, better mixed-strength support, and various GUI enhancements.

Third-party Constraints Solver. We are investigating the use of a third-party constraints solver in ACTS for better and wider constraints support. We have developed a tool to determine "combinatorial coverage metrics" of candidate test suites. We have learned that determination of combinatorial coverage of existing test suites is in great demand. We have integrated the ACTS tool for software assurance into NIST's Access Control Policy Test tool.

Combinatorial Methods for Event Sequence Testing. Our discussions with the US Air Force 46-th Test Squadron led to understanding of a new testing problem: testing sequences of events. Some software testing problems involve sequences of events. For example, an embedded system may accept multiple sensor inputs and generate output to several communication links and effectors such as machine controls. It is important to test combinations of connected components, but also to test the order in which they could be connected. We have developed a methodology and prototype tools for generating test suites for sequential combinatorial testing. A paper submitted to IEEE Transactions on Software Engineering is being revised.

Combinatorial-Based Prioritization for User-Session-Based Testing of Web. Our team has developed a prototype research tool labeled CPUT (Combinatorial-based Prioritization for User-session-based Testing) to convert web logs into user-session-based test suites so that testers can examine how users actually interact with the web application. Further, given that user-session-based test suites grow when many users access the system and testers may not be able to use all of the user-session-based test cases, CPUT provides functionality to prioritize these test suites by empirically verified criteria. CPUT allows researchers and practitioners to consider user-session-based testing and the respective prioritization techniques for their own projects. A paper on the tool was presented at the VERIFY/ATI Conference, September 26, 2011, in Arlington, VA [5].

Publications. Our NIST Special Publication "Practical Combinatorial Testing," issued in October 2010 [1], has been downloaded over 1,300 times already. We are planning to convert this publication into a published book. Our paper "A Combinatorial Approach to Detecting Buffer Overflow Vulnerabilities" [4] appeared in *Proceedings of the 41st IEEE International Conference on Dependable Systems and Networks*, Hong Kong, China, June 27-30, 2011. Our paper "A Survey of Binary Covering Arrays" [3] appeared in the *Electronic Journal of Combinatorics*.

We have presented seminars and workshops on CT at a number of conferences. We are collaborating with the NASA Independent Verification and Validation (IV&V) facility to investigate use of CT in verification and validation of NASA software systems.

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Security Risk Analysis of Enterprise Networks Using Attack Graphs

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http://csrc.nist.gov/groups/SNS/security-risk-analysis-enterprise-networks/index.html

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. Vulnerabilities are regularly discovered in software applications which are exploited to stage cyber attacks. Currently, management of security risk of an enterprise network is more an art than a science. System administrators operate by instinct and experience rather than relying on objective metrics to guide and justify decision making. The objective of this 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 now 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 allow users, vendors and researchers to evaluate methodologies and products for network security in a coherent and consistent manner.

We have approached the challenge of network security analysis by capturing vulnerability interdependencies and measuring security in the exact way that real attackers penetrate the network. Our methodology for security risk analysis is based on the model of attack graphs. We analyze all attack paths through a network, providing a probabilistic metric of the overall system risk. Through this metric, we analyze trade-offs between security costs and security benefits.

In FY 2011, we worked on validating our approach for realistic networks. We used a real network as a test bed to demonstrate the utility of this approach. The results of our experiments were published in the Proceedings of the 2011 World Congress in Computer Science, Special Track on Security and Mission Assurance [1]. We have also documented our methodology and the results of our experiments in a NIST report [2]. In FY 2012 we plan to integrate our techniques into existing attack graph-based security tools.

This work was performed in the NIST Computer Security Division with partial support from ACMD.

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Mobile Sensor Networks

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Mobile sensor networks (MSN) are envisioned to offer a novel set of applications in detecting, monitoring and tracking people, targets or events in pervasive computing environments [1]. Locations of sensors in a MSN affect both their ability to acquire information on the intended target(s) and event(s) as well as their ability to communicate this information to the intended recipient(s). The information acquisition needs, which require proximity to the target(s), often compete with the communication needs, which require proximity to the recipient(s) of the sensor information. Inherent traits of MSN such as lack of centralized control, variety of performance criteria, operational uncertainties, and possibilities of MSN topology change and sensor trapping in suboptimal locations make MSN optimization an exceedingly challenging problem.

Our previous publications [2]-[5] have proposed aligning sensor mobility with the overall MSN goals by assuming that (a) sensing and communication are optimized much faster than sensors relocation and (b) sensor relocations are governed by cost/benefit analysis, where the "cost" of sensor battery energy expenditure for sensor relocation is weighted against projected performance gains due to new sensor locations. This approach is superior to sensor mobility control based on *phenomenologically* defined potential fields and the corresponding virtual forces [6], since dissipation of the non-renewable sensor battery energy, asymmetric virtual forces due to asymmetric wireless channels, and abrupt changes in the optimal MSN topology with sensor relocation are inconsistent with the existence of a global potential field.

Practicality of the framework proposed in [2]-[5] depends on overcoming numerous challenges with the (inherently) distributed nature of MSN being the most critical. An intelligent sensor may have direct knowledge of its current life expectancy, as determined by its battery energy level and depletion rate affected by the surrounding terrain, as well as sensor infor-

mation acquisition and transmission capabilities. However, a sensor typically has no direct knowledge of the effect of its relocation on the rest of the MSN.

Our paper [7] suggests that the class of distributed subgradient projection algorithms (DSPA) [8]-[9] has potential for addressing major challenges of controlled sensor mobility in MSN. Subgradient-based iterations allow for dynamic network topology optimization. Projection of the algorithm iterations onto the set of feasible sensor locations ensures sensor information acquisition and communication needs. Most importantly, communication overhead reducing techniques allow for addressing the inherently distributed nature of MSN. While more conventional pricing-based algorithms effectively reduce the communication overhead in some particular situations, recently emerged consensus-based algorithms have low communication overhead in a more general setting.

Consensus-based algorithms differ in their approach to achieving consensus. In the first type, each agent maintains and iterates its own sequence, and consensus is achieved by communicating this sequence to the neighboring nodes, which incorporate neighbors' sequences into their own sequences through averaging. In the second type, all agents update a single sequence, and consensus is achieved by passing the sequence instances to each other. In [7] we concentrated on the first type, since updating and passing instances of a single sequence by agents to each other exposes algorithms to the risk of manipulation by malicious agents, while averaging with judiciously chosen weights can mitigate this risk.

A major difficulty with controlling sensor relocation is the possibility of sensor trapping in suboptimal locations (e.g. in non-flat terrain) due to typical non-convexity of the performance criterion [8]. A possible approach to overcoming this difficulty is allowing occasional random sensor relocations to escape the potential traps in the spirit of a simulated annealing optimization algorithm. One of the advantages of this approach [7] is in its ability to incorporate such random moves in a distributed way. Initial simulation results indicate the viability of this approach for prolonging the MSN life-span.

Future research should evaluate the pros and cons of different versions of distributed subgradient algorithms with respect to controlled sensor relocation, and provide guidelines for selection of the algorithm step size and free parameters involved in the "consensus" step. These selections affect the trade-off between the algorithm convergence rate and communication overhead. The ability to avoid traps on non-flat terrains is critical for practical implementation of controlled sensor relocation. Paper [7] suggests the possibility of achieving this by combining distributed subgradient projection and simulated annealing algorithms.

More studies are needed to realize this possibility and compare algorithm [7] with more conventional optimization algorithms [9]. Paper [9] is concerned with target monitoring using a network of collaborative mobile sensors. The objective is to compute (online) the desired sensing and communication radii of sensors as well as their location at each time instant, such that a set of prescribed specifications are met. 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, and a procedure is presented to solve it. Simulation results demonstrate the effectiveness of the proposed techniques.

In papers [10]-[11] various sensor deployment strategies are studied for effective coverage in wireless sensor networks. In [10], efficient sensor deployment algorithms are proposed to improve the coverage area in the target field. The proposed algorithms calculate the position of the sensors iteratively based on the existing coverage holes in the target field. The multiplicatively weighted Voronoi diagram (MW-Voronoi diagram) is used to discover the coverage holes corresponding to different sensors with different sensing ranges. Under the proposed procedures, the sensors move in such a way that the coverage holes in the target field are reduced. Simulation results are provided to demonstrate the effectiveness of the deployment schemes proposed in this paper.

The algorithms proposed in [11] consider the distances of each sensor and the points inside its corresponding Voronoi polygon from the edges or vertices of the polygon. Four algorithms are developed: Maxmin-vertex, Maxmin-edge, Minmax-edge, and a hybrid algorithm. The main characteristic of these algorithms is the iterative movement of the sensors. Once each destination is computed, the new local coverage area of the corresponding sensor is compared with its previous local coverage area. If the new local coverage area is larger than the preceding one, the sensor moves to the new destination; otherwise, it remains in its current location. If, on the other hand, the local coverage area by none of the sensors is improved by a certain threshold, then the iteration stops. This termination condition guarantees that the proposed algorithms arrive at the desired destination (with a prescribed accuracy which is set by the above-mentioned threshold level) in finite time. The proposed strategies outperform the existing ones in the case when some sensors are required to move toward sharp vertices.

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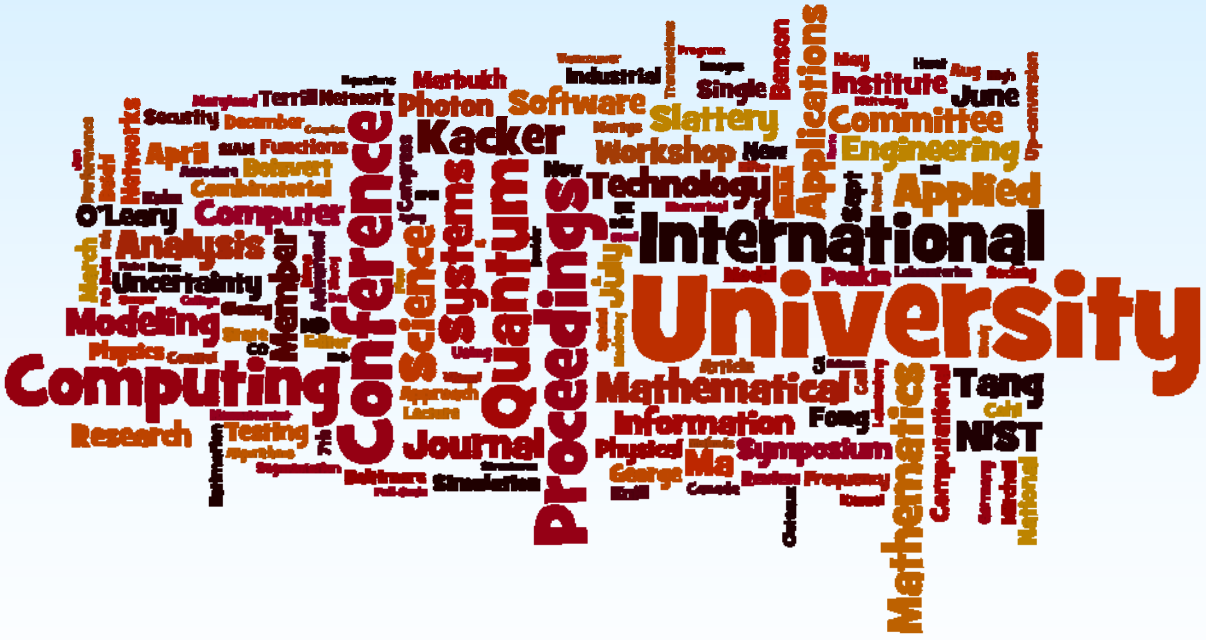
ITL Program: *Pervasive Information Systems*

Part IV

Activity Data



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17. A. Kearsley, T. Gruendling, C. Barner-Kowollik, W. Wallace, and C. Guttman, Automated Data Processing of and Quantification in Polymer Mass Spectrometry, *Mass Spectrometry in Polymer Chemistry*.

18. R. Kessel and R. Kacker, Monte Carlo Simulations Using Parallel Computing and a Client-server Model, in *Proceedings of the Conference on Advanced Mathematical and Computational Tools in Metrology and Testing (AMCTM 2011)*.

19. R. Kessel and R. Kacker, Improved Adaptive Procedure to Determine the Necessary Number of Monte Carlo Trials to Achieve the Required Numerical Tolerance, in *Proceedings of the Conference on Advanced Mathematical and Computational Tools in Metrology and Testing (AMCTM 2011)*.

20. Z. H. Levine, B. R. Galloway, A. P. Peskin, C. P. Heussel, and J. J. Chen, Theoretical Limits of RECIST in Medical CT as a Measure of Tumor Volume, *Medical Physics*.

21. Y.-K. Liu, Universal low-rank matrix recovery from Pauli measurements, in *Proceedings of Neural Information Processing Systems (NIPS)*.

22. L. Ma, O. Slattery, and X. Tang, Single Photon Frequency Up-conversion and Its Applications in Quantum Information Systems, in *Proceedings of the Single Photon Workshop 2011*.

23. V. Marbukh, Robust Cross-Layer Network Optimization for Diverse QoS Requirements: Work in Progress, *World Congress on Engineering 2011*.

24. V. Marbukh, K. Sayrafian, H. Mahboubi, A. Momeni, Ahmadreza, A. Aghdam, An Efficient Target Monitoring Scheme with Controlled Node Mobility for Sensor Networks, *IEEE Transactions on Control Systems Technology*.

25. V. Marbukh, From TCP Effective Bandwidth to Internet Performance, *IFIP Performance 2011*.

26. N. S. Martys, C. F. Ferraris, W. L. George, S. G. Satterfield, M. T. Olano, Computational Based Study of Suspension Flow in a Vane Rheometer, *83rd Annual Meeting of the Society of Rheology*.

27. 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*.

28. 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*.

29. O. Slattery, L. Ma, and X. Tang, Towards Narrow Linewidth Non-degenerate Correlated Photon Pairs, in *Proceedings of the Single Photon Workshop 2011*.
30. J. C. Wu, A. Martin, C. Greenberg, and R. Kacker, Measurement Uncertainties in Speaker Recognition Evaluation, *SPIE Defense, Security, and Sensing Conference*, Orlando, FL, April 25-29, 2011.
31. Y. Zhang, E. Knill, and S. Glancy, Asymptotically Optimal Confidences for Rejecting Local Realism, *Physical Review A*.

In Review

1. B. K. Alpert, W. B. Doriese, J. W. Fowler, and J. N. Ullom, Predicted Energy Resolution of a Running-Sum Algorithm for Microcalorimeters.
2. J. D. Benson, C. C. Chicone, and J. K. Critser, Analytical Optimal Controls for the State Constrained Addition and Removal of Cryoprotective Agents.
3. 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.
4. G. W. Bryant, N. Malkova, J. Sims, M. Zielinski, W. Jaskolski, and J. Aizpurua, Controlling the Optics of Quantum Dots with Nanomechanical Strain.
5. 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.
6. B. Cloteaux, Graphical Approximations of Degree Sequences.
7. H. S. Cohl and E. G. Kalnins, Fundamental Solution of the Laplacian in the Hyperboloid Model of Hyperbolic Geometry.
8. H. S. Cohl, On a Generalization of the Generating Function for Gegenbauer Polynomials.
9. D. L. Cotrell, P. A. Lott, and G. B. McFadden, Boundary Slip Effects on the Stability of Spiral Poiseuille Flow.
10. W. B. Doriese, B. K. Alpert, J. W. Fowler, G. C. Hilton, A. S. Hojem, K. D. Irwin, C. D. Reintsema, D. R. Schmidt, G. M. Stiehl, D. S. Swetz, J. N. Ullom, and L. R. Vale, Optimization of the Detector-bias Circuit for a TES X-ray Microcalorimeter in a Multiplexed Array.
11. T. Gerrits, M. Stevens, B. Baek, B. Calkins, A. Lita, S. Glancy, E. Knill, S.W. Nam, R. Mirin, R. Hadfield, R. Bennink, W. Grice, S. Dorenbos, T. Zijlstra, T. Klapwijk, and V. Zwiller, Generation and Characterization of Degenerate, Factorizable, Pulsed Squeezed Light at Telecom Wavelengths from pp-KTP.
12. 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.
13. D. Harris, F. Sullivan, and I. Beichl, Fast Sequential Importance Sampling to Estimate the Graph Reliability Polynomial.
14. R. D. Johnson, III, K. K. Irikura, R. Kacker, and R. Kessel, Response to Comments by Pernot and Cailliez.
15. N. Martys, M. Khalil, W. George, D. Looten, and P. Hebraud, Stress Propagation in Colloidal Suspensions under Shear.
16. M. Mullan and E. Knill, Improving Quantum Clocks via Semidefinite Programming.
17. D. P. O'Leary and B. W. Rust, Variable Projection for Nonlinear Least Squares Problems.
18. J. S. Pelc, L. Ma, C. R. Phillips, Q. Zhang, C. Langrock, O. Slattery, X. Tang, M. M. Fejer, Long-wavelength-pumped Upconversion Single-photon Detector at 1550 nm: Performance and Noise Analysis.
19. M. T. Rakher, L. Ma, M. Davanço, O. Slattery, X. Tang, and K. Srinivasan, Spectral and Temporal Manipulation of Single Photons from a Quantum Dot by Pulsed Frequency Upconversion.
20. S. Ressler, Integrating jQuery with 3D Descriptive Markup of X3DOM.
21. W. Wang, Y. Lei, S. Sampath, R. Kacker, R. Kuhn, and J. Lawrence, A Combinatorial Approach to Building Navigation Graphs for Dynamic Web Applications.
22. D. F. Williams, M. T. Ghasr, B. Alpert, Z. Shen, A. Arsenovic, R. M. Weikle II, and R. Zoughi, Improved Calculation of the Reflection Coefficient of Radiating Rectangular-Waveguide Test Ports.
23. J. C. Wu, A. F. Martin, and R. N. Kacker, Studies of Nonparametric Two-Sample Bootstrap in ROC Analysis on Large Datasets.

Sponsored Research

24. Milan Bradonjić and Iraj Saniee, Bootstrap Percolation on Random Geometric Graphs. *[Alcatel-Lucent Bell Labs]*
25. Iraj Saniee and Gabriel H. Tucci, Scaling of Congestion in Small World Networks. *[Alcatel-Lucent Bell Labs]*
26. Alonso Silva and Gabriel H. Tucci, On the Spectral Characteristics of Ad-hoc Networks and their Mobility Properties. *[Alcatel-Lucent Bell Labs]*

Presentations

Invited Talks

1. I. Beichl, Sequential Importance Sampling for Network Problems, Bell Laboratories, Murray Hill, NJ, April 26, 2011.
2. J. D. Benson, Modeling and Optimization in Cryobiology, Northwestern University, Evanston, IL, Nov. 8, 2010.
3. R. Bohn, NIST Cloud Computing Program, Texas Advanced Computing Center (TACC), Austin, TX, May 4, 2011.
4. R. Bohn, Cloud Computing Standards, *Business of Cloud Computing Forum,* San Diego, CA, June 15, 2011.
5. R. Boisvert, Mathematics at NIST, Keene State College, Keene, NH, Apr. 15, 2011.
6. J. W. Bullard, N. S. Martys, J.-L. Traore, W. L. George, and S. G. Satterfield, Computer Models as Guides through Material Design Space, *International Congress on the Chemistry of Cement,* Madrid, Spain, July 3-8.
7. T. Burns, On Modeling the Constitutive Response of Carbon Steel for High-speed Machining Simulations, *Plasticity 2011*, Vallarta, Mexico, January 3-8, 2011.
8. H. S. Cohl, The Fourier and Gegenbauer Analysis of Fundamental Solutions for the Polyharmonic Equation on Riemannian Spaces of Constant Curvature, Gdansk University of Technology, Gdansk, Poland, August 16, 2011.
9. A. Dienstfrey, Dynamic Calibration for Dynamic Metrology, *6th Dynamic Metrology Workshop*, Gothenburg, Sweden, June 20-22, 2011.
10. J. Fong, A Risk-Informed Approach to Asset Management of Aging Engineered Systems, University of Wisconsin, Madison, WI, Oct. 13, 2010.
11. J. Fong, A Risk-Informed Approach to Asset Management of Aging Engineered Systems, University of Houston, Houston, TX, Oct. 19, 2010.
12. J. Fong, A Risk-Informed Approach to Asset Management of Aging Engineered Systems, Pacific Northwest National Laboratory, Richland, WA, Nov. 15, 2010.
13. J. Fong, A New Approach to Verification and Validation (V&V) of Codes using a Statistical Plug-in for Uncertainty Estimation, *U.S. Department of Energy Training Workshop on Waste Processing Models: Material Properties Standards and Software Verification and Validation*, Germantown, MD, Nov. 30, 2010.
14. J. Fong, Uncertainty Estimation and Engineering Reliability, *Composites Workshop IV*, Stanford University, Palo Alto, CA, Jan. 24, 2011
15. J. Fong, Uncertainty Estimation and Failure Prediction of Full-Scale Structures using a Multi-Scale Approach and a Public-Domain Statistical Software Package named DATAPLOT, University of South Carolina, Columbia, SC, April 29, 2011.
16. J. Fong, Uncertainty Estimation and Failure Prediction of Full-Scale Structures using a Multi-Scale Approach, University of California, Irvine, CA, May 20, 2011.
17. J. Fong, Uncertainty Estimation and Failure Prediction of Full-Scale Structures using a Multi-Scale Approach, *First Global Forum on Structural Longevity*, Orlando, FL, July 26, 2011.
18. J. Fong, Uncertainty Estimation and Engineering Reliability, Department of Aeronautics and Astronautics, *Composites Workshop IV*, Stanford University, Stanford, CA, July 29, 2011.
19. J. Fong, Design of Experiments and Modern Statistics for Life Estimation and Extension of Full-Scale New and Aging Structures, Universidade Estadual de Campinas (State University of Campinas), Sao Paulo, Brazil, Sept. 22, 2011.
20. J. Fong, Design of Experiments and Modern Statistics for Life Estimation and Extension of Full-Scale New and Aging Structures, Embraer, Sao Paulo, Brazil, Sept. 23, 2011.
21. J. Fong, NIST Research on Materials Science and Verification and Validation, Department of Mechanical Engineering, Universidade Federal Do Rio Grande Do Norte (Federal University of Rio Grande do Norte), Natal, Brazil, Sept. 26, 2011.
22. J. Fong, Design of Experiments and Modern Statistics for Life Estimation and Extension of Full-Scale New and Aging Structures, Universidade

Federal Do Rio Grande Do Norte (Federal University of Rio Grande do Norte), Natal, Brazil, Sept. 26, 2011.

23. J. Fong, Uncertainty Estimation and Failure Prediction of Full-Scale Structures using a Multi-Scale Approach and a Public-Domain Statistical Software Package named DATAPLOT, Universidade Federal Do Rio Grande Do Norte (Federal University of Rio Grande do Norte), Natal, Brazil, Sept. 27, 2011.
24. W. L. George, N. S. Martys, and J. E. Terrill, Computational Rheology for Cement and Concrete*, Workshop on High-Performance Computing for Industry*, Rensselaer Polytechnic Institute, Troy, NY, Oct. 26, 2011.
25. W. L. George, N. S. Martys, S. G. Satterfield, M. Olano, and J. E. Terrill, Simulating the Flow of Dense Suspensions, Argonne National Laboratory exhibit, *SC Conference*, Seattle WA, Nov. 15, 2011.
26. S. Jordan, Quantum Algorithms for Quantum Field Theories, Laboratory for Physical Science, College Park, MD, May 5, 2011.
27. S. Jordan, Quantum Algorithms for Quantum Field Theories, Institute for Quantum Computation Waterloo, Canada, August 2, 2011.
28. S. Jordan, Quantum Algorithms for Quantum Field Theories, *Schloss Dagstuhl Seminar on Quantum Cryptanalysis*, Wadern, Germany, Sept. 23, 2011.
29. R. Kacker, High Strength Combinatorial Testing for Software and other Applications, Infosys Technologies Ltd., Bangalore, India, December 29, 2010.
30. R. Kacker, Evolution of Modern Approaches to Express Uncertainty in Measurement, Indian Institute of Technology-Madras, Chennai, India, Jan. 7, 2011.
31. R. Kacker, High Strength Combinatorial Testing for Software and other Applications, Indian Institute of Technology-Madras, Chennai, India, Jan. 10, 2011.
32. R. Kacker, Advanced Combinatorial Testing for Software and Systems, Technical University of Berlin, Berlin, Germany, June 27, 2011.
33. R. Kacker, Advanced Combinatorial Testing for Software and Systems, Fraunhofer Institute for Open Communication Systems, Berlin, Germany, June 28, 2011.
34. R. Kuhn and R. Kacker, Combinatorial Testing for Software and Systems, Institute for Defense Analyses, Arlington VA, Feb. 25, 2011.
35. R. Kuhn and R. Kacker, Advanced Combinatorial Testing for Software and Systems, Army Test and Evaluation Command, March 30, 2011.
36. R. Kuhn and R. Kacker, Advanced Combinatorial Testing for Software and Systems, Institute for Defense Analyses, April 6, 2011.
37. R. Kuhn and R. Kacker, Advanced Combinatorial Testing for Software and Systems, Johns Hopkins University Applied Physics Lab, April 27, 2011.
38. L. Ma, O. Slattery, and X. Tang, Single Photon Frequency Up-conversion and Its Applications in Quantum Information Systems, *Single Photon Workshop* 2011, PTB Braunschweig, Germany, June 27- 30, 2011.
39. L. Ma, O. Slattery, and X. Tang, Pulsed-pumped Up-conversion Single Photon Detectors and Their Applications, *SPIE Optics and Photonics*, San Diego, CA, Aug. 21-25, 2011.
40. W. F. Mitchell, Comparison of *hp*-Adaptive Finite Element Strategies, University of Maryland, College Park, MD, Sept. 20, 2011.
41. D. P. O'Leary, Mathematics and Computer Science in Words and Images, Women in Science Forum, Towson University, March 2011.
42. D. P. O'Leary, Where am I? Position from Incomplete Distance Information, Purdue University, April 2011.
43. D. P. O'Leary, Mathematics in Words and Images, Norbert Wiener Lecture, Tufts University, March 30, 2011.
44. D. P. O'Leary, Uncertainty Quantification for Ill-Posed Problems, Norbert Wiener Lecture, Tufts University, March 31, 2011.
45. D. P. O'Leary, Where am I? Position from Incomplete Distance Information, Norbert Wiener Lecture, Tufts University, April 1, 2011.
46. D. P. O'Leary, Where am I? Position from Incomplete Distance Information, Householder Symposium, Lake Tahoe, CA, June 2011.
47. D. P. O'Leary, Confidence in Image Reconstruction, IMA Workshop on Large-scale Inverse Problems and Quantification of Uncertainty, Minneapolis, MN, June 2011.
48. A. Reid, Object-Oriented Finite Element Materials Modeling at NIST, *3rd International Conference on Computational Methods in Engineering and Science (FEMTEC 2011)*, Stateline, NV, May 9, 2011.

49. S. Ressler, 3D Computer Graphics and the World Wide Web, Florida International University, Miami, FL, Feb. 4, 2011.

50. B. Saunders, Numerical Grid Generation Applied to Interactive Complex Function Visualization in the NIST Digital Library of Mathematical Functions, George Mason University, March 25, 2011.

51. O. Slattery, L. Ma, and X. Tang, Towards Narrow Linewidth Non-degenerate Correlated Photon Pairs, *Single Photon Workshop* 2011, PTB Braunschweig, Germany, June 27- 30, 2011.

52. O. Slattery, L. Ma, and X. Tang, Toward a Narrow Linewidth Non-degenerate Source of Correlated Photon Pairs, *SPIE Optics and Photonics*, San Diego, CA, Aug. 21-25, 2011.

53. X. Tang, L. Ma, and O. Slattery, Photon Frequency Conversion and Its Applications, *20th International Laser Physics Workshop*, Sarajevo, July 11-15, 2011.

54. X. Tang, Single Photon Frequency Up-conversion and Its Applications in Quantum Information Research at NIST, University of Maryland Baltimore County, Sept. 21, 2011.

Conference Presentations

1. B. K. Alpert, Improved High Rate Pulse Processing Algorithms for Microcalorimeters, *14th International Workshop on Low Temperature Detectors*, Heidelberg, Germany, Aug. 2, 2011.

2. T. Burns, On Modeling the Peak Temperature on the Tool-chip Interface during High-speed Machining of AISI 1045 steel, *Eighth International Conference on High-Speed Machining*, Metz, France, Dec. 8-10, 2010.

3. T. Burns, Effect on Flow Stress of a Rapid Phase Transition in AISI 1045 Steel, *ASME 2011 International Manufacturing Science and Engineering Conference*, Corvallis, OR, June 13-17, 2011.

4. A. Carasso, Effective Non-Uniqueness in Linear and Nonlinear Backward Parabolic Equations, *7th International Congress on Industrial and Applied Mathematics*, Vancouver, Canada, July 20, 2011.

5. J. Chalfoun, A. Dima, A. P. Peskin, J. Elliott, and J. J. Filliben, A Human Inspired Local Ratio-Based Algorithm for Edge Detection in Fluorescent Cell Images, *6th International Symposium on Visual Computing*, Las Vegas, NV, Nov. 29 – Dec. 1, 2010.

6. B. Cloteaux, Modeling Affiliations in Networks, *Winter Simulation Conference*, Baltimore, MD, Dec. 8, 2010.

7. B. Cloteaux, Counting the Leaves of Trees, *SECGTC 2011*, Boca Raton, FL, March 9, 2011.

8. H. S. Cohl, Gegenbauer and Fourier Series for Fundamental Solutions of the Laplacian and Powers in Hyperspherical Coordinate Systems Which Parametrize Points in Euclidean and Hyperbolic Space, *February Fourier Talks*, University of Maryland, Feb. 17-18, 2011.

9. H. S. Cohl and E.G. Kalnins, Radial Fundamental Solutions of Laplace's Equation on Riemannian Spaces of Constant Curvature, *Special Functions and Orthogonal Polynomials of Lie Groups and Their Applications*, Decin, Czech Republic, Aug. 14-20, 2011.

10. H. S. Cohl, Logarithmic Fourier Series for a Fundamental Solution of the Polyharmonic Equation in Even-dimensional Euclidean Space, *11th International Symposium on Orthogonal Polynomials, Special Functions and Applications*, Leganes, Spain, Aug. 29-Sept. 2, 2011.

11. G. Dogan, Fast Optimization Method for the Chan-Vese Model in Image Segmentation, *SIAM Conference on Computational Science and Engineering*, Reno, NV, February 28 – March 4, 2011.

12. G. Dogan, Simultaneous Segmentation and Reconstruction of Piecewise Constant Functions, *7th International Congress on Industrial and Applied Mathematics*, Vancouver, BC, Canada, July 19, 2011.

13. M. Donahue, Parallelizing a Micromagnetic Program for Multi-processor Non-uniform Memory Access Computers, *Conference on Magnetism and Magnetic Materials*, Atlanta, GA, Nov. 15, 2010.

14. S. Glancy, E. Knill, M. Girard, F. Mallet, and T. Gerrits, Lessons and Innovations in Maximum Likelihood Quantum State Tomography, *Southwest Quantum Information and Technology Workshop*, Boulder, CO, Feb. 17, 2011.

15. T. M. Hanna, E. Tiesinga, W. F. Mitchell and P. S. Julienne, Bound States of Interacting Polar Molecules in an Optical Lattice, *42nd Annual DAMOP Meeting*, Atlanta, GA, June 14.

16. F. Y. Hunt, A Mathematical Model of a Computer Protocol, Class of 1902 Lecture, *Oxtoby Centennial Conference*, Bryn Mawr College, Bryn Mawr PA., October 2, 2010.

17. F. Y. Hunt, Spectral Based Methods That Streamline the Search for Failure Scenarios in Large-

Scale Distributed Systems, *19th IASTED International Conference on Applied Simulation and Modeling*, Crete, Greece, June 22-24, 2011.

18. F. Y. Hunt, A Mathematical Model of Joint Congestion Control and Routing in Multisource Networks, *IEEE International Conference on Control Applications*, Denver, CO, Sept. 29, 2011.
19. R. Kacker and J. Lawrence, Trapezoidal and Curvilinear Trapezoidal Distributions which arise in Metrology, *International Conference on Mathematical Sciences*, St. Thomas College, Pala, Kerala, India, January 3-5, 2011.
20. R. Kacker, R. Kuhn, E. Miranda and J. Aldrich, Evolution of Advanced Combinatorial Testing for Software and Systems from Design of Experiments, Carnegie Mellon University Master of Software Engineering Professional Program, Pittsburgh, PA, June 7, 2011.
21. A. Kearsley and J. Benson, Time-Optimal Boundary Control of a State Constrained Bio-mass Transport Systems, *7th International Congress on Industrial and Applied Mathematics*, Vancouver, Canada, July 21, 2011.
22. R. Kessel, R. Kacker, and K.D. Sommer, Uncertainty Budgeting for Range Calibration, *Measurement Systems and Process Improvement*, National Physical Laboratories, Teddington, UK, April 19-20, 2010.
23. Y.-K. Liu, Quantum Property Testing for Bounded-Degree Graphs, *Workshop on Approximation, Randomization, and Combinatorial Optimization (APPROX-RANDOM)*, Princeton, NJ, Aug. 17-19, 2011.
24. D. Lozier, The NIST Handbook of Mathematical Functions: What Do Statisticians Want?, *International Conference on Mathematical Sciences*, St. Thomas College, Pala, Kerala, India, Jan. 3-5, 2011.
25. V. Marbukh, Robust Cross-layer Network Optimization for Diverse QoS Requirements: Work in Progress, *International Conference of Applied and Engineering Mathematics*, London, UK, July 6-8, 2011.
26. V. Marbukh, Towards Modeling Effect of Multiscale Stochastic Dynamics on Flow-Level Queuing Performance in the Internet, *7th International Congress on Industrial and Applied Mathematics*, Vancouver, Canada, July 18-22, 2011.
27. V. Marbukh, Cooperative Sensor Relocation in a Mobile Sensor Network by Distributed Subgradient Algorithm, *Fifth International Conference on Sensor Technologies and Applications* (SENSOCOMM 2011), Nice, France, Aug. 21-26, 2011.
28. W. F. Mitchell and M. A. McClain, Performance of *hp*-Adaptive Finite Element Methods, *SIAM Conference on Computational Science and Engineering*, Reno, NV, Feb. 27 – Mar. 4, 2011.
29. W. F. Mitchell and M. A. McClain, Comparison of *hp*-Adaptive Finite Element Strategies, Workshop on Multiresolution and Adaptivity in Numerical PDEs, *Foundations of Computational Mathematics*, Budapest, Hungary, July 13, 2011.
30. W. F. Mitchell and M. A. McClain, Comparison of *hp*-Adaptive Finite Element Strategies, *24th Chemnitz FEM Symposium*, Holzhau, Germany, Sept. 29, 2011.
31. E. Moseman, Computing Network Reliability Coefficients, *42nd Southeastern International Conference on Combinatorics, Graph Theory, and Computing*, Boca Raton, FL, March 7-11, 2011.
32. M. Mullan, Improving Quantum Clocks via Semidefinite Programming, *Southwest Quantum Information and Technology Workshop*, Boulder, CO, Feb. 17-20, 2011.
33. A. Peskin, A. Dima, J. Chalfoun, and J. Elliot, Predicting Segmentation Accuracy for Biological Cell Images, *Bioimage Informatics 2010*, Pittsburg, PA, Sept. 17-19, 2010.
34. A. Peskin, A. Dima, Modeling Clinical Tumors to Create Reference Data for Tumor Volume Measurement, *6th International Symposium on Visual Computing*, Las Vegas, NV, Nov. 29 – Dec. 1, 2010.
35. A. Peskin, A. Dima, J. Calfoun, J. Elliott, Predicting Segmentation Accuracy for Biological Cell Images, *6th International Symposium on Visual Computing*, Las Vegas, NV, Nov. 29 – Dec. 1, 2010.
36. A. P. Peskin, D. J. Hoeppner, and C. H. Stuelten, Segmentation and Cell Tracking of Breast Cancer Cells, *7th International Symposium on Visual Computing*, Las Vegas, NV, Sept. 26-28, 2011.
37. B. Rust and D. P. O'Leary, The Variable Projection Method – Back to the Roots, *7th International Congress on Industrial and Applied Mathematics*, Vancouver, Canada, July 19, 2011.
38. B. Saunders, The NIST Digital Library of Mathematical Functions: A New Resource for Mathematical and Physical Scientists, *Fall Meeting of the MD-DC-VA Section of the Mathematics Association of America*, George Mason University, Fairfax, VA, Nov. 6, 2010.

39. W.-B. Yang, K. Sayrafian-Pour, J. Hagedorn, J. Terrill, K. Y. Yazdandoost, A. Taparugssanagorn, M. Hamalainen, and J. Iinatti, Impact of an Aortic Valve Implant on Body Surface UWB Propagation: A Preliminary Study, *Fifth International Symposium on Medical Information and Communication Technology (ISMICT)*, March 27-31, 2011.
40. Y. Zhang, E. Knill, and S. Glancy, Computable and Asymptotically Optimal Lower Bounds on Confidence for Rejecting Local Realism Given Experimental Data, *Southwest Quantum Information and Technology Workshop*, Boulder, CO, Feb. 17, 2011.

Web Services

1. Digital Library of Mathematical Functions[18]: a repository of information on the special functions of applied mathematics.
2. Guide to Available Mathematical Functions[19]: a virtual repository of mathematical software components.
3. Matrix Market[20]: a repository of matrices for testing of algorithms and software for numerical linear algebra.
4. SciMark[21]: a benchmark for scientific computing in Java.

Software Released[22]

1. NGraph++[23]: a small, C++ class library for the analysis of network graphs. Version 3.9. – *R. Pozo*
2. Equiv++[24]: a template C++ package for mathematical equivalence. New. – *R. Pozo*
3. LaTeXML[25]: a LaTeX to XML converter. Multiple releases. – *B. Miller*
4. OOF2[26]: Object Oriented Finite Elements, modeling of materials with complex microstructures. Version 2.1.5 – *S. Langer*
5. PHAML[27]: Parallel Hierarchical Adaptive Multi-Level, general purpose software for 2D elliptic partial differential equations. Version 1.9.1 – *W. Mitchell*
6. Tcl packages Itcl 3.4.1 and 4.0b7, and Thread 2.6.7 – *D. Porter*
7. Tcl/Tk[28]: Tool Command Language and Toolkit. Version 8.5.10 and 8.6b2 – *D. Porter*
8. PCrawler[29]: suite of Python modules to build network graphs by crawling the World Wide Web. Version 3.0 – *R. Pozo*
9. Local Realism Analysis Engine:[30] standardizes the quantification and comparison of experiments that demonstrate failure of local realism with quantum states and measurements – *Y. Zhang, M. Knill, and S. Glancy*

Conferences, Minisymposia, Lecture Series, Shortcourses

MCSD Seminar Series

1. J. Benson (NIST), Modeling and Optimization in Cryobiology, Oct. 19, 2010.
2. I. Saniee (Bell Laboratories), The Large Scale Curvature of Networks and its Implications for Network Management and Security, Nov. 9, 2010.
3. M. Cromer, Jr. (University of Delaware), Modeling and Simulation of a Complex Fluid: Wormlike Micellar Solutions, Nov. 30, 2010.
4. E. Fried (McGill University), Dynamical Equations for the Contact Line During the Evaporation or Condensation of a Sessile Drop, Jan. 21, 2011.
5. T. Mohan (INFOSYS Technologies), Leveraging Cloud for Software Assurance, March 18, 2011.
6. J. Rinzel (New York University), Dynamics of Perceptual Bistability, March 29, 2011.
7. A. Sidi (Israel Institute of Technology), Extrapolation Methods for Vector Sequences with Applications to Large-Scale Problems, April 5, 2011.
8. A. Nurse (NIST and the University of Maryland), A Model of Force Generation in a Three Dimensional Toroidal Cluster of Cells, April 19, 2011.

[18] http://dlmf.nist.gov/
[19] http://gams.nist.gov/
[20] http://math.nist.gov/matrixmarket/
[21] http://math.nist.gov/scimark/
[22] In cases where multiple versions have been released during the year we only list the last.
[23] http://math.nist.gov/~RPozo/ngraph/index.html
[24] http://math.nist.gov/~RPozo/ngraph/ngraph_toolkit_index.html
[25] http://dlmf.nist.gov/LaTeXML
[26] http://www.nist.gov/mml/ctcms/oof/
[27] http://math.nist.gov/phaml/
[28] http://tcl.sourceforge.net/
[29] http://math.nist.gov/~RPozo/ngraph/webcrawler.html
[30] http://arxiv.org/abs/1108.2468

9. A. Gray (Georgia Institute of Technology), Machine Learning on Massive Data Sets, April 26, 2011.
10. M. Mascagni, (Florida State University), The Scalable Parallel Random Number Generators (SPRNG) Library and Modern Computer Architectures, May 4, 2011.
11. P. Johansson (National Cancer Institute, National Institutes of Health), A Genomic Portrait of Tumor Progression Using Second Generation Sequencing, May 24, 2011.
12. A. Gueye (NIST and the University of Maryland), Game Theoretic Modeling, Analysis, and Mitigation of Security Risks, June 7, 2011.
13. B. Amidan (Pacific Northwest National Laboratories), Typical Patterns, Atypical Events, and Uncertainty in Complex Systems, Sept. 15, 2011.

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, Chair, Organizing Committee, International Conference on Special Functions in the 21st Century: Theory and Applications, Washington, DC, April 6-8, 2011.

External Events Organization

1. R. Boisvert and E. Knill, Members, Program Committee, Workshop: From Quantum Information and Complexity to Post Quantum Information Security, Joint Quantum Institute, College Park, MD, Oct. 27-29, 2010.
2. B. Cloteaux, Session Organizer, Winter Simulation Conference, Dec. 11-14, 2011.
3. G. Dogan, Co-Organizer, Minisymposium on Scientific Computing in Image Processing, *SIAM Conference on Computational Science and Engineering*, Reno, NV, February 28 – March 4, 2011.
4. J. Fong, Symposium Organizer, PVP Conference, Baltimore, MD, July 17-22, 2011.
5. F. Hunt, Member, Organizing Committee, 5th Infinite Possibilities Conference, University of Maryland, Baltimore County, March 2012.
6. A. Kearsley and J. Benson, Co-Organizers, Minisymposium on Mathematical Modeling and Optimization in Cryobiology, *7th International Congress on Industrial and Applied Mathematics*, Vancouver, Canada, July 18-22, 2011.
7. V. Marbukh, Co-Organizer, NIST-Bell Labs Workshop on Large-Scale Geometry of Networks, Bell Labs, Murray Hill, NJ, April 26, 2011.
8. G. McFadden, Co-Organizer, Memorial Conference for Paul R. Garabedian, New York University, December, 2010.
9. W. Mitchell, Member, Scientific Committee, International Conference of Numerical Analysis and Applied Mathematics (ICNAAM 2011), Halkidiki, Greece, Sept. 19-25, 2011.
10. D. P. O'Leary, Member, Organizing Committee, SIAM Conference on Applied Linear Algebra (LA12), Valencia, Spain, June 18-22, 2012.
11. Y. Parker and J. Terrill, Co-Organizers, NIST booth, SC10, the 2010 International Conference for High Performance Computing, Networking, Storage and Analysis, New Orleans, LA, Nov. 13-19, 2010.
12. Y. Parker and J. Terrill, Co-Organizers, NIST booth, SC11, the 2011 International Conference for High Performance Computing, Networking, Storage and Analysis, Seattle, WA, Nov. 13-19, 2010.
13. B. Rust and K. Mullen, Co-Organizers, Minisymposium on Recent Advances in Separable Nonlinear Least Squares, *7th International Congress on Industrial and Applied Mathematics*, Vancouver, Canada, July 18-22, 2011.

Other Professional Activities

Internal

1. I. Beichl, NIST Research Advisory Committee.
2. R. Boisvert, NIST Scientific Computing Steering Group.
3. R. Boisvert, ITL Diversity Committee.
4. S. Glancy, NIST Boulder SURF Committee.
5. W. Mitchell, ITL Awards Committee.
6. A. O'Gallagher, ITL Diversity Committee.
7. A. Peskin, Boulder Research Advisory Council.
8. S. Ressler, NIST Lobby Display Advisory Council.

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, Computing Research Repository (CoRR) preprint service.[31]
5. A. Dienstfrey, Associate Editor, *International Journal of Uncertainty Quantification*.
6. D. Lozier, Associate Editor, *Journal of Numerical Analysis, Industrial and Applied Mathematics*.
7. G. McFadden, Associate Editor, *Journal of Crystal Growth*.
8. G. McFadden, Associate Editor, *Interfaces and Free Boundaries*.
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, *Computing in Science & Engineering*.
14. D. P. O'Leary, Department Editor, Your Homework Assignment, *Computing in Science & Engineering*.
15. R. Pozo, Associate Editor, *ACM Transactions on Mathematical Software*.

Boards and Committees

1. I. Beichl, Member, IEEE Electronic Products and Services Subcommittee.
2. J. Benson, Member, Planning Committee, Society for Cryobiology.
3. R. Bohn, Member, Cloud Computing Scoping Subcommittee, President's National Security Telecommunications Advisory Committee (NSTAC).
4. R. Bohn. Co-chair, Faster Administration of Science and Technology Education and Research (FASTER) Community of Practice, Networking and Information Technology R&D (NITRD) Program.
5. R. Boisvert, Chair, International Federation for Information Processing's (IFIP) Working Group 2.5 (Numerical Software).
6. R. Boisvert, Co-chair, Publication Board, Association for Computing Machinery (ACM).
7. R. Boisvert, Member, Program Review Committee, Center for Computing Sciences, Institute for Defense Analysis.
8. R. Boisvert, Member, External Review Committee, Computer Science Department, George Washington University.
9. R. Boisvert, Member, Fast Track Action Committee on Modeling and Simulation, Office of Science and Technology Policy.
10. E. Knill, Member, Technical Advisory Panel, Quantum Computer Science Program, IARPA.
11. D. Lozier, Secretary, Activity Group on Orthogonal Polynomials and Special Functions, Society for Industrial and Applied Mathematics (SIAM). Term ended December 2010.
12. D. Lozier, Member, Steering Committee, Painleve Project.
13. D. P. O'Leary, Chair, Committee on Committees, Association for Women in Mathematics.
14. D. P. O'Leary, Member, Oversight Committee, Gene Golub SIAM Summer Schools, 2010-2014.

[31] http://www.arXiv.org/

15. B. Miller, Member, Math Working Group, WWW Consortium.
16. D. Porter, Member, Tcl Core Team.
17. S. Ressler, Member, Declarative 3D for the Web Architecture Community Group[32].
18. B. Saunders, Member, MAA Committee on Business, Industry, and Government Mathematics.
19. J. Terrill, Member, Federal High End Computing Implementation Task Force.
20. J. Terrill, Member, High End Computing Research and Development, and Infrastructure Interagency Working Groups, Networking and Information Technology R&D (NITRD) Program.

Reviewing

Division staff members referee manuscripts for a wide variety of journals including *ACM Transactions on Mathematical Software, Acta Materialia, The Annals of Applied Statistics, BIT, Computational Statistics and Data Analysis*, *Inverse Problems, Computer Physics Communications, European Physical Journal D: Atomic, Molecular, Optical and Plasma Physics, IEEE Transactions on Information Theory, IEEE Transactions on Instrumentation & Measurement*, *IEEE Transactions on Magnetics, International Journal of Uncertainty, Journal of Applied Physics*, *Journal of Computational and Applied Mathematics*, *Journal of Computational Physics, Journal of Fluid Mechanics*, *Journal of Mathematical Analysis and Applications, Mathematical Reviews*, *Mathematics of Computation, Nature, New Journal of Physics*, *Numerical Mathematics, Numerical Methods for Partial Differential Equations, Optical Engineering, Optics Communications, Physical Review*, *Physical Review A, Physical Review B, Physical Review Letters*, *Quantum Information and Computation, SIAM Journal on Matrix Analysis and Applications*, *SIAM Journal of Scientific Computing*.

In addition, Division staff members served as reviewers for a variety of conferences, including 2011 Winter Simulation Conference, QIP (Quantum Information Processing) 2011, 22nd Annual IEEE International Symposium on Personal, Indoor and Mobile Radio Communications 2011 (PIMRC'11), Symposium on the Foundations of Computer Science (FOCS).

ACMD staff also reviewed proposals for the following agencies/competitions during FY 2011: DOE, Netherlands Organization for Scientific Research, NSF.

[32] http://www.w3.org/community/declarative3d/

External Contacts

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

Industrial Labs

21st Century Medicine
Agilent
Alcatel-Lucent Bell Laboratories
Balance R&D (Australia)
CD-adapco
CLO Virtual Fashion, Inc.
Enig Associates
ExactData, LLC
Google Summer of Code
Gradient Effects
IBM Entity Analytics
Intel
The Jackson Laboratory
Northrop Grumman
Orbital Sciences Corporation
Palantir Technologies
Plastic Technologies Inc.
Synarch
Tech-X Corporation
Volume Graphics GmbH

Government/Non-profit Organizations

Aberdeen Proving Grounds
Army Research Lab
Association for Computing Machinery
Association for Women in Mathematics
Cambridge Healthtech Institute
CNRS/ESPCI, France
DARPA
Department of Energy
Ecole Nationale Superieure de Chimie de Rennes (France)
Environmental Protection Agency
IARPA
IDA Center for Computing Sciences
IEEE Computer Society
Institute for Mathematics and Its Applications
Lawrence Livermore National Laboratory
Leibniz Inst. for Solid State and Matls. Res. (Germany)
Library of Congress
Maui High Performance Computing Center
NASA Goddard Space Flight Center
NASA Langley Research Center
National Institutes of Health
National Physical Laboratory (UK)
Nuclear Decommissioning Authority (UK)
Nuclear Regulatory Commission
National Security Agency

Oak Ridge National Laboratory
Office of Science and Technology Policy
Pacific Northwest National Laboratory
Royal Melbourne Institute of Technology
Sandia National Laboratories
Santa Fe Institute
Society for Industrial and Applied Mathematics
Swedish Metrology Institute
Theiss Research
World Wide Web Consortium

Universities

Boston University
California Institute of Technology
Cambridge University
College of William and Mary
Concordia University (Canada)
Cornell University
Delft University of Technology (The Netherlands)
Durham University (UK)
Frederick University (Cyprus)
George Mason University
George Washington University
Georgia Institute of Technology
Heriot-Watt University (UK)
Indiana University
Jacobs University, Bremen (Germany)
Johns Hopkins University
King Abdullah Univ. of Sci. and Tech. (Saudi Arabia)
Linkoping University (Sweden)
Murdoch University (Australia)
New York University
Oregon State University
Polish Academy of Science
Renssalear Polytechnic University
State University of New York at Binghamton
University of Antwerp (Belgium)
University of Birmingham (UK)
University of California, Davis
University of Colorado
University of Connecticut
University of Delaware
University of Luxembourg
University of Maryland
University of Maryland Baltimore County
University of Minnesota
University of Nebraska -- Lincoln
University of Nevada, Reno
University of New Mexico
University of Oulu (Finland)
University of Pittsburgh
University of Sheffield (UK)
University of South Africa
University of Texas at Arlington
University of Technology (The Netherlands)
University of Utah
University of Virginia
University of Wisconsin
Virginia Tech

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 special appointments. The following list reflects all appointments held during any portion of the reporting period. (*) Denotes staff at NIST Boulder.

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
*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

NIST-ARRA Postdoctoral Fellows
Asha Nurse, Ph.D. (Mechanical Engineering), Brown University, 2011
Ismet Sahin, Ph.D. (Electrical and Computer Engineering), University of Pittsburgh, 2006

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

P. Aaron Lott, Ph.D. / Lawrence Livermore National Laboratory
Bruce Murray, Ph.D. / SUNY Binghamton
Asha Nurse, Ph.D. / University of Maryland (ARRA Postdoctoral Fellow)
Sita Ramamurti, Ph.D. / Trinity Washington University
Ismet Sahin, Ph.D. / University of Maryland (ARRA Senior Fellow)
Christoph Witzgall, Ph.D., *NIST Scientist Emeritus*

Mathematical Software Group

Daniel Lozier, *Leader,* Ph.D. (Applied Mathematics), University of Maryland, 1979
Javier Bernal, Ph.D. (Mathematics), Catholic University, 1980
Valerie Coffman, Ph.D. (Physics), Cornell University, 2006
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
Howard Cohl, Ph.D. (Mathematics), University of Auckland, 2010

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)
Gunay Dogan, Ph.D. / Theiss Research
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
Stephen Jordan, Ph.D. (Physics), Massachussetts Institute of Technology, 2008
*Emanuel Knill, *NIST Fellow,* Ph.D. (Math), University of Colorado at Boulder, 1991
Yi-Kai Liu, Ph.D. (Computer Science), University of California, San Diego, 2007
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
Elizabeth Moseman, Ph.D. (Mathematics), Dartmouth College, 2007
James Shook, Ph.D. (Mathematics), University of Mississippi, 2010

NIST-ARRA Postdoctoral Fellows
Assane Gueye, Ph.D. (Computer Science), University of California, Berkeley, 2011

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)
Stephen Bullock, Ph.D. / IDA Center for Computing Sciences
Robert Carpenter / NIST (retired)
*Bryan Eastin, PhD. / Northrup Grumman
Paulina Kuo, Ph.D. / Joint Quantum Institute, University of Maryland
Francis Sullivan, Ph.D. / IDA Center for Computing Sciences

Students (Name, Degree / Home Institution)
Amada Crawford / University of Colorado
Mark Girard / Trinity University
*Michael Mullan / University of Colorado at Boulder
*Adam Meier / University of Colorado at Boulder
*Yanbao Zhang / University of Colorado at Boulder

High Performance Computing and Visualization Group

Judith Terrill, Leader, Ph.D. (Information Technology), George Mason University, 1998
Yolanda Parker, Office Manager
William George, Ph.D. (Computer/Computational Science), Clemson University, 1995
Terence Griffin, B.S. (Mathematics), St. Mary's College of Maryland, 1987
John Hagedorn, M.S. (Mathematics), Rutgers University, 1980
John Kelso, M.S. (Computer Science), George Washington University, 1984
*Adele Peskin, Ph.D. (Chemical Engineering), University of Colorado at Boulder, 1985
Sandy Ressler, M.F.A. (Visual Arts), Rutgers University, 1980
Steven Satterfield, M.S. (Computer Science), North Carolina State University, 1975
James Sims, Ph.D. (Chemical Physics), Indiana University, 1969

Faculty Appointees
Marc Olano / University of Maryland Baltimore County

Guest Researchers (Name, Degree / Home Institution)
Dennis Backhaus / Fachhochschule Wiesbaden (Germany)
Styvens Belloge / ISIMA, Campus de Clermont-Ferrand, France
Pradeep Gaddam / Core Projects and Technologies PVT LTD, India
Stanley Hagstrom, Ph.D. / Indiana University
Marlene Hildebrand / Polytech Nice-Sophia, France
Clement Rey / ISIMA, Campus de Clermont-Ferrand, France
Jean-Loup Traore / Université Blaise Pascal Clermont Ferrand II, France

Students (Name / Home Institution)
Luis Catacora / Montgomery Blair High School
Matthew Du / Thomas Wootton High School
William Hess / Purdue University
Kevin Rawlings / Carnegie Mellon University
Anshu Rustagi / University of Illinois
Poorva Singal / Franklin W. Olin College of Engineering
Becky Song / Richard Montgomery High School

Glossary of Acronyms

A&S	Abramowitz & Stegun (NBS *Handbook of Mathematical Functions*, 1964)
ACM	Association for Computing Machinery
ACMD	NIST/ITL Applied and Computational Mathematics Division
ACTS	Advanced Combinatorial Test Suites (software)
AI	artificial intelligence
AISI	American Iron and Steele Institute
AMS	American Mathematical Society
ANSI	American National Standards Institute
ANTD	ITL Advanced Networking Technology Division
APD	avalanche photo diode (photon detector)
APS	American Physical Society
ARRA	American Recovery and Reinvestment Act
arXiv	preprint archive housed at Cornell University (http://arxiv.org/)
ASME	American Society of Mechanical Engineers
BAN	body area network
BLAS	Basic Linear Algebra Subprograms
CAIDA	Cooperative Association for Internet Data Analysis
Caltech	Califonial Institute of Technology
CGM	conjugate gradient method
CI	configuration interaction
CMOS	complementary metal-oxide semiconductor
CNRS	Centre National de la Recherche Scientifique
CNST	NIST Center for Nanoscale Science and Technology
CODATA	Committee on Data for Science and Technology
CPA	cryoprotective agent
CPU	central processing unit
CPUT	combinatorial-based prioritization for user-session-based testing
CT	combinatorial testing
CT	computed tomography
CVSS	Common Vulnerability Scoring System
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
DOC	Department of Commerce
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
DPD	dissipative particle dynamics
DSPA	distributed subgradient projection algorithm
EL	NIST Engineering Laboratory
EPG	error probability per gate
ESPCI	École Supérieure de Physique et Chimie Industrielles de la Ville de Paris
FASTER	Faster Administration of Science and Technology Education and Research
FDA	Food and Drug Administration
FDS	Fire Dynamics Simulator
FEM	finite element method
FFT	fast Fourier transform
FY	fiscal year
F90gl	Fortran 90 interface to OpenGL graphics standard
GAMS	Guide to Available Mathematical Software
GCN	Government Computer News
GPS	generalized processor sharing
GUI	graphical user interface

HEC	high-end computing
HIM	helium ion microscope
HTML	hypertext markup language
Hy-CI	Hylleraas-Configuration Interaction technique
IAS	information assurance and security
IDA	Institute for Defense Analysis
IEEE	Institute of Electronics and Electrical Engineers
IFIP	International Federation for Information Processing
IMS	Innovations in Measurement Science
INCITE	Innovative and Novel Computational Impact on Theory and Experiment (DOE Program)
ISIMA	Institut Supérieur d'Informatique, de Modélisation et de leurs Applications (France)
IT	information technology
ITL	NIST Information Technology Laboratory
JILA	joint NIST-University of Colorado physics research institute
JAMA	Java Matrix package (software)
LaTeX	a math-oriented text processing system
LaTeXML	LaTeX to MathML translator
MAA	Mathematical Association of America
MALDI/TOF	matrix assisted laser desorption/ionization time-of-flight (mass spectrometer)
MathML	Mathematical Modeling Language (W3C standard)
MGI	Materials Genome Initiative
MIT	Massachusetts Institute of Technology
MKM	mathematical knowledge management
MLE	maximum likelihood estimation
MML	NIST Material Measurement Laboratory
MPI	Message Passing Interface
MRAM	magneto-resistive random access memory
MRI	magnetic resonance imaging
MSN	mobile sensor network
muMAG	Micromagnetic Activity Group
NASA	National Aeronautics and Space Administration
NBS	National Bureau of Standards
Ngraph	Network Graph (software)
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
NL	The Netherlands
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)
OSPF	open shortest path first
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
PTB	Physikalisch-Technische Bundesanstalt
QD	quantum dot
QDPD	quarternion-based dissipative particle dynamics
QIS	quantum information science

QKD	quantum key distribution
QoS	quality of service
R&D	research and development
REGEN	software for modeling of cryocoolers
RIP	restricted isometry property
RF	radio frequency
SBIR	Small Business Innovative Research
SEM	scanning electron microscope
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
SRM	standard reference material
STEP	NIST Student Temporary Employment Program
SUNY	State University of New York
SURF	Student Undergraduate Research Fellowship
SVT	singular value thresholding
TES	transition-edge sensor
TNT	Template Numerical Toolkit (software)
TPM	transition probability matrix
TSA	Transportation Security Administration
TV	total variation
UCSD	University of California at San Diego
UK	United Kingdom
UMBC	University of Maryland Baltimore County
URL	universal resource locator
UTA	University of Texas at Arlington
UWB	ultra-wide band
VRML	virtual reality modeling language
W3C	World Wide Web Consortium
WebGL	Web-based Graphics Library
X3D	Extensible 3D
X3DOM	an open-source frameword for integrating X3D and HTML5
XML	Extensible Markup Language