Part III

Project Summaries

Mathematical Modeling of Mechanical Systems and Processes

OOF: Object-Oriented Finite Elements

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

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

See feature article, page 37.

Modeling Fluid Flow in Materials Processing

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

See feature article, page 39.

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

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

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

While there are many Kolsky bars in laboratories at universities, U.S. Government (DOD and DOE) facilities, and defense contractors, the NIST Kolsky bar has the unique capability of pulse-heating a test specimen from room temperature to a significant percentage of its melting temperature in tens of milliseconds, which mimics the rapid heating that occurs in thin cutting regions during a high-speed machining operation. The development of this capability was initially funded in large part by the NIST Intramural ATP Program, and new and/or improved instrumentation for this work continues to be supported by MEL, MSEL, and ITL.

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

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

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

Modeling Time Delay Effects for Machine Tool Chatter Control

David E. Gilsinn
Sita Ramamurti (Trinity University)

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

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

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

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

References

[1] D. E. Gilsinn and F. A. Potra, "Integral Operators and Delay Differential Equations" *Journal of Integral Equations and Applications* **18** (3), Fall 2006, pp. 297-336.
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Numerical Modeling of Deformation and Diffusion

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

through a combination of modeling, analysis, and computations.

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

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

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

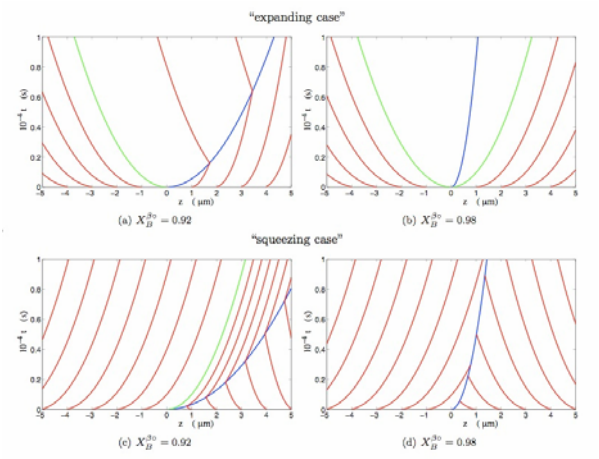

Figure 26. *Trajectories of Kirkendall markers on the original interface (green) and at other initial positions (red). The blue trajectory is the position of the two-phase boundary.*

References

[1] W. J. Boettinger, G. B. McFadden, S. R. Coriell and R. F. Sekerka, J. A. Warren, Lateral Deformation of Diffusion Couples, *Acta Materialia* 53 (2005) 1996-2008.

[2] J. A. Dantzig, W. J. Boettinger, J. A. Warren, G. B. McFadden, S. R. Coriell and R. F. Sekerka, Numerical Modeling of Deformation and Diffusion, *Metallurgical and Materials Transactions* 37A (2006), pp. 2701-2714.

Modeling of Contact Dynamics of Silicon Cantilevers

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

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

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

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

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

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

Characterization of Microdomain Lattice Defects in Block Copolymer Thin Films

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

Complex System Failure Analysis

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This research began in February 2004 when ITL and BFRL were awarded a 5-year joint Innovations in Measurement Science project. The objective was to create the scientific basis for building failure investigation procedures that (a) will allow NIST to accomplish its mission under the National Construction Safety Team Act (P.L. 107-231, Oct. 1, 2002), and (b) will be likely, over time, to be applicable for failure analysis and uncertainty determination of a broad range of complex physical, chemical, biological, and engineered systems of interest throughout NIST and beyond.

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

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

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

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

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

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

View of the NIST campus in Gaithersburg, Maryland.

Mathematical Modeling of Electromagnetic Systems

Optical Coherence Tomography for Biomedical Imaging

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See feature article, page 27.

Micromagnetic Modeling

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

Michael Donahue and Donald Porter in MCSD have developed a widely used public domain computer code for doing computational micromagnetics, the Object-Oriented Micromagnetic Modeling Framework (OOMMF). OOMMF serves as an open, well-documented environment in which algorithms can be evaluated on benchmark problems. OOMMF also provides a fully functional micromagnetic modeling system, handling both two and three-dimensional problems, with sophisticated extensible input and output mechanisms. OOMMF has become an invaluable tool in the magnetics research community. In fiscal year 2006 alone, the software was downloaded more than 2,700 times, and use of OOMMF was acknowledged in 85 peer-reviewed journal articles.

OOMMF is part of a larger activity, the Micromagnetic Modeling Activity Group (μMAG), formed to address fundamental issues in micromagnetic modeling through two activities: the development of public domain reference software, and the definition and dissemination of standard problems for testing modeling software. MCSD staff members are involved in development of the standard problem suite as well. There are currently four standard problems in the suite, testing both static and dynamic magnetization properties. Additional standard problems dealing with issues such as thermal effects and the effect of representation errors when boundaries do not align with the computation grid are in development.

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

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

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

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

Time-Domain Algorithms for Computational Electromagnetics

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Acoustic and electromagnetic waves, including radiation and scattering phenomena, are increasingly modeled using time-domain computational methods, due to their flexibility in handling wide-band signals, material

inhomogeneities, and nonlinearities. For many applications, particularly those arising at NIST, the accuracy of the computed models is essential. Existing methods, however, typically permit only limited control over accuracy; high accuracy generally cannot be achieved for reasonable computational cost.

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

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

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

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

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

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

Modeling of Optical Spectra

Peter Ketcham
Eric Shirley (NIST PL)

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

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

Mathematical Modeling for Chemical and Biological Applications

An Accurate Model for Measuring Fluorophore Photodegredation Dynamics

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See feature article, page 41.

Optical Coherence Tomography for Biomedical Imaging

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Paul Williams (NIST MSEL)

See feature article, page 27.

Simulation of Bioregulatory Networks Involved in Cell Cycle Control

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Mirit Aladjem (National Institutes of Health)
Kurt Kohn (National Institutes of Health)

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

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

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

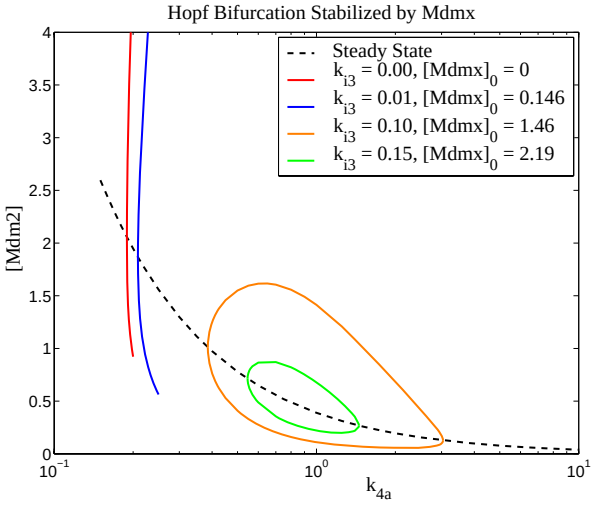

Figure 27. *Bifurcation diagram showing the concentration of Mdm2 in the system as a function of the kinetic parameter k4a.*

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

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

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

Virtual Measurements in Quantum Chemistry

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

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

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

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

References

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Systems Identification and Parameter Estimation for Environmental Applications

Bert W. Rust

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

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

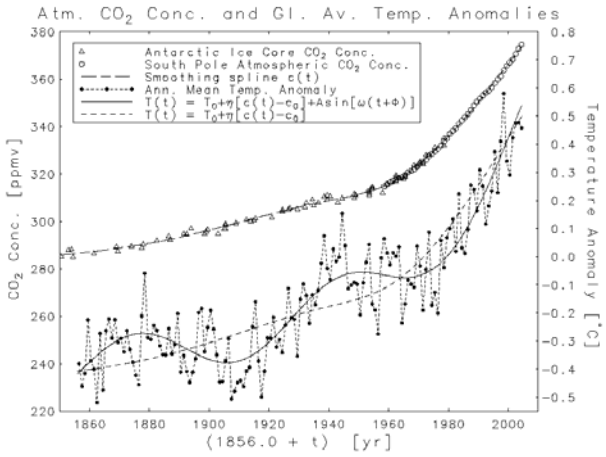

Figure 28. *Atmospheric CO_2 concentration and global average temperature anomalies.*

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

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

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

Improvement in Modeling Cryocoolers

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

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

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

Mathematics of Metrology

Numerical Optimization of Complex Instrumentation

Anthony J. Kearsley
William E. Wallace

See feature article, page 43.

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

Alfred S. Carasso

See feature article, page 23.

Nonlinear Image Analysis and the Mumford-Shah Functional

Alfred S. Carasso

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

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

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

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

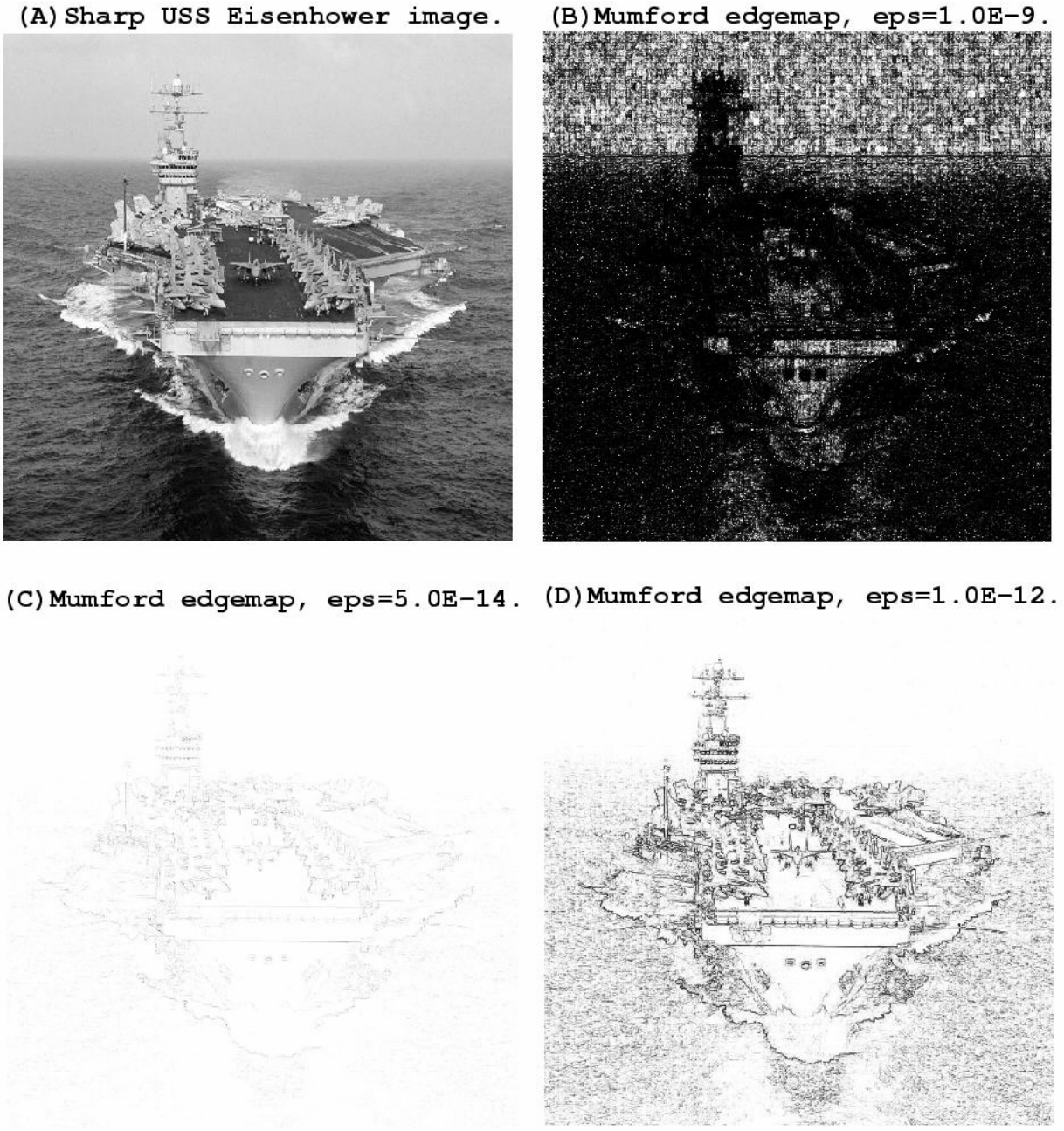

Figure 29. *Correct choice of regularization parameter ε is crucial for obtaining useful Mumford-Shah edge map. (A) Sharp image. (B) Computed edgemap with ε too large smears edges and obscures result. (C) Too small a value for ε makes edgemap almost invisible. (D) Correct value* $\varepsilon = 1 \times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

Sparse Representations in High Dimensional Geometry

Bradley Alpert
Yu Chen (New York University)

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

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

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

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

Applications in Security

Isabel Beichl

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

This work was supported by the National Security Agency.

Automated Combinatorial Testing for Software (ACTS)

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

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

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

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

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

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

Quantum Information

Benchmarks for Quantum Computing with Ion Traps

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

See feature article, page 35.

Quantum Computing Theory

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

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

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

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

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

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This work is supported in part by the Defense Advanced Research Projects Agency (DARPA) and the NIST Innovations in Measurement Science Program.

Optical Quantum Metrology and Quantum Computing

Scott Glancy
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Tracy Clement (NIST EEEL)
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Marty Stevens (NIST EEEL)

Members of the MCSD are contributing to the development of an experimental research program in optical quantum metrology and quantum computing. This project is developing expertise in the preparation, manipulation, and measurement of exotic quantum states of light, such as entangled states of N photons and Schrödinger Cat states. The entanglement properties of

these states can be exploited for high precision interferometry, quantum communication, and quantum computation. All of these technologies require the ability to control and measure very delicate and sensitive quantum states, and they will all benefit from this project. Quantum optical technology is potentially useful in medical imaging because of the improved depth resolution possible using entangled photons. Nanotechnology could benefit from methods for focusing light to better than the diffraction limit. This project will significantly expand NIST capabilities in quantum optical metrology, enabling us to expand our position as the global leader in measurement and enabling technology as applied to quantum optics.

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

Our plans include experiments to prepare and characterize squeezed light, Schrödinger cat states, entangled states of a few photons, and the demonstration of the violation of Bell's inequalities. Many of these elements will be integrated in a versatile optics testbed capable of performing these and many other quantum optics tasks.

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

High Performance Computing

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

James Sims
Stanley Hagstrom (University of Indiana)

See feature article, page 33.

Computation of Nano-structures and Nano-optics

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

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

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

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

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

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

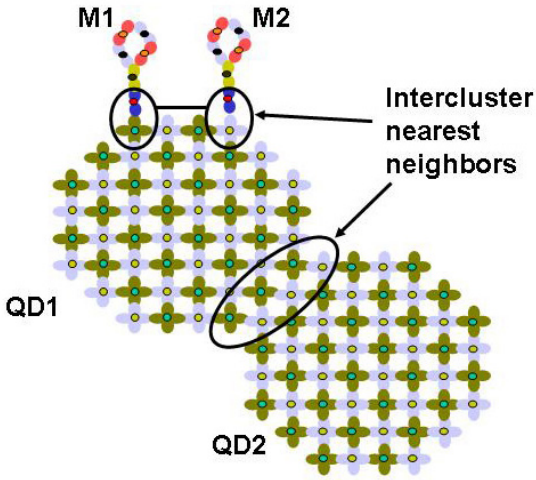

Figure 30. *Illustration of intercluster nearest neighbors in a nanosystem with four subsystems: two quantum dots (QD1 and QD2) and two conjugating molecules (M1 and M2).*

Computational Modeling of the Flow of Concrete

William George
Julien Lancien
Christine McKay
Nicos Martys (NIST BFRL)

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

Understanding the flow properties of complex fluids like suspensions (e.g., colloids, ceramic slurries and concrete) is of technological importance but presents a significant theoretical challenge. The computational modeling of such systems is challenging because of the difficulty in tracking boundaries between different fluid/fluid and fluid/solid phases. We are utilizing a new computational method called dissipative particle

dynamics (DPD), which has several advantages over traditional methods while naturally accommodating necessary boundary conditions. In DPD, the interparticle interactions are chosen to allow for large time steps so that physical behavior on time scales many orders of magnitude greater than that possible with molecular dynamics may be studied. Our algorithm (QDPD) is a modification of DPD, which uses a velocity Verlet method to update the positions of both free particles and the solid inclusions. In addition, the rigid body motion is determined from the quaternion-based scheme of Omelayan (hence the Q in QDPD). Parallelization of the algorithm is important in order to adequately model size distributions, and to have enough resolution to avoid finite size effects.

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

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

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

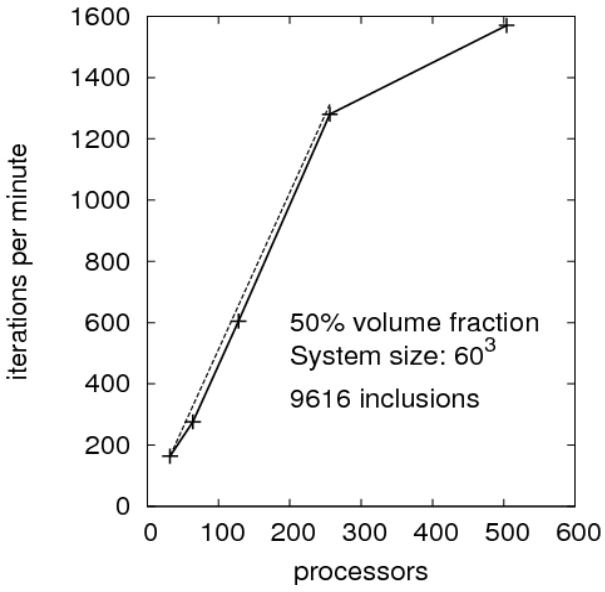

Figure 31. *Scaling of new parallel algorithm on Columbia system. Above ~300 processors, the algorithm could handle a larger system size.*

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

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

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

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

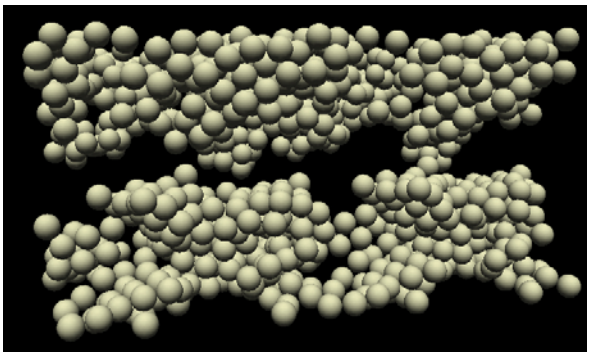

Figure 32. *Separation of particles into two clusters in above image is a confinement effect due to small system size*

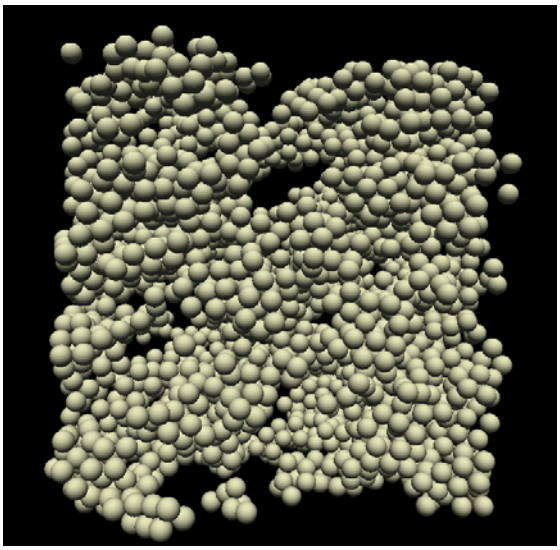

Figure 33. *The above image shows same system when the resolution is increased. The resolution is adequate to allow the natural clusters to form.*

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

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

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

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

Screen Saver Science

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

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

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

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

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

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

Interoperable MPI

William George
John Hagedorn
Judith Terrill

http://impi.nist.gov

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

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

We consulted with Dr. Yutaka Ishikawa, Professor of Computer Science at the University of Tokyo, and Dr. Motohiko Matsuda of the Grid Technology Research Center of Japan's National Institute of Advanced Industrial Science and Technology (AIST). These researchers are involved in the development of GridMPI, a Grid-focused version of MPI that currently uses IMPI (see http://www.gridmpi.org/gridmpi-0-6/). In cooperation with the OpenMPI developers, they have agreed to implement and contribute full IMPI support for the OpenMPI library. As a result, Drs. Ishikawa and Matsuda attended an OpenMPI developer's workshop in April 2006, sponsored by Cisco Systems, to help finalize the addition of IMPI to the OpenMPI library distribution. Small changes were proposed to the OpenMPI library to better support the IMPI protocols as implemented by Drs. Ishikawa and Matsuda. After these changes were made to OpenMPI, the testing of IMPI support within OpenMPI revealed minor additions to the OpenMPI library are needed to complete the IMPI support within OpenMPI. These are in progress.

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

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

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

High Performance Visualization

Measurement and Analysis of Tissue Engineering Scaffolds

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

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

See feature article, page 29.

Virtual Measurement and Analysis Laboratory

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

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

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

Measurement Science in the Virtual World

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

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

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

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

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

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

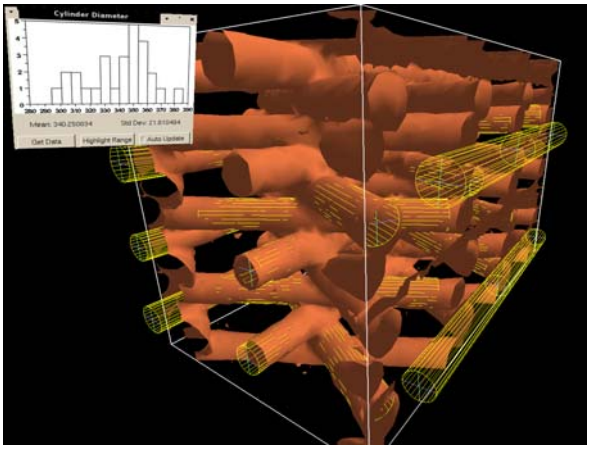

Figure 34. *Cylinder measurement and analysis tool used on rendered objects derived from measured data taken from a tissue engineering scaffold.*

Virtual Cement and Concrete Testing Laboratory

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

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

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

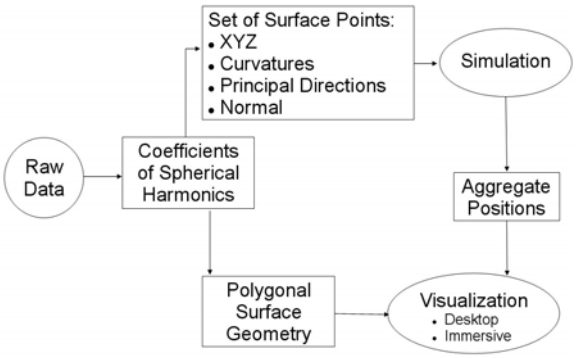

Figure 35. *The raw data from the X-ray tomography of each aggregate is processed into one data set that is input into the simulation, and another data set that is used in the visualization.*

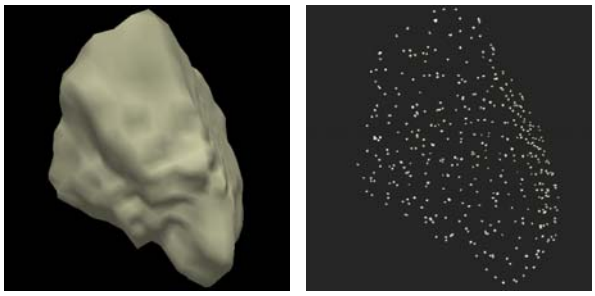

Figure 36. *On the left is the polygonal representation used in the visualization; on the right is the point representation used in the simulation.*

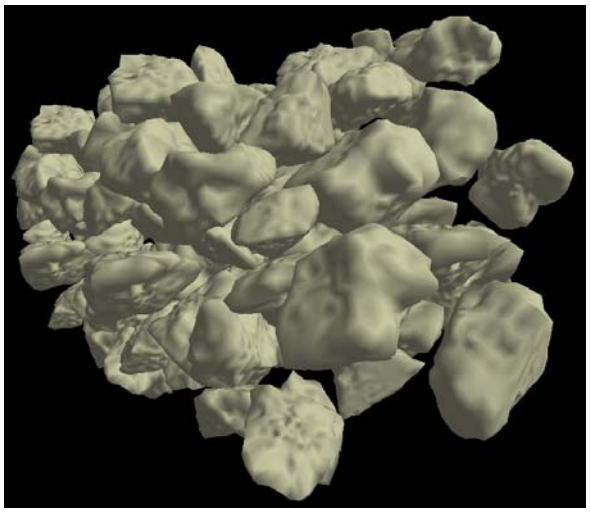

Figure 37. *Snapshot from a computer simulation of a sheared suspension of cement particles. The cement particles shapes were obtained via X-Ray microtomography and are approximately 10-50 micrometers in size. These simulations play an important role in understanding how particle shape influences the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

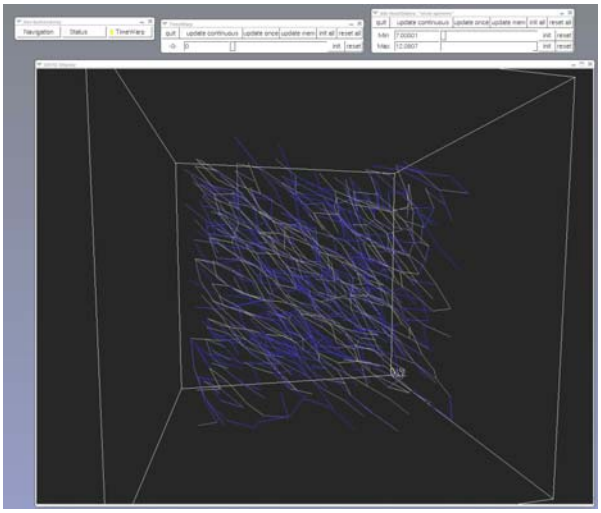

Figure 38. *A snapshot of the sfvis tool.*

Visualization of Stress in Aggregate Flow. A high performance dissipative particle dynamics code for the modeling of aggregate flow developed jointly by MCSD and BFRL is being used to study the motion of hard spheres under stress. Visualizations of the normal stress and shear stress computed by this model were requested by our VCCTL consortia partners, who were interested in understanding the spatial distribution of stresses in a suspension at the onset of a jamming transition. While it is known that there are large stress fluctuations at the onset of jamming, it is not clear where the stresses occur. We developed a visualization that would depict the stresses among neighboring spheres in a suspension. This capability has already proven quite useful. For example, as a result of viewing our visualizations, it became clear that instead of the stresses being carried along a few "chains" which span the system, the stresses were, unexpectedly, homogeneously distributed at the onset of jamming. Such behavior, over long length scales, is indicative of a dynamical phase transition.

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

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

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

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

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

Visualization of a Coal Mine

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

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

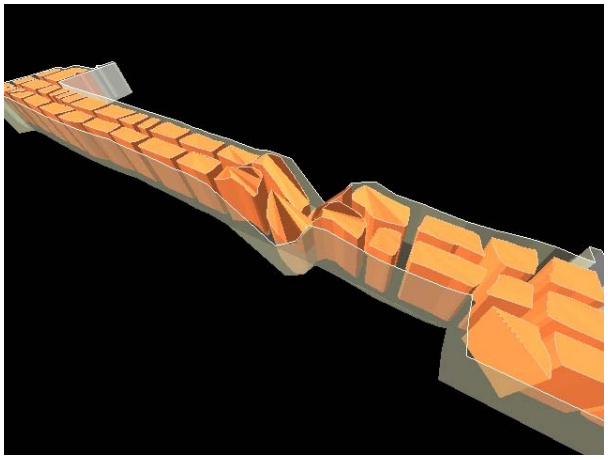

Figure 39. *3D Visualization of a coal mine. Sunken area in middle is clearly visible.*

Visualization of Nano-structures and Nano-optics

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

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

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

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

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

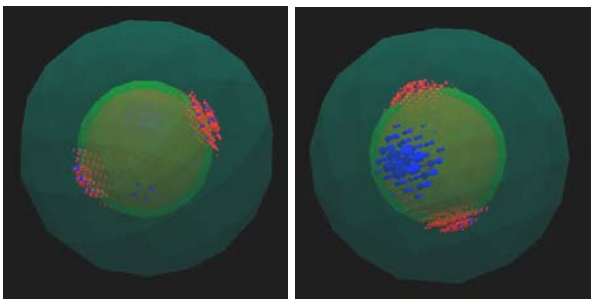

Figure 40. *Two different views of atomic state density of an electronic state trapped in the well region of a nanohetereostructured nanocrystal.*

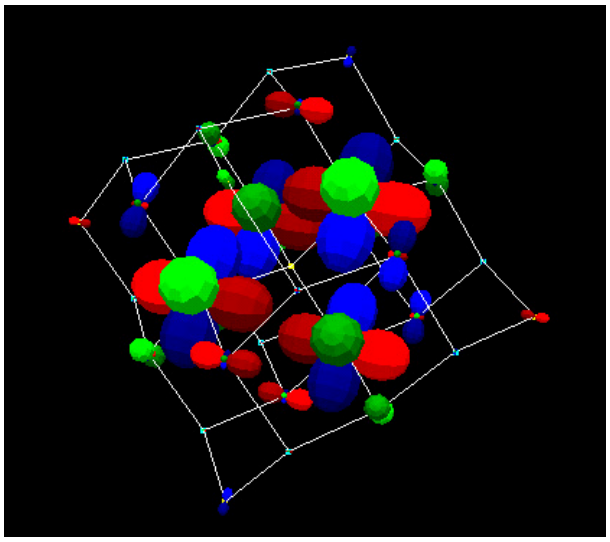

Figure 41. *Image of p orbitals. The white lines in the figure are the nearest neighbors of each atom.*

Feature Detection

Adele Peskin
Judith Terrill

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

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

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

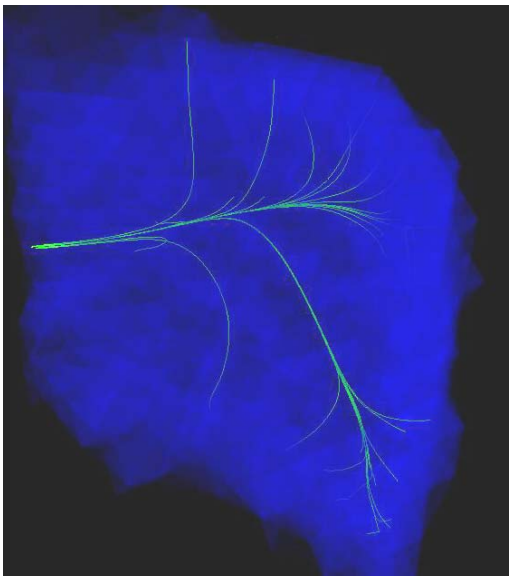

Figure 42. *Curve-skeleton from an image file of a rock.*

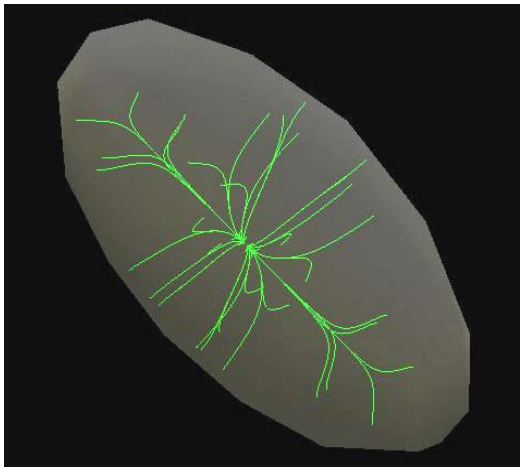

Figure 43. *Curve-skeleton made from the divergence field on an ellipsoid.*

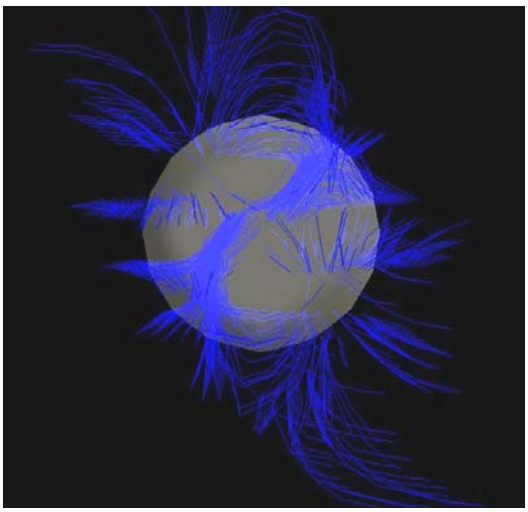

Figure 44. *Streamlines of the electric field around an array of atoms in a nanostructure.*

3D Chemical Imaging at the Nanoscale

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

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

A quantitative understanding of the distribution of chemical species in three dimensions including the internal structure, interfaces and surfaces of micro and nanoscale systems is critical to the development of successful commercial products in nanotechnology. Current nanoscale chemical 3D measurement tools are in their infancy and must overcome critical measurement barriers to be practical. This project is developing intermediate voltage electron microscope measurement approaches to attain three-dimensional chemical images at nanoscale resolution. These will be broadly applicable to nanoscale technologies from microelectronics to pharmaceuticals and subcellular biomedical applications. MCSD collaborators are working on computational, visual analysis, and data management techniques and tools to enable the analysis of imagery to be generated by this project. Among the particular capabilities under development are: techniques for the visualization of 3D data in an immersive environment, techniques for interactions with immersive visualizations, algorithms and analysis, and parallelization of simulation codes

We recently completed a port of the 3D chemical imaging application EPQ to our parallel distributed software environment, SSS. EPQ is a Monte Carlo application that is a simulation of a scanning electron microscope, tracking the trajectories of electrons and determining the output of the detectors given a description of the target material. It was implemented in a mix of Java and Python, and was developed and run primarily in the MS Windows environment. Increased computational demands on this application, due to larger multidimensional simulations being attempted, have necessitated the move to a parallel/distributed algorithm. Test runs of this application have begun on 32 processors of the ITL/PL Raritan cluster.

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

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

One paper was written on this work:

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

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

Fundamental Mathematical Software Development and Testing

OOF: Object-Oriented Finite Elements

Stephen Langer
Andrew Reid
Seung-Ill Han (UMBC)
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Valerie Coffman (Cornell University)
R. Edwin Garcia (Purdue University)

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

See feature article, page 37.

Parallel Adaptive Refinement and Multigrid Finite Element Methods

William F. Mitchell
Eite Tiesinga (NIST PL)
Pascal Naidon (NIST PL)

http://math.nist.gov/phaml

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

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

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

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

References

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

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

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

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

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

Sparse BLAS Standardization

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

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

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

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

Among the most significant components of the updated BLAS standard is support for sparse matrix computations. R. Pozo of MCSD served as chair of the Sparse BLAS subcommittee during the standardization process. NIST was first to develop and release a public domain reference implementation for early versions of the standard, which were critical in shaping the final specification.

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

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

Roldan Pozo
Bruce Miller

http://math.nist.gov/scimark

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

The current SciMark results database contains entries from more than 3,500 submissions representing computational platforms from Palm devices to high-end servers, and contains reports from nearly every operating system and virtual machine environment currently in use, including Solaris, FreeBSD, MacOS, Sun OS, IRIX, OSF1, Linux, OS/2, and Windows 95, 98, 2K, ME, NT, and XP.

SciMark and its kernel components have become a pseudo-standard in industry and academia. They were adopted by the Java Grande Benchmark Forum.; Sun Microsystems used SciMark 2.0 to demonstrate the floating-point improvements to their Java Virtual Machine version.[5] Currently, SciMark inclusion in SPECjvm2006 is under development.

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

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

TNT: Object Oriented Numerical Programming

Roldan Pozo

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

NIST has a history of developing some of the most visible object-oriented linear algebra libraries, including Lapack++, Iterative Methods Library (IML++), Sparse Matrix Library (SparseLib++), Matrix/Vector Library (MV++), and most recently the Template Numerical Toolkit (TNT). This package has been downloaded by thousands of developers (more than 15,000 downloads in calendar 2006, for example) and is currently in use in several industrial and commercial applications. This year saw a major redesign and the introduction of two new components.

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

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

Recent developments in the latest design of TNT (version 3.2) provide support for both multidimensional arrays and integrate linear algebra modules which include fundamental algorithms (LU, Cholesky, SVD, QR, and eigenvalues), sparse matrix support, and support for iterative methods in solving linear systems with dense or sparse matrices. In particular, a new interface proposal for iterative methods has been presented and new implementations are under development to integrate TNT with other software libraries.

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

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

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

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

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

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

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

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

Mathematical Knowledge Management

Visualization of Complex Function Data

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Daniel Lozier
Frank W. J. Olver

http://dlmf.nist.gov/

See feature article, page 31.

Representation and Exchange of Mathematical Data

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

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

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

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

Mathematical Knowledge Management (MKM) is a growing international field of research at the interface between mathematics and computer science. MCSD is becoming a significant contributor due to its development of the Digital Library of Mathematical Functions. The DLMF project has gained recognition within the MKM community as the most ambitious content development effort anywhere in the world. The DLMF project team at NIST is facing all of the questions in the list above, and has developed partial answers to most of them.

Progress was made in FY 2006 on authoring and conversion of LaTeX documents to web formats, and on difficult questions involving mathematical representation. Employing the DLMF as a research laboratory, future work will center on developing more general techniques and tools for delivery of serious mathematics to advanced users.

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

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

Math Search Techniques and Systems

Abdou Youssef
Bruce Miller

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

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

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

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

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

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

Digital Library of Mathematical Functions

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Nico Temme (CWI, Amsterdam)

30 authors under contract
25 validators under contract

http://dlmf.nist.gov/

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

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

The Digital Library of Mathematical Functions has two main goals. First, we are reviewing the published literature on special functions, selecting the

properties most relevant to current applications, and publishing an up-to-date handbook of the traditional sort. The handbook will consist of 33 chapters devoted to individual classes of special functions plus 4 chapters on algebraic and analytical methods, asymptotic approximations, numerical methods, and computer algebra. The most recent comprehensive handbook was published in 1964 by the National Bureau of Standards. Still in print and in widespread use, it is badly out-of-date with respect to recent mathematical research, current scientific applications of special functions, and computational methods. Second, we will disseminate the same information, with significant augmentations, from a Web site at NIST. The augmentations include live links to available online software and references, a math-aware search capability, a facility for downloading formulas into word processors and computer software systems, and interactive visualizations.

The project is large, and the contributors fall into several categories. The *editorial board* consists of 4 principal and 8 associate editors. They are responsible for the selection and presentation of the technical information in book and Web formats. Since the beginning of the project, the principal editors have met frequently to review progress and to make midcourse corrections when necessary. *Authors* consist of expert individuals selected for their published research achievements and their ability to write for the intended audience of scientists, engineers and mathematicians. Their contributions are being carefully edited and, in many cases, extensively revised by the principal editors to achieve uniformity of content and presentation across all chapters. *Validators*, like the authors, consist of expert individuals selected for their research accomplishments. Their responsibility is to check the work of the authors and editors. This is a vital step to uphold the worldwide reputation of NIST as a reliable source of accurate, useful and timely scientific reference information. The *project staff* consists of highly qualified mathematicians and computer scientists whose responsibilities, broadly, are (i) construction of a mathematical database that encodes the entire technical content of the DLMF, (ii) application of advanced visualization methods and tools that enable users to display and manipulate complex functional surfaces, (iii) development of software tools to facilitate the production of the book and Web site, (iv) research into advanced techniques for the faithful translation of mathematical formulas and facts among different computer systems, (v) proof-of-concept integration of software tool prototypes into the DLMF Web site, (vi) research into the frontiers of technical search methodology to enable effective queries involving fragments of technical mathematics, and (vii) integration of a prototype math-aware search tool into the DLMF Web site. The *support staff* consists of individuals capable in the use of advanced mathematics document processors, symbolic and numerical computation packages, and bibliographic tools such as the ones provided by the American Mathematical Society.

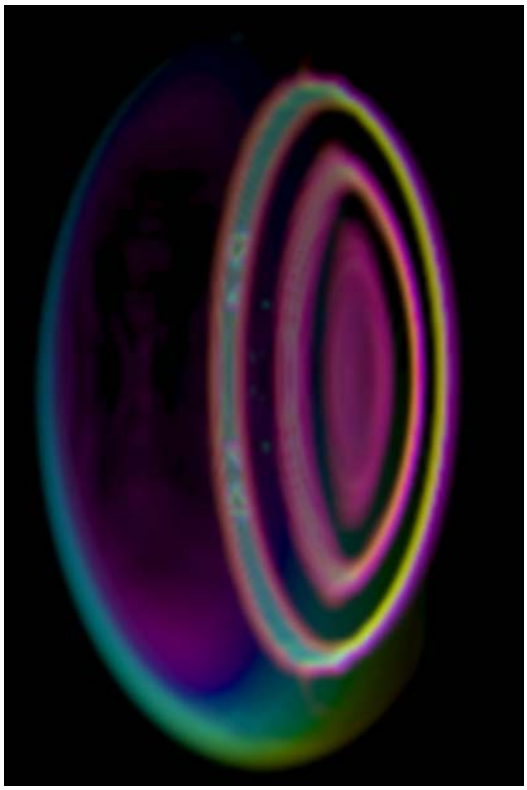

Figure 45. *Many nonlinear ordinary and partial differential equations have solutions that may be expressed in terms of Jacobian elliptic functions. These include the Schrödinger equation. This equation can be used to model the formation of vortex rings in Bose Einstein condensates. Results of such a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

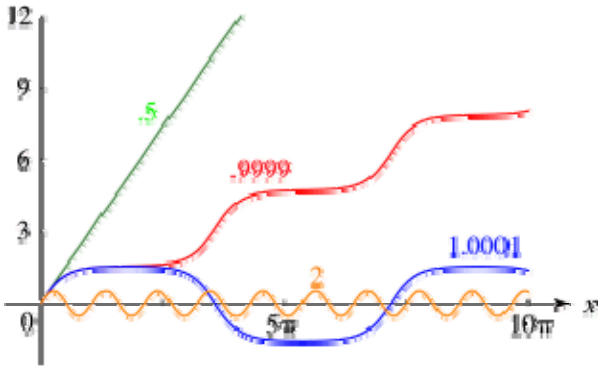

Figure 46. *The Jacobian* am*(x,k) function for four values of the parameter k. These functions arise in the classical analysis of the dynamics of pendulums.*

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

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

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

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

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

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

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

Mathematical Software Reference Databases

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

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

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

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

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