

CSE 2013

“Big Data” and “Planet Earth” Take Leading Roles at SIAM CSE Conference

The SIAM Conference on Computational Science and Engineering has seen dramatic growth since its inception in 2000. CSE13, held in Boston, was no exception—it was in fact the largest SIAM conference to date. The registered attendance of 1370 reflects a 65% increase over CSE11 and a four-fold increase in attendance since the 2000 conference.

The program for CSE13 offered an enormous diversity of topics across computational science and engineering. Popular themes among the 270 minisymposia included methods for multiscale and multiphysics problems, numerical methods for PDEs, high-performance computing, scientific software, fast algorithms, numerical linear algebra, model reduction, uncertainty quantification, optimization, inverse problems, and CSE education. The 61 presentations in the poster session ranged across a similar set of themes.

The conference had two special themes: Computational Mathematics for Planet Earth and Big Data. These themes were chosen to reflect the designation of 2012 as a year of emphasis on Mathematics, Statistics, and the Data Deluge and of 2013

as the year of Mathematics of Planet Earth. *SIAM Journal on Scientific Computing*, in conjunction with CSE13, will devote a section of an upcoming issue to the themes Planet Earth and Big Data; guest-edited by Tamara Kolda (Big Data) and Irad Yavneh (Planet Earth), the section will feature high-quality scientific-computing papers in one or (optimally) both of these areas.

The invited plenary talks at CSE13 were a chance to see inspiring examples of CSE in real applications: medicine (Natalia Trayanova), astrophysics (Joshua Bloom), reservoir simulations (Jan Dirk Jansen), and computational chemistry (Emily Carter). Invited plenary speakers also presented cutting-edge methods in reduced-order modeling (Jan Hesthaven), multiphysics problems (Barbara Wohlmuth), and big networks (Tamara Kolda), and provided forward-looking thoughts for the challenges of exascale (William Gropp, Paul Fischer). The articles in this and upcoming issues of *SIAM News* expand on some of these highlights.

A particular success of CSE13 was its engagement with SIAM student members. The conference attendance numbers include 250 registered students. Special events for students included a lunch-time CSE careers panel sponsored by The MathWorks and IBM, which drew more than 100 students (a student’s-eye view of the event can be

Former SIAM president Cleve Moler presented the 2013 SIAM/ACM Prize in Computational Science and Engineering to Linda Petzold at CSE13. Petzold, a professor of computer science and mechanical engineering at the University of California, Santa Barbara, was honored for her “pioneering research in methods for the computational solution of differential–algebraic equations, their incorporation into widely distributed software and scientific applications, and her significant accomplishments in pioneering computational science and engineering education.”

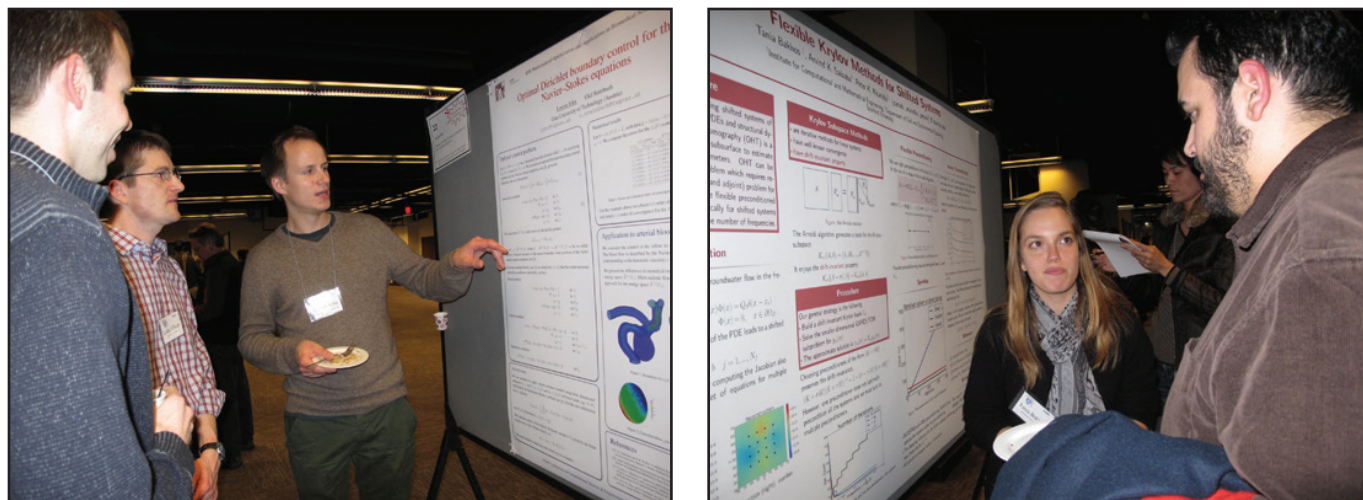


found on page 8). The MIT Center for Computational Engineering sponsored a prize for the Best Student Poster, and the Bavarian Graduate School of Computational Engineering (BGCE) Prize competition was held for the fourth time. Local SIAM Student Chapters from MIT and Tufts were actively engaged in helping with conference operations, and the students also organized tours to the MIT campus for those willing to brave the wintry Northeast weather. We were thrilled to see the next generation of computational mathematicians, scientists, and engineers so energetically involved.

Going into the conference, the organizers had concerns regarding the unexpected large attendance, which resulted in an

unprecedented 20 parallel sessions running for a full five days. The actual conference atmosphere was overwhelmingly positive, however, reflecting the upside of a large conference—a great variety of session topics to choose from at all times, and excellent networking opportunities, given the significant portion of the community in attendance. The SIAG business meeting saw a vigorous discussion of the future of the CSE conference, including possible structural changes that may be needed if the conference continues to grow. How that plays out remains to be seen at CSE15.—Karen Willcox, MIT, and Hans Petter Langtangen, Simula Research Laboratory and University of Oslo.

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Prize-winning student posters in CSE. Top prize went to Lorenz John and Olaf Steinbach of Graz University of Technology for “Optimal Dirichlet Boundary Control for the Navier–Stokes Equations.” Left-hand photo, John highlighted the poster’s fine points for Bedrich Sousedik and Luke Olson. Second-prize recipients Tania Bakhos, Arvind Saibaba, and Peter K. Kitanidis of Stanford University were recognized for “Flexible Krylov Subspace Methods for Shifted Systems.” Right-hand photo, Bakhos was on hand at the session to discuss her group’s research. The competition, which was sponsored by the MIT Center for Computational Engineering, opened with a “poster-blitz,” in which student presenters, in rapid succession, conveyed the essence of their posters in 1–2 minutes. Photos by Susan Whitehouse.

CSE 2013

Quantum Mechanics Without Wavefunctions

By Matthew G. Reuter and Lin-Wang Wang

Quantum mechanical effects are inherent to molecular or material systems in which electronic structure plays a critical role, and computational simulations of these systems help elucidate the properties of chemicals and materials. For example, quantum mechanics describes both physical structure (perhaps the lengths and angles of chemical bonds) and dynamics (including chemical reactions). It is unsurprising, therefore, that quantum mechanical calculations have a myriad of applications, ranging from understanding enzyme catalysis to discovering novel superconducting materials.

Computationally, these simulations aim to solve the Schrödinger wave equation for the wavefunction, the “state variable”

of quantum systems [2]. Even though the Schrödinger equation is a linear, second-order PDE and is reasonably simple to write down, it has proven very difficult to solve for all but the simplest systems. Exact solutions are known for some systems with a single electron (the hydrogen atom, for instance); numerical approaches have been required for all other systems. In these cases, the key computational difficulty in solving the Schrödinger equation is the number of degrees of freedom; if the system has N electrons, the wavefunction is a function of $3N$ variables.

Over the years, various approximations have been developed to make calculations of the wavefunction more tractable; most of them balance computational cost with physical accuracy [3]. The costliest of these, which is generally the most accurate, scales as $\mathcal{O}(N!)$, where-

as others scale polynomially (at least cubically). Computational bottlenecks in these methods include solving generalized eigenvalue problems and/or manipulating high-order tensors. Accordingly, simulations of large systems, perhaps an entire protein with thousands of atoms and even more electrons, are considered heroic and remain intractable for most approximations. Efforts to calculate larger systems have continually pushed the bounds of computational science, garnering several Gordon Bell prizes along the way [4].

The density functional theory (DFT) is an alternative to these wavefunction-based methods that reformulates quantum mechanics in terms of the electron density, ρ [8]. Unlike the wavefunction, ρ is a function of only three variables (regardless of the number of electrons), and for this reason

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1 "Big Data" and "Planet Earth" Take Leading Roles at SIAM CSE Conference

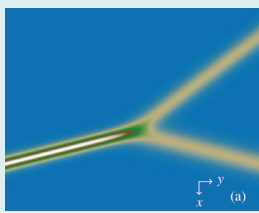
1 Quantum Mechanics Without Wavefunctions

3 Taming Snakes and Dragons in the Earth

3 Ready for the Bigger Picture? Become a Program Director at NSF!

4 Nonlinear Ocean-Wave Interactions on Flat Beaches

Tapping both aesthetically and practically into the enduring fascination of water waves, M.J. Ablowitz and D.E. Baldwin report on interacting waves they have seen and photographed. "A well-known nonlinear wave equation," they explain, "has solutions that are remarkably similar to what we observed."



4 "Setting the Default to Reproducible" in Computational Science Research

"Computational science is facing a credibility crisis," write the authors of an article on the need for reproducibility in computational work, who go on to present three recommendations that emerged from a week-long ICERM workshop on the subject.

5 Large-scale Network Analysis at SIAM CSE Conference

From the theoretical to the practical "and everything in between," Tamara Kolda and Ali Pinar touch on challenges arising in the analysis of today's large, complex, and evolving data sets.

6 Federal Funding Prospects for the Math Sciences in 2014

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Obituaries

Frank W.J. Olver, professor emeritus at the Institute for Physical Science and Technology and the Department of Mathematics at the University of Maryland, and faculty appointee of the National Institute of Standards and Technology, passed away in Maryland on April 23, 2013, at the age of 88. A foreign member of the Royal Society of Sciences, Sweden, and a fellow of the UK Institute of Mathematics and its Applications, Frank was renowned for his contributions to asymptotics, numerical analysis, and special functions.

Born in 1924 in Croydon, UK, Frank showed deep interest in mathematics and proved himself a mathematical talent at a young age. He received a bachelor's degree with first-class honors in mathematics from the University of London in 1944, followed by a master's degree in 1948 and a DSc in mathematical analysis in 1961. At the age of 19, on completion of his undergraduate studies, Frank was assigned to the British Admiralty Computing Service, where he was introduced to numerical analysis. It was at that time that his research interest in special functions began to take shape.

Frank later joined the National Physical Laboratory, where he became a founding member of the Mathematics Division. NPL turned out to be a milestone in his career and life. There, his work in compiling numerical tables of zeros of Bessel functions marked the beginning of his life-long interest in asymptotics and special functions. There too, he met his first wife, Grace. They were married in 1948 and had three children, Peter, Linda, and Sally.

Frank was invited to spend the year 1957–58 at the National Bureau of Standards (now the National Institute of Standards and Technology) in Washington, DC, where he wrote "Bessel Functions of Integer Order," a chapter for the *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, edited by Milton Abramowitz and Irene Stegun. When he returned to NPL, it was with an open invitation to work at NBS; persuaded by Grace to accept, Frank moved to the U.S. in 1961 and spent the rest of his life there. In 1969, he joined the University of Maryland as research professor; on his retirement, in 1992, he was appointed professor emeritus.

Frank wrote numerous papers on asymptotics, numerical analysis, and special functions, and served on the editorial boards of several leading journals in mathematical and numerical analysis. Very active in SIAM, he was one of the founders of *SIAM Journal on Mathematical Analysis* and its first managing editor, from 1970 to 1975. His first book, *Asymptotics and Special Functions*, published in 1974 by Academic Press, became a standard reference in those fields. It was translated into Russian in 1990 and reprinted in 1997.

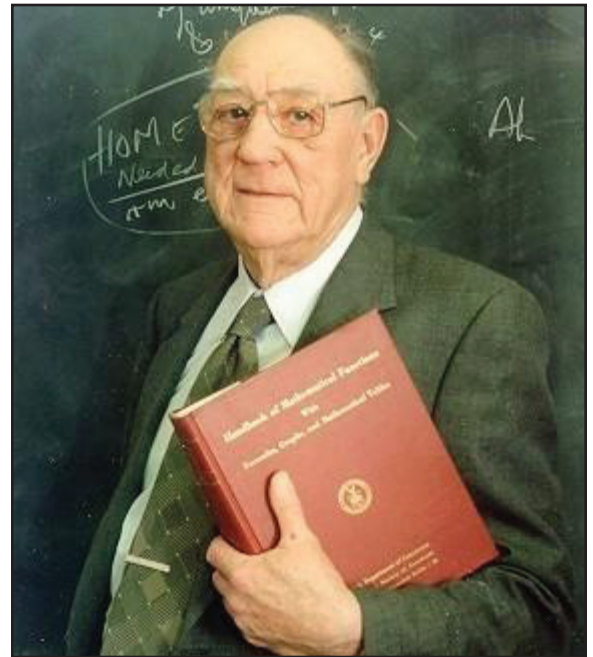
Among his many contributions, one that could be lauded as his "lifetime achievement" was his involvement, as editor-in-

chief and mathematics editor, in the *NIST Handbook of Mathematical Functions* and its web counterpart, the *NIST Digital Library of Mathematical Functions* (DLMF), both published in 2010. This daunting task took Frank, together with editorial and production staff at NIST and about 50 international authors and validators, 10 years to complete. The new publications continued the legacy of their predecessor, the Handbook edited by Abramowitz and Stegun, as an authoritative publication on special functions. The DLMF project, under his leadership, earned the group of nine NIST contributors the Gold Medal of the U.S. Department of Commerce; DLMF was also chosen as one of 10 Government Computer News Award Winners for "Outstanding Information Technology Achievement in Government."

In addition to his important contributions to mathematics, Frank's seriousness about accuracy earned him great respect and appreciation. Everyone who worked with him, read his work, or knew him personally will agree that he was meticulous and precise. When proofreading, he would read every formula backward to ensure that no error was missed. For the book *Asymptotics and Special Functions*, after reading all the galley proofs and page proofs, he traveled to New York to proofread the final manuscript before printing. "He is amazing," says his son Peter, a mathematician at the University of Minnesota. "I don't know any other mathematician who has paid that much attention to detail."

As editor of the NIST Handbook, Frank went through every single chapter and every single line several times, whether the text had been written by him or by other scholars. He read each chapter eight or nine times to pick up even the most minor errors, always refining the language to make it as perfect as possible. Leonard Maximon of George Washington University, an associate editor of the project who worked closely with Frank, once said that Frank's "commitment to assuring that the NIST Handbook was as perfect and coherent a work as is possible involved a Herculean task; I know of no one else that could have accomplished it."

In the mid-1950s, Frank wrote a series of papers on what is now known as uniform asymptotic expansions that appeared in the *Philosophical Transactions of the Royal Society of London* [4–7]; the papers caught the attention of mathematicians who were working in asymptotic analysis as well as of applied mathematicians who were using asymptotics for their applied problems. In the early 1960s, Frank began to work on the construction of numerical bounds for truncation errors associated with asymptotic expansions. Among existing bounds, those provided by Frank still seem to be most realistic and computable.



Frank W.J. Olver, 1924–2013

Although known largely for his work in asymptotic analysis, Frank also made substantial contributions to numerical analysis. In fact, many of his early papers were either on the numerical computation of special functions or on error analysis of recurrence algorithms (e.g., [8,9]). In the late 1970s and early 80s, Frank returned to numerical analysis, constructing with Jim Wilkinson [10] a posteriori error bounds for Gaussian elimination, and proposing with Charlie Clenshaw [2,3] a new number system for computer arithmetic, which they called the level-index system. In 1989, in an important paper [1] that presented a new interpretation of the Stokes phenomenon, Sir Michael Berry adopted the view that the change in form of a compound asymptotic expansion occurs smoothly, although very rapidly, as a Stokes line is crossed. Berry's argument is based on R.D. Dingle's theory of terminants, and is hence quite formal. In a series of papers, Frank developed new analysis to place the theories of Dingle and Berry on rigorous mathematical foundations.

In 2000, commemorating Frank's impressive contributions to mathematics, a two-volume collection of his selected papers was published. The 1074-page collection consists of 56 papers covering his most important contributions in the areas of asymptotic analysis, special functions, and numerical analysis, during the years from 1949 to 1999.

Frank will be remembered as one of the great mathematicians of our time, for his profound influence on the development of special functions, as an editor admirable for his attention to details, and as an inspiring scholar for the standards and references he created for succeeding generations of mathematicians.

Frank is survived by his second wife, Claire, his brother, Terence, son Peter and daughter Sally, their spouses, Cheri and Neal, and five grandchildren, Parizad, Krista, Sheehan, Brian, and Noreen.

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CSE 2013

Taming Snakes and Dragons in the Earth

By Alison Malcolm and
Andreas Fichtner

As most of recorded human history had it, the Earth's interior was ruled by giant snakes and dragons. Only with pioneering studies of surface-exposed rocks (J. Hutton, 1726–1797) did our planet come to be perceived as a complex superorganism that could be understood without the invocation of mystical creatures. The initially descriptive geosciences have gradually been complemented by physical models of plate tectonics, mantle convection, and seismic wave propagation, among many others. Over the past few decades, the tools of mathematics have been increasingly exploited to improve our understanding of these models, as well as to shape their development. As with many fields, continuously increasing computer power is producing new tools with which we can explore our planet. In recent years, computational science and applied mathematics have evolved—from mere tools, they have become major drivers of geoscientific progress. The ongoing mathematization of Earth system studies was clear in Boston at this year's SIAM Conference on Computational Science and Engineering, where cutting-edge research was presented in numerous sessions on such diverse topics as 4D imaging, flow in porous media, adjoint methods, ice sheet modeling, uncertainty quantification, and climate simulation.

Seismic modeling and inversion are two of the principal Earth-science beneficiaries of advances in computational mathematics. New methods that harness the power of modern HPC allow us to address key problems related to these topics, including the assimilation of massive data sets, 3D frequency-domain wave propagation and imaging, nonlinear inversion with multiple scattering, multiscale seismic wavespeed tomography, uncertainty quantification, and the search for optimal misfit functionals for full-waveform inversion.

As discussed at CSE 2013, today's seismic acquisition systems produce immense quantities of waveform data that are increasingly difficult to handle and to model. To reduce the computational burden of seismic waveform inversion, F.J. Herrmann has used ideas from compressive sensing to design an iterative method in which updates are computed from random data subsets via curvelet-domain sparsity promotion. In a closely related effort to minimize the number of forward simulations in waveform inversion, K. van den Doel and colleagues used experimental design techniques to develop optimal source encoding strategies that model multiple seismic sources simultaneously, without loss of information about subsurface structure.

Whether the seismic inverse problem should be solved in the time or the frequency domain continues to be a subject of active debate. The first quantitative and objective comparison of the time- and frequency-domain approaches was presented at CSE 2013 by R. Brossier, whose group concluded that 3D full-waveform inversion in the frequency domain is feasible and competitive. Additional impetus to frequency-domain modeling was provided

by B. Engquist, who developed “sweeping preconditioners” for the Helmholtz equation, for which the number of operations scales approximately linearly in the number of unknowns.

Owing to the extreme computational requirements, uncertainty quantification in full-waveform inversion has long been considered infeasible. G. Stadler described a practical solution to this problem, based on second-order adjoints, which he and colleagues used to construct a low-rank approximation of the Hessian that carries information on the posterior covariance. The approximated posterior distribution can then be sampled to provide a range of plausible Earth models (see Figure 1).

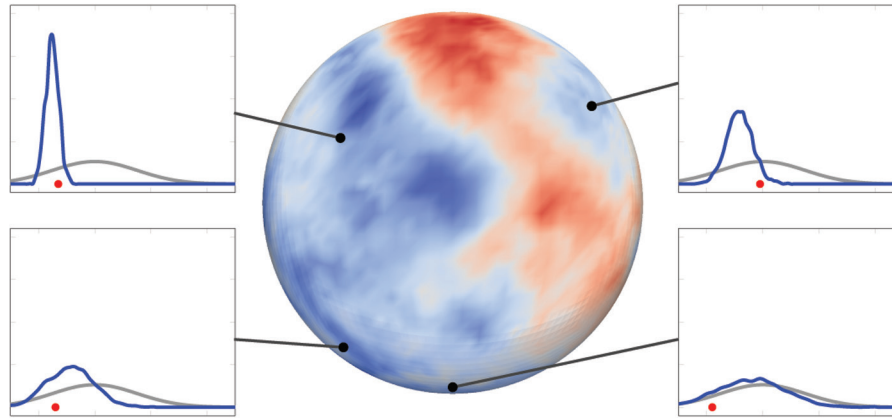


Figure 1. Sample from the posterior probability density of local wave speed at 70 km depth, resulting from a synthetic full-waveform inversion. Receivers were located only in the northern hemisphere. The gray lines in the graphs are the prior point marginals, the blue lines the posterior point marginals. Red dots indicate the point value of the sample. In the northern hemisphere, the posterior variance is reduced significantly compared to the prior variance. Only small variance reductions are observed in the southern hemisphere, where no receivers are located.

ing models, and of developing objective functions that are less susceptible to local minima. Along these lines, W. Symes illustrated how linear modeling can be extended to exploit the redundancy in the data and how this extension can be merged into full-waveform inversion to recover the low-frequency part of the model and thus avoid local minima. L. Demanet and V. Jugnon discussed a method that also aims to address this problem, using correlations between different parts of the data set. Both approaches seem to indicate that it is in new ways of combining complementary techniques and ideas that we can expect to overcome this problem.

A similar thread was visible in other sessions addressing geophysical problems. We heard from A. Malcolm and A. Richardson and from S. Fomel that, in some cases, adaptations of older imaging techniques can be superior to current techniques, although in different contexts. Malcolm and Richardson showed how including multiply-scattered events separately in an approximate method can sometimes result in a better image than processing all events simultaneously, as is done in more complete methods. S. Fomel stepped even further back, to the simplest of all imaging techniques, known as time migration, and showed how it can be improved via techniques of modern geometry.

Unlike seismic exploration, for which abundant regularly sampled data are available, global seismology suffers from a strongly heterogeneous distribution of sources and receivers over a wide range of spatio-temporal scales (1–10,000 km, 1–1000 s). Assimilating these data into a consistent Earth model requires the devel-

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Ready for the Bigger Picture? Become a Program Director at NSF!

This column is addressed not so much to students and junior faculty as to more experienced mathematical scientists who are looking for new challenges and wish to use their accumulated knowledge and experience to serve the community. That is how I saw myself, after a long career as a researcher (including a stint as division director) in the Mathematics and Computer Science Division at Argonne National Laboratory.

In 2001, having served on a number of review panels and a Committee of Visitors for the Division of Mathematical Sciences at the National Science Foundation, I was asked whether I would be interested in joining DMS as a program director. (Then, as now, several positions were about to open up.) At Argonne, working as an applied mathematician in a multidisciplinary research environment, I had become familiar with all sorts of mathematical and computational problems in physics, materials science, chemistry, and engineering, and found inspiration in diverse applications for my research, mainly in the area of differential equations. Becoming a program director would be an interesting opportunity to put this accumulated knowledge to work in a different environment, so I accepted the invitation and became a “rotator”—a temporary staff member, on assignment from my home institution. The idea was to give it a try for a year and see whether I would like it. As it turned out, I loved it; I stayed for three years and then signed on for another three.

In this column I describe some of my experiences as a program director in applied mathematics (I was one of four), and as a participant in some larger programs within DMS and in several NSF-wide multidisciplinary programs. I hope to convince you

that serving the community as a rotator can be both challenging and exciting.

At the Micro-level— DMS Applied Mathematics Program

As program director in the DMS applied mathematics program, my primary responsibility was to manage a portfolio of research projects within a given budget. With four

program directors and about 300 proposals submitted to the program each year, each of us handled between 75 and 90 proposals (the numbers increase as you become more experienced). During

my tenure, I handled all proposals dealing with applications of dynamical systems and many proposals in various other areas of applied and computational mathematics (materials, inverse problems, and so on). By “handling” I mean making sure that the proposals are in compliance with the required format, that they are appropriate for the program, that they are reviewed fairly and expertly, and that the review process is thoroughly documented. If you think that a proposal may be of interest to other programs, within the division or in other divisions, you contact the program director and coordinate a joint review.

Putting review panels together is serious business, because you want to make sure not only that the panelists' expertise matches the proposals under review, but also that the panel has enough diversity (in more ways than one). Fortunately, our community takes its responsibilities seriously, and I found that, although not all panelists were equally adept at putting their thoughts in writing, the opinions were always informative and helpful. As program director, you learn to read between the lines. I certainly enjoyed this part of the job and admit that running a panel was one of my favorite

activities. I also enjoyed taking a panel to dinner one evening at a local restaurant, as was the custom. My favorite restaurant was Taste of Morocco, where the food was different, the atmosphere relaxed, and the biggest surprise came at 8 o'clock, when the belly dancer made her entrée. Panelists who were unaware of this extra attraction reacted in various ways, but all remembered the occasion.

Sometimes we had to solicit extra reviews if a panel could not reach consensus on the merits of a particular proposal. But once the recommendations of the panel and the reviews were in, it was time for tough decisions: to consider each proposal and decide whether to recommend a declination (a “dec”) or an award. Although the success rate is higher in DMS (about 30%) than in most other divisions, there are always more declinations than awards. When a proposal is declined, you need to be sensitive to the expectations of the principal investigator, or PI, who needs to be made aware of the reasons for the declination. These reasons can vary. Only the “best” projects can be funded (the standard expression is that a proposal needs to be “compelling”), but as program director you need to keep in mind that a portfolio needs to be balanced by topic area, by seniority of the PIs, by geographic distribution of the institutions, and so on. This is where experience and judgment come in.

Of course, it is always a pleasure to recommend an award, especially if the project is proposed by a junior researcher. The budget, which is part of a funding recommendation, requires something that is euphemistically called “negotiation.” In most cases, the negotiation is one-way; considering the scope of the proposed project, you give a bottom-line figure to the PI, who must then figure out how to allocate the dollars to the various budget items.

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Obituaries

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—Roderick Wong, City University of Hong Kong.

Nonlinear Ocean-Wave Interactions on Flat Beaches

By M.J. Ablowitz and D.E. Baldwin

People have always been fascinated by waves, particularly water and ocean waves. The mathematical study of water waves goes back to the origins of differential equations. While linear equations are often good models for small-amplitude waves, nonlinear equations are needed for larger amplitudes. We have seen and photographed interacting nonlinear waves that occur daily at two relatively flat beaches; a well-known nonlinear wave equation has solutions that are remarkably similar to what we observed.

Even Newton (1642–1727) was interested in providing a mathematical description of water waves, but many years would pass before this was feasible. In 1757 Euler derived the inviscid equations of fluid dynamics. Soon afterward, Laplace and Lagrange found linear approximations to the water-wave equations. In 1816 Cauchy's study of the linear initial-value problem of water waves won a prize from the French Academy of Sciences. This work, an early application of Fourier analysis, was not well understood at the time. But in general, water-wave dynamics satisfy nonlinear equations because the wave amplitudes are not sufficiently small.

In 1847 Stokes derived the correct nonlinear boundary conditions on the water's free surface and used it to show that the

speed of a traveling wave in deep water depends on its amplitude. In the 1870s, understanding that the nonlinear water-wave equations are simplified when the water is shallow or the waves are long, Boussinesq derived (1+1)-dimensional equations (one space and one time dimension); he found a solitary wave solution that is localized and nonperiodic. In 1895 Korteweg and his student de Vries followed Boussinesq's pioneering path and derived a unidirectional (1+1)-dimensional nonlinear equation for shallow water, usually called the Korteweg–de Vries (KdV) equation. They also found special periodic solutions, which they called cnoidal waves, that can be written in terms of Jacobian elliptic functions. The cnoidal wave, in a special limit, becomes a solitary wave. A solitary wave had been observed in 1834 by Russell, a naval engineer; he found that the wave's speed depends on its amplitude, which agrees with the KdV equation's solitary wave.

Between 1895 and 1960, most applications of the KdV equation involved water waves. But in the 1960s mathematicians found that the KdV equation is universal: It arises in wave problems with weak dispersion and weak quadratic nonlinearity. Besides water waves, the KdV equation arises in stratified fluids, plasma physics, elasticity, and lattice dynamics, among other settings. It was lattice dynamics that

motivated Kruskal and Zabusky in 1965 to carry out a numerical study of the KdV equation. They discovered that these KdV solitary waves have special interaction properties: Their amplitudes before and after interaction are preserved, but there is a phase shift. They called these special solitary waves solitons. Soon afterward, in 1967, Gardner, Greene, Kruskal, and Miura developed a method—later named the inverse scattering transform (IST) method—for finding the solution. They also found a spectral interpretation for solitons. Their work spurred great interest, and many researchers made important contributions.

Equations solvable with the IST method, like the KdV equation, are often called integrable. In 1970 Kadomtsev and Petviashvili (KP) found a multidimensional (two-space, one-time) generalization of the KdV equation; it is also integrable and can be derived from the water-wave equations in shallow water with surface tension included. Like the KdV equation, it has soliton solutions that can be written explicitly. The simplest is a plane-wave solution, which is essentially one-dimen-

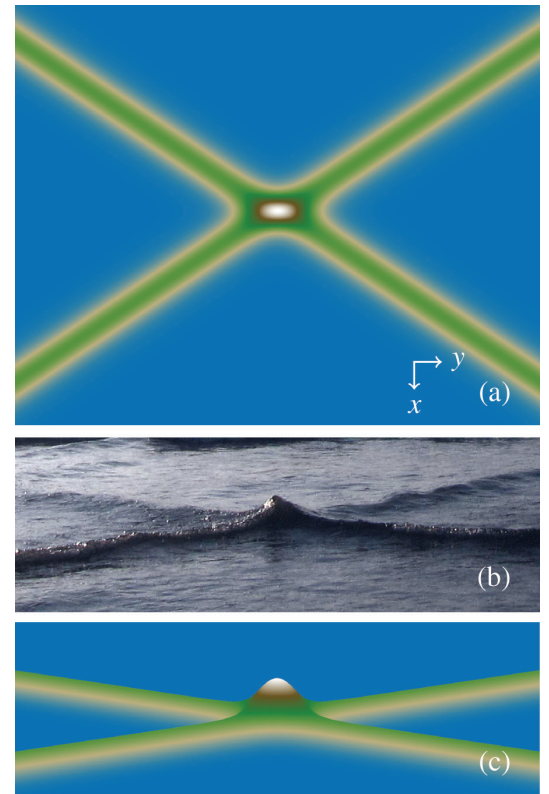


Figure 1. Short-stem X-type interaction; see also [2]. (a) Contour plot of an analytical line-soliton interaction solution of the KP equation (here $e^{\phi} \approx 2.3$). (b) Photograph taken in Mexico, December 31, 2011. (c) 3D plot of the solution shown in (a).

sional and satisfies the KdV equation.

See **Waves** on page 5

“Setting the Default to Reproducible” in Computational Science Research

Following a late-2012 workshop at the Institute for Computational and Experimental Research in Mathematics, a group of computational scientists have proposed a set of standards for the dissemination of reproducible research.

By Victoria Stodden, Jonathan Borwein, and David H. Bailey

Computation is now central to the scientific enterprise, and the emergence of powerful computational hardware, combined with a vast array of computational software, presents novel opportunities for researchers. Unfortunately, the scientific culture surrounding computational work has evolved in ways that make it difficult to verify findings, efficiently build on past research, or even apply the basic tenets of the scientific method to computational procedures.

As a result, computational science is facing a credibility crisis [1,2,4,5]. The enormous scale of state-of-the-art scientific computations, using tens or hundreds of thousands of processors, presents unprecedented challenges. Numerical reproducibility is a major issue, as is hardware reliability. For some applications, even rare interactions of circuitry with stray subatomic particles matter.

In December 2012, more than 70 computational scientists and stakeholders, such as journal editors and funding agency officials, gathered at Brown University for the ICERM Workshop on Reproducibility in Computational and Experimental Mathematics. This workshop gave a broad cross section of computational scientists their first opportunity to discuss these issues and brainstorm ways to improve on current practices; the result was a series of recommendations for establishing really reproducible computational science as a standard [13]. Three main recommendations emerged from the workshop discussions:

1. It is important to promote a culture change that will integrate computational

reproducibility into the research process.

2. Journals, funding agencies, and employers should support this culture change.

3. Reproducible research practices and the use of appropriate tools should be taught as standard operating procedure in relation to computational aspects of research.

Changing the Culture

Early in their careers, bench scientists and experimental researchers are taught to maintain notebooks or computer logs of every work detail—including design, procedures, equipment, raw results, processing techniques, statistical methods of analysis. Unfortunately, few computational experiments are documented so carefully. Typically, there is no record of workflow,

computer hardware and software configuration, parameter settings, or function invocation sequences. Source code is often either lost or revised with no record of the revisions. These practices not only cripple the reproducibility of results; ultimately, they impede the researchers' own productivity.

The research system must offer institutional rewards for producing reproducible research at every level, from departmental decisions to grant funding and journal publication. The current academic and industrial research system places primary emphasis on publication and project results, with little attention to reproducibility. It penalizes those who devote the time needed to produce really reproducible research. It is regrettable that software development is often discounted. It has been compared to, say, constructing a telescope, rather than doing *real science*. Thus, scientists are discouraged from writing or testing code. Sadly, NSF-funded projects on average remain accessible on the web only about a year after funding ends. Researchers are busy with new projects and lack the time or money to preserve the old. With the ever-increasing importance of computation and software, such attitudes and practices must change.

Support from Funding Agencies, Journals, and Employers

Software and data should be “open by default,” in the absence of conflicts with other considerations, such as confidentiality. Grant proposals involving computational work should be required to provide such details as standards for: dataset and software documentation, including reuse (some agencies already have such requirements [11]); persistence of resulting software and dataset preservation and archiving; standards for sharing resulting software among reviewers and other researchers.

Funding agencies should add “reproducibility” to the specific examples, such as “Broader Impact”

statements, that proposals could include. Software and dataset curation should be explicitly included in grant proposals and recognized as a scientific contribution by funding agencies. Templates for data management plans that include making software open and available could be provided, perhaps by funding agencies, or by institutional archiving and library centers [7].

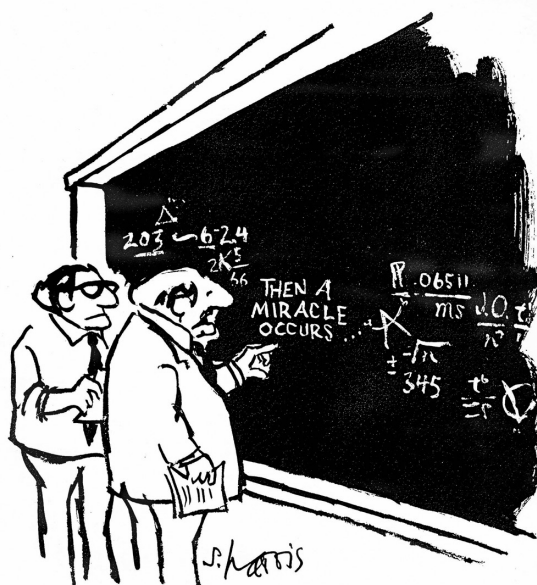
Editors and reviewers must insist on rigorous verification and validity testing, along with full disclosure of computational details [6]. Some details might be relegated to a website, with assurances that this information will persist and remain accessible. Exceptions arise, as in the case of proprietary, medical, or other confidentiality issues, but authors need to state this upon submission, and reviewers and editors must agree that the exceptions are reasonable. Better standards are needed for including citations of software and data in the references of a paper, instead of inline or as footnotes. Proper citation is essential both for improving reproducibility and for ensuring credit for work done in developing software and producing data, which is a key component in encouraging the desired culture change [10].

The third source of influence on the research process stems from employers—tenure and promotion committees and research managers at research labs. Software and dataset contributions, as described above, should be rewarded as part of expected research practices. Data and code citation practices should be recognized and expected in computational research.

Teaching and Tools for Reproducible Research

Proficiency in the skills required to carry out reproducible research in the computational sciences should be taught as part of the scientific methodology, along with modern programming and software engineering techniques. This should be a standard part of any computational research curriculum, just as experimental or observational scientists are taught to keep laboratory notebooks and follow the scientific method. Students should be encouraged and formally taught to adopt appropriate tools. Many tools are available or under development to help in replicating earlier results (of the researcher or others). Some tools ease literate programming and publishing of computer code,

See **Reproducibility** on page 6



“I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO.”

Courtesy of S. Harris, ScienceCartoonsPlus.com.

CSE 2013

Large-scale Network Analysis at SIAM CSE Conference

By Tamara G. Kolda and Ali Pinar

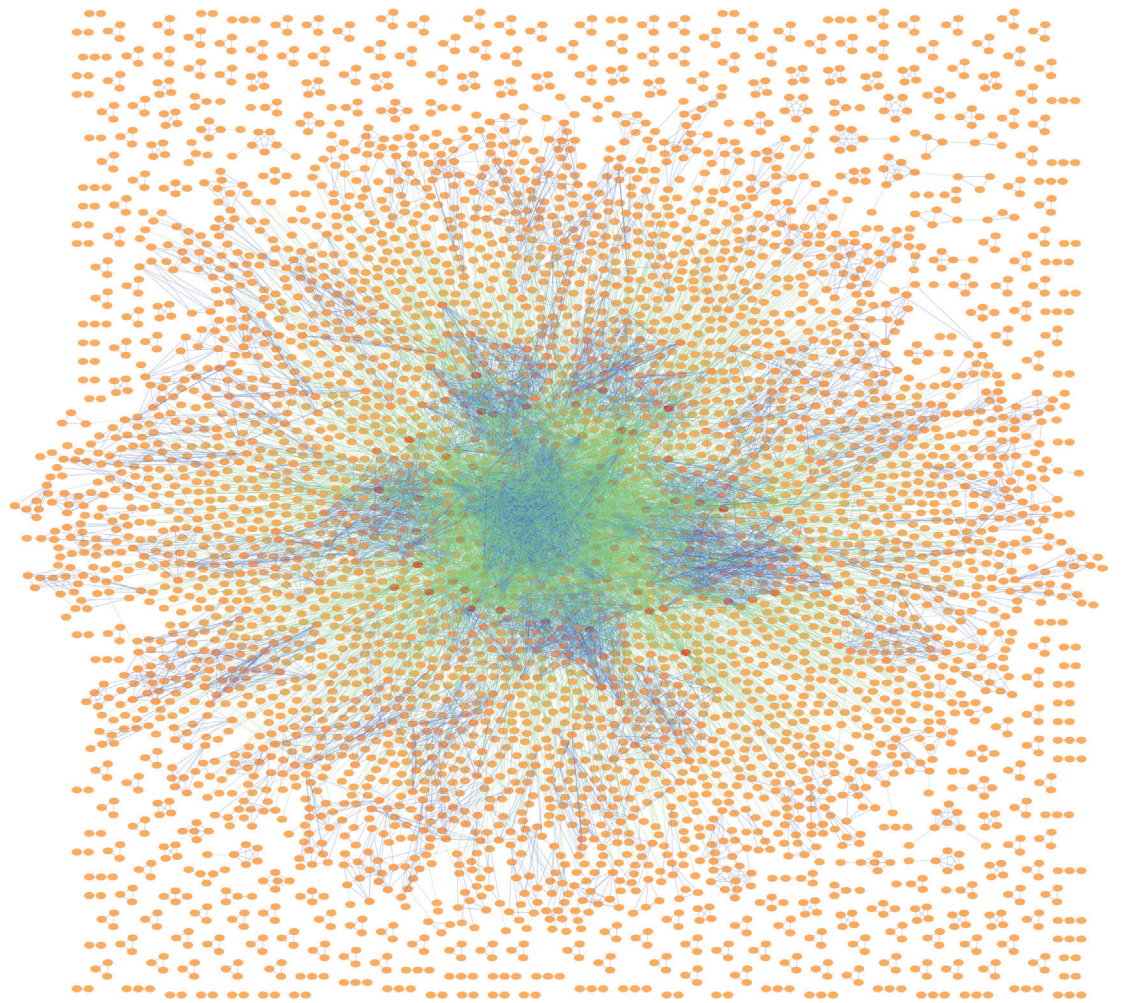
The organizers of the 2013 SIAM Conference on Computational Science and Engineering chose “Scalable Algorithms for Big Data” as one of the main conference themes. We can better understand many real-world data sets by looking at their connectivity (i.e., the network or graph) rather than at static features. The early success of Google’s PageRank analysis, for instance, showed that incorporating connectivity in web search was much more effective than keyword analysis alone. Today, network analysis plays an important role in a wide variety of application domains, including biology, chemistry, economy, communications, transportation systems, cybersecurity, sociology, and even sports analysis.

Large-scale networks are ubiquitous: Consider social networks; graphs of links between web pages; the power grid; graphs of phone, e-mail, or text communications; graphs of purchasing and/or financial transactions; player interaction networks in multiplayer online games; and computer network traffic between various IP addresses. These networks are not described simply by nodes and edges, but by *attributed* graphs, whose nodes and edges carry (possibly changing) properties. Moreover, the edges may have both timestamps and directionality, which appears (and disappears) based on the interactions between nodes.

The size of such networks is already quite large. For instance, public data sets available for research have graphs as large as 100 million nodes and 4.5 billion edges, and these are tiny compared to many graphs that companies like Facebook and Google are analyzing. Moreover, these data sets continue to grow in size—far outstripping analysis capabilities.

Several talks at CSE13 focused on ways to handle these large, complex, and evolving data sets. The challenges ranged from the theoretical (e.g., generating uniformly random instances of graphs) to the practical (e.g., discovering computer malware) and everything in between. Here are a few highlights:

BTER graph model. The nodes are color-coded—darker nodes are of higher degree. The blue edges correspond to affinity blocks, and the green edges to “random” connections. Image by Nurcan Durak, courtesy of Tamara Kolda.



■ In her plenary talk, Tamara G. Kolda discussed the challenge of modeling large-scale networks in a way that captures both the connectivity of the nodes (i.e., the degree distribution) and the community structure (i.e., the degree-wise clustering coefficients). Ultimately, her team’s proposed BTER (block two-level Erdős-Renyi) model was able to capture these properties on a simple graph with more than 4 billion edges, although specialized techniques were needed just to compute the clustering coefficients of such large-scale graphs. For directed graphs, she showed that the situation is much more complicated because of the

impact of the reciprocity of edges on the community structures.

■ Graph modeling was the focus of several other talks as well. Dmitri Krioukov (UC San Diego) presented a hyperbolic model of evolving networks that achieves good clustering coefficients. Pierre-André Maugis (University College London) and Sonja Petrović (Penn State) both considered the problem of correctly estimating parameters for multiplicative probability models of edges. Maugis discussed the use of these parameters to find hubs. Petrović turned to polyhedral geometry to discover whether a solution even exists, and also used ran-

dom walks to modify networks. Similarly, Ali Pinar considered how many moves are needed in a Markov setting to guarantee sufficient distance from the original graph.

■ The theme of graph analysis for cybersecurity surfaced in several talks. John R. Johnson (Pacific Northwest National Laboratory) discussed the “pass the hash” attack that adversaries use to gain increasing levels of access within a network. The researchers’ goal was to analyze the vulnerability of a network, but they needed to use graph minors (an aggregated ver-

See **Large-scale Networks** on page 7

Waves

continued from page 4

The well-known two-soliton solutions, first found in the 1970s, are more interesting; surprisingly, similar interactions are visible on a daily basis on relatively flat beaches. It is useful to write the two-soliton solution of the KP equation, with small surface tension, with a phase-shift parameter that we label e^ϕ . We concentrate on four cases: e^ϕ order one, e^ϕ large, e^ϕ zero, and e^ϕ small. Remarkably, we have seen each of these types at the beach; we call them short-stem X-, long-stem X-, Y-, and H-type interactions, respectively.

Before our recent observations, there was only one known photograph—of a long-stem X-type interaction, taken on the Oregon coast in the 1970s (see [1], page 291). MJA saw and photographed short- and long-stem X-type and Y-type interactions in Nuevo Vallarta, Mexico; he also occasionally saw and photographed more complex multisoliton interactions. Motivated by this and the KP equation’s analytic solutions, DEB traveled to Venice Beach, California, where he saw and photographed not only interactions of the types seen by MJA, but also H-type interactions. We observed these soliton interactions daily on relatively flat beaches, in shallow water, within about two hours of low tide. Being near a jetty helps

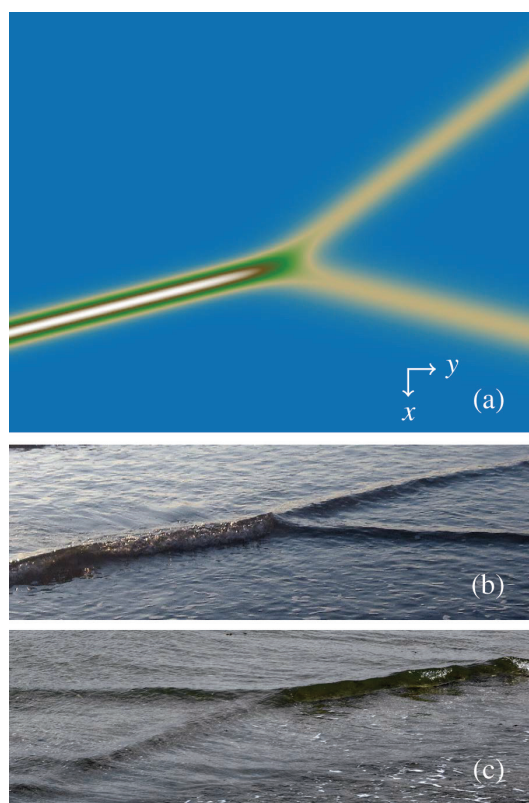


Figure 2. Contour plot (a) and photographs (b), (c) of a Y-type interaction ($e^\phi = 0$); see also [2]. (b) Taken in Mexico, January 6, 2010. (c) Taken in California, May 3, 2012.

the development of cross-waves but is not necessary if there is a good crosswind. We have seen mainly two-soliton interactions but occasionally have spotted more complex soliton interactions as well. Additional details and photos can be found in our paper [2], and we have also posted photos

and videos on our websites (<http://www.markablowitz.com/line-solitons> and <http://www.douglasbaldwin.com/nl-waves.html>).

Along with the phase shift, some of these distinctive nonlinear interactions are explained in part by the stem height: Not just the sum of the wave heights away from the interaction, it can be considerably higher. This can be important in descriptions of tsunami propagation, which in certain cases can be modeled with the KP equation. Indeed, satellite images reveal local X- and Y-type interactions for the 2011 Japanese earthquake-induced tsunami. This made the effects of the tsunami even worse. Because the Japanese tsunami was close to shore, nonlinearity did not have time to amplify

the stem height; other tsunamis might occur well away from shore, in which case nonlinear effects could become important. In such cases X- and Y-type tsunami interactions could be extremely destructive.

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- M.J. Ablowitz is a professor of applied mathematics at the University of Colorado, Boulder, from which D.E. Baldwin recently received a PhD.*

MPE2013 Daily Blog

Among the activities of Mathematics of Planet Earth 2013 is a daily English-language blog devoted to the themes of the worldwide project. Along with climate change and sustainability, themes include geophysics, ecology, epidemiology, biodiversity, and the global organization of the planet by humans. Since the beginning of the year, more than 100 entries have been posted. Recent posts discuss the mathematical modeling of flow through porous media (Todd Arbogast, University of Texas, Austin), water management in California’s Central Valley (participants in a workshop held at the American Institute of Mathematics), and atmospheric waves and the organization of tropical weather (Joseph Biello, UC Davis).

A recent post, “Nonlinear Waves and the Growth of a Tsunami” (<http://mpe2013.org/2013/02/28/4914/>), mentioned work of Mark Ablowitz and Douglas Baldwin, illustrated with a picture of a long-stem X-type interaction. The item caught the attention of *SIAM News*; Mark Ablowitz accepted our invitation to tailor an article on the subject for our readers, and the result is the accompanying article.

Contributions to the MPE2013 daily blog are welcome. It’s easy to participate: Think of an interesting MPE-related topic, consider how it relates to mathematics, and describe it in 200–500 words. Adding a picture or link to a video will attract even more readers. Blog entries can be submitted via e-mail to blog@mpe2013.org.

Federal Funding Prospects for the Math Sciences in 2014

On April 10, President Obama released his budget request for fiscal year 2014. Although unlikely to become reality, the budget is interesting to our community as a reflection of the Administration's priorities for research in the coming years. It continues strong support for basic research, alongside a marked emphasis on programs and initiatives in such areas as clean energy, "big data," cybersecurity, advanced manufacturing, materials research, neuroscience, robotics, and STEM education. We can expect new solicitations and federal agency plans in several of these areas in coming months.

One notable change for FY 2014 is a proposal to consolidate all federal educational fellowship programs, including the Department of Energy's Computational Science Graduate Fellowship (CSGF) program, and move them to the National Science Foundation's Directorate for Education and Human Resources. Such a consolidation may make sense on some level—simplifying the application process and providing greater visibility for the programs—but it may not be optimal for a program that, like CSGF, places fellows in national laboratories as part of the research experience.

In broad-brush summary, the Administration has proposed the following significant FY 2014 investments in agencies and programs critical to the applied mathematics and computational science research communities:

■ NSF. The requested FY 2014 budget of \$7.63 billion is 3.2% above the estimated FY 2013 level; DMS would see an increase of 2.9% over the FY 2012 actual level (a 0.19% decrease from the FY 2013 request).

■ DOE's Office of Science. The \$5.15 billion

requested for FY 2014 (5.1% above the estimated FY 2013 level) includes a 5% increase over the FY 2013 estimate for Advanced Scientific Computing Research.

■ Department of Defense Basic Research. At \$2.16 billion, the FY 2014 request is 1.6% above the estimated FY 2013 level; DARPA basic research would increase by 1.9% over the FY 2013 request.

■ National Institutes of Health. The request of \$31.3 billion for FY 2014 represents a 0.9% increase over the estimated FY 2013 level.

National Science Foundation

In FY 2014, Research & Related Activities at NSF would receive \$6.212 billion, a 3.8% increase over FY 2013; Education and Human Resources would receive \$880 million, 1.7% below FY 2013 funding.

At \$244.5 million, the FY 2014 request for the Division of Mathematical Sciences represents a decrease of 0.19% from the FY 2013 request, but a \$6.8 million increase (2.9%) over the FY 2012 actual level. Compared with the other MPS divisions (Astronomy, Chemistry, Materials, and Physics), DMS would receive the smallest increase over FY 2012 levels; Chemistry and Materials would lead, with increases of 8.4% and 6.8%, respectively.

In a mid-April phone call, Fleming Crim, recently appointed NSF assistant director for the Mathematical and Physical Sciences, emphasized his support for core programs, pointing out that DMS core programs have been protected to a large extent from funding decreases. New funds for a division, he noted,

are usually associated with an initiative or focus area.

An example is DMREF (Designing Materials to Revolutionize and Engineer our Future), an NSF-wide program introduced in 2013 as part of the ongoing Materials Genome Initiative. The response of the mathematical sciences community to DMREF was relatively low, despite a call for proposals from DMS. Low response rates to Administration priorities generally lead to lower participation in these initiatives and, hence, to smaller budget growth.

About 53% of the FY 2014 request for DMS would be for new research grants to individual researchers. The following are details of some of the other proposed DMS activities for FY 2014:

■ Participation in the NSF-wide CIF21 (Cyberinfrastructure Framework for 21st Century Science and Engineering). DMS would increase its contribution by \$1.3 million, to \$7.66 million, in part to support the development of models and computational tools to help meet scientific challenges involving massive and complex data sets. This would expand on existing efforts in analyzing large data sets, developing new algorithms, and developing new computational methods in mathematics and statistics, as well as training activities.

■ Increased participation in BioMaPS (Research at the Interface of the Biological, Mathematical and Physical Sciences). DMS would contribute \$4.2 million, a \$1.3 million increase from the FY 2013 request and a \$2.2 million increase from the FY 2012 actual level for innovative research at the interface of the

mathematical and physical and the biological sciences.

■ Participation in the expanded NSF-wide SEES (Science, Engineering, and Education for Sustainability) initiative. DMS's contribution of \$3.5 million (up approximately \$1.0 million from FY 2012) would support the development of potentially transformative mathematical, statistical, and computational methods needed for data analysis, modeling, and simulation related to climate, hazards, sustainability, and energy.

■ Participation in the cross-cutting SaTC (Secure and Trustworthy Cyberspace) initiative. DMS would continue its participation in this program by investing in efforts related to cryptography, new algorithms, risk assessment, and mathematical and statistical efforts related to cybersecurity.

■ The Materials Research Division and DMS would collaborate in addressing "complex problem solving to support strategic investments in cyberinfrastructure, instrumentation, and fundamental science to enable development of grand challenge communities."

■ The Science and Technology Policy Institute would continue to work with DMS on a pilot report on the NSF-funded mathematical institutes.

Discussions of the budgets for NSF's Computer and Information Science and Engineering Directorate, and for other federal agencies, are for another article, in another issue of *SIAM News*. (We note *See Budget on page 7*)

Reproducibility

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either as commented code or notebooks. Others capture the provenance of a computation or the complete software environment. Version control systems are not new, but current tools facilitate their use for collaboration and archiving complete project histories. For a description of current tools, see the workshop report [13] or wiki [8].

One of us teaches a graduate seminar that requires students to replicate results from a published paper [9]. This is one way to introduce tools and methods for replication into the curriculum, and it gives students first-hand appreciation for the importance

of incorporating principles of reproducibility into the scientific research process.

Conclusions

Recent events in economics and psychology illustrate the current scale of error and fraud in scientific research [3]. Following the lead of the United Kingdom, Australia, and others, the United States recently mandated public release of publicly funded research, including data [12]. We hope that this will help bring about the needed cultural change in favour of consistently reproducible computational research. While different types and degrees of reproducible research were discussed at the ICERM workshop, an overwhelming majority argued that the commu-

nity must move to "open research": research that uses accessible software tools to permit (a) auditing of computational procedures, (b) replication and independent verification of results, and (c) extension of results or application of methods to new problems.

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Earth

continued from page 3

opment of multiscale methods for seismic inversion, as in the work presented by A. Fichtner, in which multiple nested inverse problems on various scales are solved simultaneously (see Figure 2).

Progress in the mathematical and computational Earth sciences is extraordinarily rapid. Problems like the assimilation of massive seismic data sets into 3D full-waveform inversions would have been considered a luxury only a few years ago. The snakes and dragons of Hutton's time are definitely tamed. Nevertheless, numerous

challenges remain: Researchers in seismic imaging and inversion will have to abandon computationally less expensive acoustic approximations to fully exploit the wealth of information contained in seismic recordings. The transition to elastic modeling and inversion needs to go hand in hand with the development of powerful wave equation solvers that honor the complexities of the real Earth, including irregular topography, fluid–solid interfaces, anisotropy, and poroelasticity. With increasing complexity in modeling and inversion come new challenges for uncertainty quantification. Current methods rely on local approximations of the misfit functional, and they are effective for

single-parameter problems. Future methods for uncertainty quantification must be able to detect the presence of multiple local minima, and to operate in multi-parameter inversions that constrain not only isotropic wave speeds, but also anisotropy, attenuation, and density. Such methods, in turn, will alleviate many problems related to local minima of the misfit function.

Alison Malcolm is an assistant professor of geophysics in the Department of Earth, Atmospheric, and Planetary Sciences at MIT. Andreas Fichtner is an assistant professor in the Department of Earth Sciences at ETH Zurich.

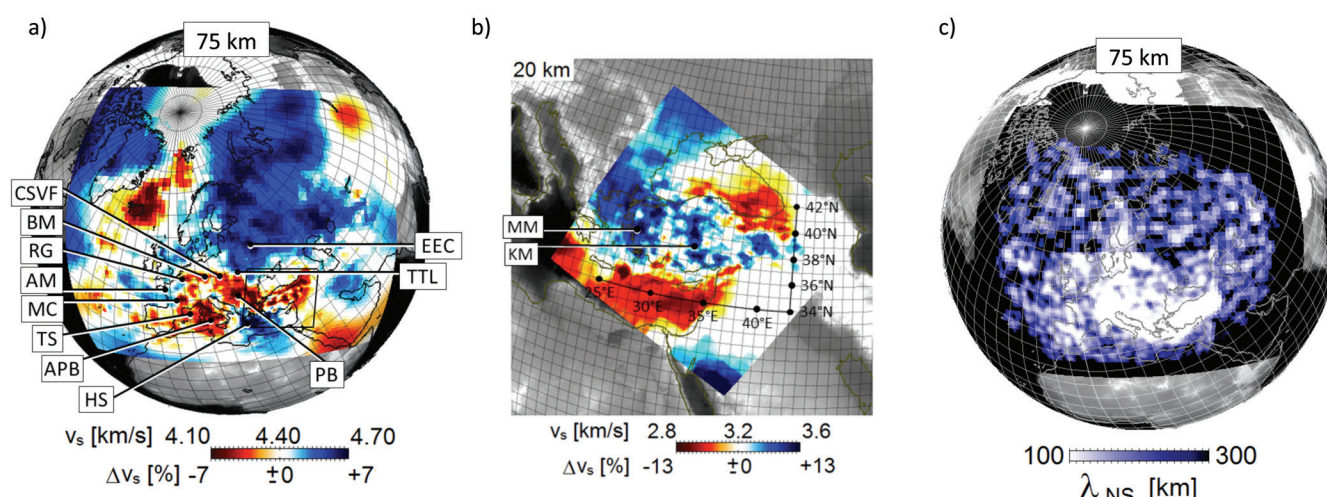


Figure 2. Multiscale full-waveform inversion with resolution analysis. (a) Shear velocity at 75 km depth beneath Eurasia. (b) Zoom-in view of the crustal velocity structure beneath Anatolia at 20 km depth. (c) Resolution length in N–S direction at 75 km depth, derived with second-order adjoints. AM, Armorican Massif; APB, Alghero–Provençal Basin; BM, Bohemian Massif; CSVF, Central Slovakian Volcanic Field; EEC, East European Craton; HS, Hellenic Slab; KM, Kirsehir Massif; MC, Massif Central; MM, Mendere Massif; PB, Pannonian Basin; RG, Rhine Graben; TS, Tyrrhenian Sea; TTL, Tornquist–Teisseyre Line.

Budget

continued from page 6

here that the substantial growth in the CISE budget is actually in large part a reflection of the relocation of the Office of Cyber-infrastructure to CISE.)

Conclusions

Several themes emerge from discussions of the Administration's FY 2014 budget. First, it is clear that national priorities continue to play a major role in driving research budgets. New initiatives, many of which support these research priorities, remain the means for enhancing the budgets of related research areas. Sastry Pantula, director of DMS, and Hank Warchall, deputy director of DMS, have emphasized the need for exciting new ideas—suggestions for research that supports national priorities and has the potential to drive new initiatives, as well as to advance the discipline. Pantula and Warchall have addressed these budget issues during presentations at the Conference Board of

the Mathematical Sciences and the Joint Policy Board for Mathematics, respectively.

How can the community help? We can communicate new ideas to leaders in the appropriate agencies. The SIAM Committee on Science Policy can support the community in these efforts.

A second theme that emerges is the need for the community to respond as vigorously as appropriate to calls for proposals. The magnitude of the response ("proposal pressure") can play a role in determining future allocations for a given initiative or program.

Finally, while in general our community has enjoyed strong funding support from the federal agencies, it is increasingly important to show how research advances in our discipline are essential to progress in science and engineering, as well as how research in our field is ultimately important to society. We need to tell our story. *SIAM News* continues to welcome such stories from the community.—*JMC (with the assistance of Lewis-Burke Associates in preparing the background material for this report).*

Careers

continued from page 3

If the division director concurs with your recommendation, it goes to the NSF Division of Grants and Agreements, which formalizes the award in a contract between NSF and the proposer's university. Details may be tweaked, but in the end it is your recommendation as program director that is decisive. I found this part of the work most satisfying; it seemed to strike a nice balance between autonomy and responsibility.

At the Meso-level—Division of Mathematical Sciences

DMS has a team of about 30 program directors. Some are permanent, some are rotators; the split, about 40–60 during my time at NSF, has shifted lately to about 50–50. There are good reasons for this arrangement; ideally, permanent program directors are the institutional memory, and rotators bring in the fresh ideas. In fact, it works pretty much as stated. In DMS, the permanent program directors and rotators worked very well together. Some of us were more outgoing than others, and some worked harder than others, but nobody considered DMS a sinecure. I appreciated the help I got from my permanent colleagues when I first came to DMS. They guided me through the labyrinth of data bases and helped me conquer the vagaries of Windows.

As a DMS program director, you are expected to participate in the management of various programs that have been developed to foster collaboration and communication among mathematical scientists. I was particularly interested in the Focused Research Groups (FRGs), a program that funds teams of researchers to address well-defined problems or problem areas in the mathematical sciences. Proposals submitted to this program go through a more extensive review process than proposals from individual researchers, and the eventual recommendation must be endorsed in a joint meeting of all the DMS program directors. The panel reviews and any supplementary ad hoc (mail) reviews must be strongly positive, and somehow you have to make the argument that "your" proposal is as compelling as strong proposals from other areas of mathematics. It is a bit like comparing apples and oranges, and your responsibility is to convince your colleagues that your shining apples are as deserving of support as their bright oranges. The colleagues are friendly, but the competition is stiff, and you have to know how to make your case.

Major programs in DMS are handled by a "Management Team," which consists of two to five program directors, depending on the size of the program. In my second term I became a member of the Institutes Management Team, which is responsible for overseeing the portfolio of Mathematical Sciences Institutes supported by DMS. This was a fascinating and most rewarding experience. The institutes are the "major facilities" of the mathematical sci-

ences research community and the jewels in the crown of DMS. Each institute has its own character, and collectively they demonstrate the breadth and depth of current mathematics and statistics. I particularly enjoyed participating in site visits to review the organization of programs and the quality of governance. These visits were very illuminating, as well as exciting and—because of the high visibility of the institutes within the universities—a bit intimidating. Lots of good things happened, but nothing is perfect, and the challenge was always to make every visit a constructive experience for all involved.

At the Macro-level—National Science Foundation

Managing a portfolio of research projects in applied mathematics was only part of my job. I quickly became involved in several activities beyond DMS. This was probably natural, given my prior experience in a multidisciplinary research environment. In my first term I particularly enjoyed my involvement in the three ongoing NSF-wide initiatives: Nano-science and Technology, Information Technology Research (ITR), and Bio-complexity. My responsibilities included participating in the management of these programs, handling proposals, organizing reviews, and negotiating with colleagues in other disciplines about funding recommendations. These activities gave me first-hand experience in managing a broad portfolio of research proposals in areas in which I had only limited expertise.

Programs like Nano, ITR, and Bio-complexity reflect a national research agenda, which is set by the U.S. Congress and implemented at the level of NSF. As a program director, you don't have much influence over the goals of such programs, but you do have significant influence over how they are implemented and managed. Other NSF-wide programs emerge from the research community, and this is where I found that program directors can have a much more direct influence. As program director, you are in touch with the research community, you pick up ideas, and discuss these ideas internally with colleagues in NSF, usually in NSF working groups. The ideas are tested out in workshops with outside experts, worked out in white papers and reports, and, if all goes well, eventually endorsed and supported by upper-level management.

During my tenure at NSF I participated in several such working groups. A working group in the Mathematical and Physical Sciences (MPS) Directorate on cyber-science eventually led to the NSF-wide program Cyber-enabled Discovery and Innovation (CDI), another to the MPS-wide program Approaches to Combat Terrorism (ACT), the latter with significant support from the intelligence community. Both programs ran for several years and supported several interesting research projects in the mathematical sciences. One of my lasting legacies is a Dear Colleague Letter (still active but in need of updating) issued joint-

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ly with my colleague Eduardo Misawa in the Engineering Directorate soliciting proposals from mathematicians and engineers for collaborative research in complex systems.

The Global Perspective

After serving a little more than six years as program director, I asked myself whether I had made a difference. My answer was unambiguous: yes. I had been able to support good science that will eventually benefit society and help up-and-coming scientists who may become leaders in our discipline. At a personal level, I had become familiar with a broader range of mathematics. It was often hard work, but most of it had been rewarding. And I had really enjoyed interacting with my colleagues, who were smart, interesting, and focused on doing a good job for the research community. Without hesitation, I recommend that you give it a try. If your expectations are realistic, and you approach the job with

curiosity and an open mind, you will find it an enriching experience.

Hans Kaper is an applied mathematician who wears many hats. He is currently affiliated with Georgetown University and is co-director of the "Mathematics and Climate Research Network" (MCRN). Kaper is a corresponding member of the Royal Netherlands Academy of Sciences and a Fellow of the Society for Industrial and Applied Mathematics, class of 2009. He is editor-in-chief of SIAM News, chair of the SIAM Activity Group on Dynamical Systems, and a member of the SIAM Committee on Science Policy. Kaper received a PhD in Mathematics and Physical Sciences from the University of Groningen, the Netherlands. He can be reached at kaper@mathclimate.org.

Sue Minkoff (sminkoff@utdallas.edu), of the University of Texas at Dallas, is the editor of the Careers in the Math Sciences column.

Large-scale Networks

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sion of the graph) to make the problem tractable. Benjamin A. Miller and Matthew C. Schmidt (MIT Lincoln Laboratory) discussed methods for anomaly detection in time-varying graphs and its utility for finding real-world malicious activity in a graph of computer connections.

■ High-performance computing was a theme in many talks. Big graphs pose challenges that differ from those of traditional scientific computing. David A. Bader (Georgia Tech) is involved in the Graph 500 Benchmark, which has a goal of guiding the design of hardware and software architectures that are appropriate for network science. Henning Meyerhenke (Karlsruhe Institute of Technology) discussed HPC clustering methods.

■ Several speakers described new packages for working with graphs. Jason Riedy (Georgia Tech) tackles the big-data problem with streaming analysis via the STINGER

package, keeping only a small part of the data in memory at any time. Aydin Buluç (Lawrence Berkeley National Laboratory) presented the Knowledge Discovery Toolbox, which is accessible to domain scientists, but uses the Combinatorial BLAS library for high performance. Joseph Gonzalez (UC Berkeley) discussed GraphLab, which uses clever hashing and approximations for fast graph computations.

CSE13 was remarkable for demonstrating both the growing importance of network analysis itself and the role of applied mathematics within network analysis.

Tamara G. Kolda and Ali Pinar are Members of the Technical Staff at Sandia National Laboratories in Livermore, California.

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CSE 2013

Navigating the Paths to a Career in CSE

By Andrew D. Davis

The interdisciplinary nature of many academic questions and the wide array of applications can make choosing a career path in computational science and engineering difficult. Theoretical tools are constantly being developed and must be implemented and used in the seemingly endless array of applications. This year's SIAM Conference on Computational Science and Engineering scheduled a panel discussion (sponsored by The MathWorks and IBM) to help undergraduate and graduate students navigate this diverse field and choose a career path. The four panelists, Kirk E. Jordan, Tamara G. Kolda, Jill Reese, and Gilbert Strang, served as representatives of careers in academia, industry, and national labs. The discussion focused on the progression of typical careers in each of the three areas, the chal-

lenges faced in switching career tracks, and ways to supplement graduate school with internships.

Many in the audience were interested in pursuing tenure-track jobs at research universities. Some had questions about how to apply for such jobs. Specifically, one student wanted to know the departments to which computational science and engineering students should apply. As for many in the audience, this student's research was a blend of mathematics, computer science, and an application. Because many universities do not have computational science departments, it was unclear whether the student should apply for a professorship in mathematics, computer science, or an engineering discipline. The panel's suggestion: Rather than pick a single department, look for openings in any department that has a computational component, the logic being

that an applicant's current research and research interests will determine whether s/he matches what the department wants. The interdisciplinary nature of computational applications means that students with similar educational backgrounds can pursue academic careers in very different fields.

Industrial companies often hire students with degrees in CSE. Students in the audience who were interested in pursuing research-based careers asked how research at a company was different from research at a university. One student, in particular, wanted to know how difficult it would be to transition from industry to academia. The panel pointed to the importance of journal publications for success in academia, whereas the ability to publish in an industrial job depends on the job and the company. Students pursuing industrial careers, but with an interest in moving to academia later in their careers, were encouraged to look for jobs that would allow them to publish. Two of the panelists had had graduate students work for them, either as interns or in collaboration with a professor; they suggested that pursuing jobs with such opportunities would facilitate a switch from industry to academia.

Labs account for many of the career options for students graduating with degrees in CSE. One student asked the panel to compare being a researcher at a lab to being a professor. A major difference identified by the panel was the effect of not having students on the research group structure. At universities, professors use their advisees to create a research direction for the group. At labs, which do not have students, the panel described a system based more on peer-

to-peer collaboration. Often, each person involved in a lab project is an expert in a different field, as opposed to universities, where the students in a group are studying similar subjects.

Students were also interested in learning about more short-term career options. A few students had completed or been offered internships. Should graduate students take internships? Or should they focus more on their dissertations? The panel began by pointing out that internships can often be designed to relate to students' research, especially if their advisers have engaged in industrial collaborations. Two panelists had supervised graduate interns, and one had had internships as a graduate student. They argued that such experiences, by exposing students to jobs outside academia, might help them decide which of the three typical career paths best suits them. Students then asked how to approach their advisers about accepting internships. The panel encouraged a direct approach; advisers, they pointed out, often have collaborative projects that provide internship opportunities. Additionally, advisers can make sure that an internship does not interfere with the student's graduation time line.

Overall, students wanted to know what they could do to maximize their opportunities for career advancement. Among other concerns were how to choose a PhD program and how long a potential employer would expect a PhD to take. The panelists conveyed diverse points of view on how students could become successful computational scientists. In the end, their advice was to remain passionate and curious and to pursue any appealing opportunity that arises.

Andrew D. Davis is a PhD student at MIT, working under the supervision of Youssef Marzouk and Patrick Heimbach. His dissertation research is in large-scale parameter inference for prediction.



Organizers of the Student Careers Panel (from left): Luke Olson, University of Illinois at Urbana-Champaign, Karen Willcox, MIT, and Gianluigi Rozza (chair), SISSA, International School for Advanced Studies, Trieste, Italy. Photo by Susan Whitehouse.

Quantum Mechanics

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DFT has become a route to scalable quantum mechanical methods. In the traditional Kohn-Sham DFT, ρ is constructed from single electron orbitals, which are analogous to the wavefunctions mentioned above. With only one electron, these orbitals have three degrees of freedom and thus greatly simplify the calculations. Nevertheless, the computational cost increases cubically with N because of the need to calculate and orthogonalize N orbitals. This cubic scaling has limited Kohn-Sham DFT calculations to systems with a few thousand atoms, and there has been a lasting push to develop linear scaling methods using both physical and computational approximations [1].

At CSE 2013, Emily Carter of Princeton University discussed recent work of her group to develop orbital-free DFT (OF-DFT) methods, which eschew the use of orbitals in quantum mechanical calculations. The new methods use only the electron density to perform the calculations. One of the benefits of orbitals is that they simplify the calculation of the electrons' kinetic energy; however, there is no physical requirement to use orbitals. In principle, the kinetic energy can be written as a functional of ρ , and the main challenge in advancing OF-DFT is finding suitable—that is, physically accurate and computationally feasible—forms for this functional. One example is

$$KE[\rho] =$$

$$\int d\mathbf{r}_1 \int d\mathbf{r}_2 \rho(\mathbf{r}_1)^{5/6} F(\mathbf{r}_1, \mathbf{r}_2; \rho) \rho(\mathbf{r}_2)^{5/6}.$$

The Carter group, which has been developing these functionals for the last fifteen years [5,9], has exposed two computational hurdles in evaluating them for OF-DFT applications.

First, in the simplest approximation, F is a function of only $|\mathbf{r}_1 - \mathbf{r}_2|$ and the

functional can be viewed as a convolution integral with a nonlocal kernel (F). Evaluation of the kinetic energy functional can then be carried out with Fourier transforms. Although the fast Fourier transform has a computational complexity of $\mathcal{O}(n \log(n))$, its requirement of global all-to-all communications intrinsically limits the parallel scalability of OF-DFT methods. Fine-tuning of the FFT's communication patterns is one way to help with this scaling; exploiting the physics of the OF-DFT application is another. Specifically, the kernel $F(\mathbf{r}_1, \mathbf{r}_2)$ is short-range, or can, at least, be made short-range without a significant loss of accuracy. As a result, small-box local FFTs can be used instead of global FFTs.

Second, the utility of the FFT is potentially hampered by the form of F . It is not guaranteed (or expected) that $F(\mathbf{r}_1, \mathbf{r}_2)$ will be a function simply of $|\mathbf{r}_1 - \mathbf{r}_2|$; it might also depend on ρ . For example, the kernel may be $f(k_f |\mathbf{r}_1 - \mathbf{r}_2|)$, where k_f is proportional to $[\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)]^{1/6}$ or $[\rho(\mathbf{r}_1) + \rho(\mathbf{r}_2)]^{1/3}$. Due to this dependence on ρ , FFTs cannot be directly applied to evaluate the functional (in general). The Carter group has overcome this problem by employing Taylor expansions of F with respect to ρ about the average value of ρ . The FFT can then be used on each term in the expansion; multiple FFTs are required to evaluate the functional. Unfortunately, the Taylor expansions might break down or converge slowly, particularly in systems with large fluctuations in ρ (such as insulators). Better ways to deal with this problem would be welcome.

Armed with this OF-DFT approach to quantum mechanical simulations, Carter demonstrated its applicability to numerous physical systems, including metals, insulators, and molecules. Owing to the favorable scaling of OF-DFT methods, some of the simulated systems had millions of atoms [6], showing that some large, "holy grail"

systems are coming into reach (at least on supercomputers). For one example (shown in Figure 1), Carter detailed how OF-DFT calculations can probe the mechanical properties of nanomaterials under strain [7].

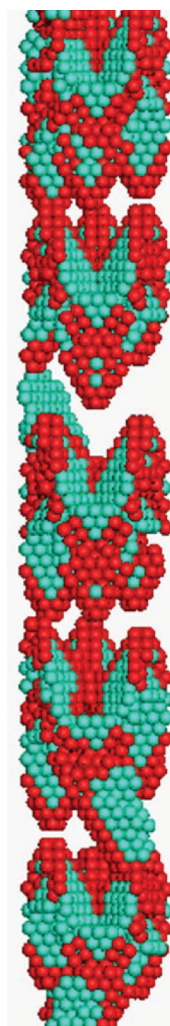


Figure 1. Structure of an aluminum nanowire being stretched. OF-DFT calculations of large systems help illuminate the mechanical properties (here, sliding planes) of materials. See [7] for more details. Figure used with permission of Emily Carter.

Extrapolating from the successes of quantum chemistry programs in the last twenty years, computational investigations of these types should help guide experimental efforts to understand and design quantum systems. Simulations of large biomolecules might lead to better pharmaceuticals, and

high-throughput computations of materials (as called for in the Materials Genome Initiative) could reduce the parameter space for building better batteries. At the end of the day, the quest for bigger, faster, and more accurate quantum mechanical simulations offers great scientific advances and poses ongoing challenges to the physical, chemical, mathematical, and computational communities.

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