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Paleo-structure of the Earth's Mantle: Derivation from Fluid Dynamic Inverse Theory

By Hans-Peter Bunge

Mantle convection is vital to our Earth system. The relentless deformation produced inside the Earth's mantle by slow, viscous creep has a far greater impact on our planet than might be immediately evident. Continuously reshaping the Earth's surface, mantle convection provides the enormous driving forces necessary to support large-scale horizontal motion in the form of plate tectonics and the associated earthquake and mountain-building activity. At the same time, mantle convection induces substantial vertical motion in the form of topography dynamically maintained by lateral pressure gradients beneath tectonic plates. This vertical motion, on the order of 1 km or so, is perhaps the most spectacular manifestation of mantle convection—and its most enduring impact upon the entire Earth system. It is expressed ultimately on all scales—local, regional, global—through sea level variations and flooding events known from the geologic record to have reached deep into the interiors of continents (see Figure 1), with profound consequences for the opening and closure of marine pathways and their impact on the global climate system. The link between deep mantle processes and their surface manifestations is an issue of direct practical relevance, in particular concerning the evolution of sedimentary basins and their paramount economic importance in terms of hydrocarbon and other resources (see [4] for a recent review).

The time scale of geologic processes, typically on the order of millions of years, is sufficiently long that the Earth's mantle, although stronger than steel and capable of transmitting seismic shear waves, can be treated as a fluid. Mantle convection is thus governed by hydrodynamic field equations expressing the fundamental principles of mass, momentum, and energy conservation. Here, the form of the momentum equation is of particular interest. Because of the very high viscosity of the Earth's mantle (in the range of 10^{21} Pa·s), the momentum conservation law simplifies to the Stokes equation, where the inertia terms can be ignored owing to the negligible flow velocities (on the order of cm/year) and accelerations. The resulting instantaneous balance of frictional and buoyancy forces is represented by an elliptic partial differential equation, with driving forces for the flow arising from lateral density anomalies in the mantle. Time-dependence enters the mantle convection system through the energy equation, which describes the transport of heat inside the Earth's mantle by advection and conduction.

A rich spectrum of physics is compatible with the governing equations. Powerful computer models are available for simulating the mantle convection process (see [12] for a recent review), and software development now under way opens a path to exascale computing [3,8]. But grave uncertainties compromise our knowledge of crucial material parameters (temperature, composition, strength) in the mantle. In principle, it is possible to resolve these uncertainties by testing mantle convection models against data, such as paleo-shorelines or variations in the structure of sedimentary basins, gleaned from the geologic record. But geologic events—by definition—happened in the past. Modeling paleo-mantle convection currents so that they can be linked explicitly to the geologic record thus requires knowledge of the state of the convective system in the past, which, of course, is not available to us.

Over the past two decades, geophysicists have constructed *mantle circulation models* (MCMs) to overcome the initial condition problem [1]. Such models (see Figure 2) compensate for the lack of initial condition information by postulating a priori a pattern of mantle heterogeneity for an earlier geologic period. In this approach a given model is integrated forward to the time of interest, with a model for the history of past plate motion (see [10] for a recent review) serving as the surface boundary condition for velocity in the momentum equation. It would be impossible to obtain meaningful MCMs without the geologic record of past plate motion: Tectonic plates cover 80% of the total surface area of the mantle, with the core–mantle boundary (CMB) accounting for the other 20%. Thus, past plate motion models constrain the history of mantle

See **Mantle Convection** *on page 8*

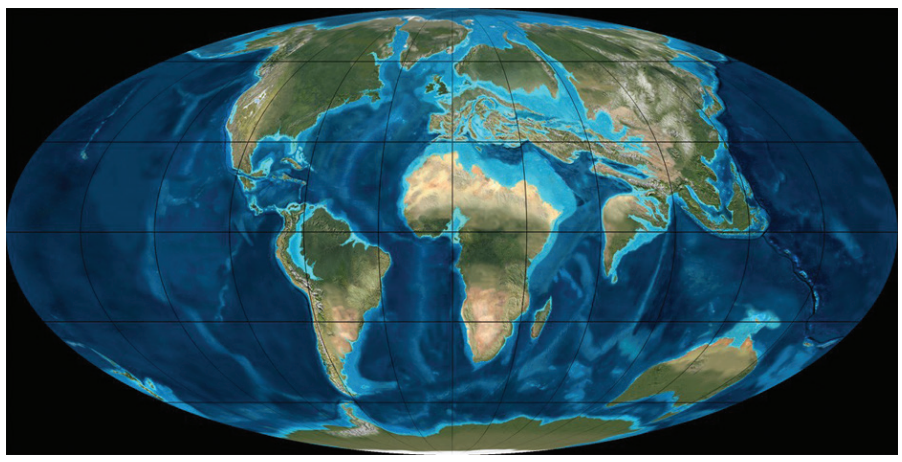

Figure 1. *Schematic representation of Earth's paleogeography corresponding to conditions in the Eocene, some 50 million years ago. In the comparatively recent Eocene epoch (less than 1% of Earth's history has occurred since), the Earth system differed substantially from today, with extended inland seas covering portions of the continents, e.g., in northern Africa, central Europe, and parts of Russia. In these regions Earth's mantle experienced substantial change because of active subduction of the ancient Tethys ocean. Subsidence in the Tethys realm had a profound impact on ocean circulation and climate, enabling the formation of equatorial marine pathways that are mostly closed now and serving as a major depositional centre. Whereas the distribution of marginal (inland) seas can be inferred reasonably well from paleo-shorelines, greater uncertainty is associated with the subarial paleotopography depicted here. Image from the paleogeography maps of R. Blakey, Northern Arizona University; www2.nau.edu/rcb7.*

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The 2013 Nobel Prize in Chemistry Celebrates Computations in Chemistry and Biology

By Tamar Schlick

Progress in science depends on new techniques, new discoveries and new ideas, probably in that order.

—Sidney Brenner (2002 Nobel laureate in physiology or medicine)

It was an exciting day for the fields of computational chemistry and biology when news of the 2013 Nobel Prize in Chemistry filtered in early on the morning of October 9, 2013. Awarded to Martin Karplus, Michael Levitt, and Arieh Warshel for the "development of multiscale models for complex chemical systems," the prize provided a welcome "seal of approval" to a field that historically struggled behind experiment. This is not unlike the traditional division between pure and applied mathematics, stemming from the difference between using *exact* theories to solve *ideal* problems versus *approximating* complex physical systems to solve *real* problems. Historically, the results of simulations for biological and chemical systems were judged by their ability to *reproduce* experimental data. Thus, computational predictions had to pass the scrutiny of experimentalists, who employ direct, though not error-free, measurements, especially for large systems. If results from computations agreed with experiment, they were considered uninformative, but if they predicted properties ahead of experiment, they were considered unverifiable and hence unpublishable!

In time, however, just as applied mathematics and computational science evolved into huge successful fields in their own right, computations in chemistry and biology are finally recognized not only as valid for making predictions and generating insights into physical systems, but as necessary for addressing complex problems we face in the 21st century. In fact, clever modeling ideas and methods for the design of appropriate algorithms are *essential* for discovering the information missing from products of current high-throughput technologies; this is because genome sequencing, microarrays, and other technologies and instrumentation produce voluminous amounts of genomic sequences and related data for systems whose structures, functions, and interactions are largely unknown.

This is not the first time the Nobel committee celebrated computations. In 1998, the Nobel Prize in Chemistry was awarded to Walter Kohn for the development of density-functional theory, and to John Pople for the development of computational techniques and the pioneering program GAUSSIAN for quantum chemistry calculations. But this year's prize-winning contributions are more general and perhaps more far-reaching. The separate work of the three laureates, and their interactions with each other and with others in the community, offer an opportunity to examine the history of the field and view how people, ideas, and technologies come together to shift existing paradigms. The prize also provides an exceptional occasion to look into the bright future of a field whose three powerful arms—physical experimentation, theory, and computer simulation—can lead to the solution of key problems ranging from the workings of individual proteins to the packaging of DNA, DNA repair and RNA editing processes, and interactions among and within cells, organs, and organisms (Figure 1).

Field Trajectory

The roots of molecular modeling reside with the notion that molecular geometry, energy, and many related properties can be calculated from mechanical-like models subject to basic physical forces. These molecular mechanics concepts of molecular bonding and van der Waals and electrostatic forces arose naturally from quantum

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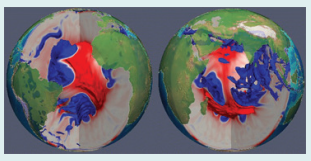
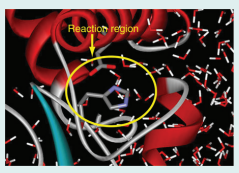
SIAM Elections
At press time, the results of the fall elections are in: Officers elected or re-elected to terms beginning in January 2014 are **Pam Cook** (president elect),

Simon Taverner (secretary), and **Daniel Szyld** (vice president at large). **Tim Kelley**, **Bob Kohn**, and **Randy LeVeque** won election to the Board of Trustees, and **Liliana Borcea**, **Angelika Bunse-Gerstner**, **Oscar Bruno**, and **Felix Otto** to the Council.

1 Paleo-structure of the Earth's Mantle: Derivation from Fluid Dynamic Inverse Theory



1 The 2013 Nobel Prize in Chemistry Celebrates Computations in Chemistry and Biology



2 Models and Algorithms for Exascale Computing Pose Challenges for Applied Mathematicians

5 Mathematics, Management Consulting, and Emerging Markets
With master's degrees in engineering and applied math, background in IT and computational science, and an MBA, this issue's Careers columnist entertained thoughts of "a nontraditional professional path." Management consulting—the profession he chose as "providing the greatest long-term flexibility"—is "the practice of helping organizations improve their performance"; analytical skills top the list of qualities sought by recruiters.

2 Obituaries

7 Professional Opportunities

Obituaries

Jan Willems passed away on August 31, 2013, after fighting a serious illness for several years.

He will be deeply missed by his former students and his many collaborators and colleagues, in Groningen and around the world, in his beloved field of systems and control. Although he played a prominent role in shaping the field over an exceptionally long period, he was as happy talking to young scientists as to top scientists. His door was always open to all.

Jan Willems was born on September 18, 1939, in Bruges, Belgium. After finishing his studies in engineering at the University of Ghent, he moved to the United States, where he obtained an MSc in electrical engineering from the University of Rhode Island in 1965, and a PhD in electrical engineering from the Massachusetts Institute of Technology in 1968. His doctoral dissertation, on input/output stability, appeared as the monograph *The Analysis of Feedback Systems* (MIT Press, 1971). From 1968 to 1973, as an assistant professor in the Department of Electrical Engineering at MIT, he made fundamental contributions to the subject of optimal control, in particular linear quadratic problems with indefinite cost and the associated algebraic Riccati equation. His ground-breaking papers "Least Squares Stationary Optimal Control and the Algebraic Riccati Equation" (*IEEE Transactions on Automatic Control*, 1971), and "Dissipative Dynamical Systems, General Theory" and "Dissipative Dynamical Systems, Linear Systems with Quadratic Supply Rates" (*Archive for Rational Mechanics and Analysis*, 1972) led to the notions of dissipative systems and linear matrix inequality, which are generally considered the main concepts and tools for analysis in robust control, for both linear and nonlinear systems.

Jan Willems, 1939–2013

In 1973, Jan was appointed professor in the Department of Mathematics at the University of Groningen in the Netherlands to set up the new specialization of Systems and Control. During this period he worked in subjects from differential games, realization theory, and physical systems. By the end of the 1970s his research interests had shifted, to a geometric approach to control and to problems of disturbance decoupling. The latter research area attracted considerable attention at the time. In the late 70s he introduced the notions of almost controlled invariant and almost conditioned subspaces, which made it possible to resolve problems of approximate disturbance decoupling by high-gain feedback and singular linear quadratic problems. During this time, Jan was a founder (with Roger Brockett) of the journal *Systems and Control Letters*, which first appeared in 1981; he was a managing editor of the journal from 1981 to 1994. From 1989 to 1993, he was editor-in-chief of *SIAM Journal on Control and Optimization*.

In the early 80s, Jan became conscious of the limitations of input/output thinking as the framework for the analysis and synthesis of open and interconnected systems. This uneasiness eventually led him to develop what is called a behavioral approach, in which a dynamical system is simply viewed as a family of trajectories. This work also emphasizes the importance—in, for example, object-oriented modeling—of latent variables in addition to the manifest variables that are the model's main concern. In the behavioral setting, interconnection is viewed as variable sharing, and control is viewed as interconnection, with feedback as an important special case. The original ideas were introduced in an early paper in the Italian journal *Ricerche di Automatica*. More extensive development followed in a three-part paper in *Automatica* (1986 and 1987), for which he received an *Automatica* outstanding paper award in 1988. An important resource for his behavioral ideas is also the textbook (co-authored with Jan Willem Polderman) *Introduction to Mathematical Systems Theory: A Behavioral Approach* from 1998.

In 1998 Jan received the IEEE Control Systems Award and the *IEEE Control Systems Magazine* Outstanding Paper Award for "300 Years of Optimal Control, from the Brachystochrone to the Maximum Principle" (co-authored with Hector Sussmann).

During his years in Groningen, Jan played an important role in the systems and control community within the Dutch universities. Drawing on his natural charm and skills in diplomacy and persuasion, he was one of the founders and (from 1986 to 1996) chairperson of the Dutch Network of Systems and Control. The main goal was a national graduate school that would offer courses in systems and control theory—an ambition that was realized. The network was the precursor of the Dutch Institute of Systems and Control, which was

See **Obituaries** *on page 3*

Models and Algorithms for Exascale Computing Pose Challenges for Applied Mathematicians

By Jeffrey Hittinger, Sven Leyffer, and Jack Dongarra

Computer architectures are changing, from the PC under your desk to the world's largest supercomputers. Processor clock speeds have been stagnating since 2002, and future performance gains are expected to come from increased concurrency through larger numbers of cores or specialized processing units. For supercomputers, constraints on power are expected to reduce the amount of memory per core, alter the organization of the memory, and reduce resilience [3]. These changes in hardware architecture present opportunities for applied mathematicians to develop new models and algorithms with the new constraints in mind.

For several years, the U.S. Department of Energy, whose critical missions rely heavily on high-performance computing, has been preparing for these changes. Numerous DOE workshops [2] have been held, with the focus mainly on the groundbreaking science that could be achieved at the exascale and on the computer science challenges that need to be addressed. It has become clear, however, that the full benefits of computing at the exascale cannot be achieved without substantial research on new algorithms and models, which will require close collaboration between applied mathematicians, computer scientists, and application domain experts.

DOE's Exascale Mathematics Working Group

The Advanced Scientific Computing Research Program in DOE's Office of Science has formed the Exascale Mathematics Working Group; the group's mission is to identify opportunities for mathematical and algorithmic research that will enable scientific applications to harness the full potential of exascale computing. EMWG is composed of applied mathematicians from across the DOE national laboratories. In the spring of 2013, EMWG issued a call to the greater applied mathematics community for position papers on exascale computing research challenges.

Of the 75 position papers received, 40 were selected for presentation and discussion at a workshop held in Washington, DC, August 21–22, 2013. More than 70 participants from DOE laboratories, universities, and U.S. government agencies attended the workshop. Topics of the position papers presented include scalable mesh and geometry generation, multiphysics and multiscale algorithms, in situ data analysis, adaptive precision, asynchronous algorithms, optimization, uncertainty quantification, and resilience.

Three main themes emerged at the workshop: hierarchies in models, algorithms, and decision processes that improve parallel performance; new approaches for exposing additional concurrency; and algorithmic approaches that address the resilience challenges. We summarize these ideas here; more details can be found in the original position papers and workshop presentations available on the EMWG website [1].

Hierarchies in Models and Algorithms

Many mathematical models live within hierarchies based on scales or physical fidelity. Exascale computing will provide an opportunity not only to develop hybrid models and algorithms that couple across scales, but also to use the hierarchy to accelerate or improve expensive algorithms at the fine scales. New algorithms will improve our understanding of the scale coupling and dynamics of the hierarchical physical processes. Hierarchical algorithms, such as multigrid and hierarchical adaptivity of mesh or order, should promote scalability

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Obituaries

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founded in 1995 and whose board Jan chaired from 1995 to 1999.

In 1993 Jan was the general chair of the European Control Conference, which was held in Groningen, and he served as president of the European Union Control Association from 1994 to 1996. From 1994 to 1996, he was president of the Dutch Mathematical Society.

In 2003, Jan Willems became an emeritus professor of the University of Groningen and moved to Antwerpen, Belgium. There he was warmly welcomed at K.U. Leuven as a guest professor in the Department of Electrical Engineering, part of the research group Signals, Identification, System Theory, and Automation.

After his formal retirement from Groningen, Jan remained active as ever, fruitfully collaborating with many colleagues and actively participating in conferences and workshops all over the world. Until very recently he was an active participant in the annual IEEE Conference on Decision and Control, enjoying conversations with old friends and colleagues, but also inspiring young researchers with suggestions and (usually) positive criticism. His unquenchable scientific energy is manifest in the nearly one hundred publications he co-authored after his official retirement. Many of these later publications show his very deep thinking, scientific maturity, and clear vision on the field of systems and control. An example is the paper "The Behavioral Approach to Open and Interconnected Systems," which appeared in *IEEE Control Systems Magazine* in 2007.

It is hard to imagine a world without Jan Willems, even though the products of his scientific activity, his contributions in shaping the field of systems and control, and his influence on the scientific taste and thinking of his students will remain.—*Harry Trentelman, University of Groningen.*

Exascale Challenges

continued from page 2

by providing a means to decompose and coordinate efficient solution of problems.

Finding Additional Concurrency

Several position papers discussed the development of parallel-in-time algorithms. In parallel-in-time schemes, the space–time problem is decomposed in parallel and organized in a hierarchical, iterative (but physical) way such that, for a sufficiently large number of processors, one achieves additional parallel speed-up by exploiting concurrency in the temporal direction. Related approaches presented include pipelined Krylov solvers that hide synchronization and hierarchical, tree-based techniques for sparse linear systems that reduce communication; iterative techniques effectively introduce a "pseudo-time," which may provide an additional dimension over which to decompose with relaxed synchronization. Exascale architectures should make it possible to raise the level of abstraction, from basic forward simulation to optimal design and control and/or to uncertainty quantification; this should lead to additional scope for exploiting algorithmic concurrency. In situ data analysis also offers an opportunity to increase concurrency locally and to reduce global communication and synchronization.

Fault Tolerance and Resilience

A persistent undercurrent in the discussions was fault tolerance. It is still unclear how (un)reliable an exascale computer may be, but scalable means for recovering from faults like node failures will be needed to ensure scientific productivity. Currently, fault recovery is achieved predominantly by synchronous checkpointing/restarting, which will not be feasible with extreme concurrency. Algorithmic techniques for recovering from faults while preserving accuracy may become more important as hardware experts sort out the extent of low-level fault detection support that may be provided.

Conclusions

The road ahead contains a rich set of theoretical, algorithmic, and modeling challenges and opportunities brought about by the paradigm shift in computing architectures. There is much work to be done to develop the theory behind the stability, consistency, and accuracy of algorithms as we increase asynchrony, reduce communication, and decompose problems in search of more concurrency. Concerns about resilience are only one aspect of the greater issue of correctness, and applied mathematicians will need to reconsider verification and validation for hybrid, multiphysics, multiscale algorithms. The exascale challenges and opportunities will not only affect computation at the highest scale, but are expected to influence computational science at all scales and levels.

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[2] http://science.energy.gov/ascr/news-and-resources/program-documents/.

[3] P. Kogge, ed., CSE Department Tech. Rep. TR–2008–13, University of Notre Dame, September 28, 2008.

Jeffrey Hittinger is a computational scientist in the Center for Applied Scientific Computing at Lawrence Livermore National Laboratory. Sven Leyffer is a senior computational mathematician in the Mathematics and Computer Science Division at Argonne National Laboratory. Jack Dongarra is a university distinguished professor in the Department of Electrical Engineering and Computer Science at the University of Tennessee and a distinguished research staff member in the Computer Science and Mathematics Division at Oak Ridge National Laboratory.

Nobel Prize

continued from page 1

chemistry theory developed in the 1920s, leading to several different Nobel Prizes in Physics: to Bohr, de Broglie, Dirac, Heisenberg, Planck, and Schrödinger. In particular, quantum chemistry led to the Born–Oppenheimer approximation, in which atomic nuclei can be considered fixed on the time scale of electronic motion. Quantum chemistry was also the basis of Linus Pauling's fundamental research on the nature of the chemical bond and its application to the elucidation of the structure of biological molecules, as recognized by the 1954 Nobel Prize in Chemistry. In fact, ahead of his time, and relying in part on quantum chemistry (concepts of orbital hybridization, ionic bonds, and aromatic compounds) mastered during his earlier studies with Bohr and Schrödinger, Pauling correctly predicted a planar peptide bond in 1951. Based on this notion, he used paper cutouts to predict the α-helix and β-sheet as the primary structural motifs in protein secondary structure. Watson and Crick used wire models around that time to deduce the structure of DNA. While the first molecular mechanics calculations, notably of Frank Westheimer, date to the 1940s, computers were not yet available for practical applications. Other early contributors to molecular modeling include Kenneth Pitzer and James Hendrickson, as highlighted in [5].

In the early 1960s, work on the development of systematic force fields began independently in three laboratories around the world. These pioneers were the late Shneior Lifson of the Weizmann Institute of Science, Harold Scheraga of Cornell University, and Norman Allinger of Wayne State University and later the University of Georgia. At Weizmann, a second-generation computer was already available to the researchers, called Golem for a powerful but soul-less hero in Jewish folklore. Scheraga and Allinger used a CDC-1604 computer and an IBM 360/65 machine, respectively, in those early days.

With their talented co-workers—notably Némethy with Scheraga, Warshel, who was Lifson's graduate student, and Levitt, who came to Lifson at Weizmann with a Royal Society fellowship—the groups pursued the arduous task of selecting functional forms and parameters for bonded and nonbonded interactions from spectroscopic information, heats of formation, structures of small compounds, other experimental data, and quantum-mechanical information. Importantly, hydrogen bonds were expressed by simple electrostatic interactions. A comparison of calculated structures and energies for families of compounds composed of the same basic chemical subgroups with experimental observations led to an iterative process of force-field refinement. The three resulting empirical force fields—consistent force field (CFF) [13], empirical conformational energy program for peptides (ECEPP) [15], and the molecular mechanics family MM1, MM2, . . . [2] formed the basis for numerous programs and applications in the decades to come.

While the Lifson/Warshel and Allinger schools used energy minimization to calculate molecular properties, Scheraga and co-workers pursued the ideas of statistical mechanics to generate conformational ensembles of molecules that approach the statistically correct Boltzmann distribution. These concepts are now prevalent in modern Monte Carlo and molecular dynamics simulations. Scheraga also combined his expertise in experimental physical chemistry with theory in very early investigations of many biological problems, such as protein stability and folding pathways [19].

In their pioneering Cartesian coordinate CFF treatment [13], Levitt, Lifson, and Warshel calculated energies, forces (first derivatives), and curvature (Hessian) information for the empirical potential function. Levitt and Lifson soon reported the first energy calculation of entire protein molecules (myoglobin and lysozyme) [11]; they used not only the empirical potentials but also experimental constraints to guide the minimization, by the steepest descent method. Levitt and Warshel later followed with a pioneering coarse-grained protein simulation [12], with atoms grouped into larger units and normal modes used to escape from local minima. Levitt and the late Tony Jack of Cambridge also pursued the idea of using molecular mechanics force fields with energy minimization as a tool for refining crystal structures [7]. Konnert (in 1976) and Hendrickson (from 1980) extensively developed macromolecular crystal refinement [6], based on methods of Waser (from 1963).

More than two decades later, minimization with constraints or restraints has become a practical and widely used tool for refining experimental diffraction data from X-ray crystallography, by optimization and, more effectively, by simulated annealing and molecular dynamics [3]. (I had the good fortune to work with Lifson as a postdoctoral fellow in 1989 for a few months during an NSF mathematical sciences postdoc at the Courant Institute. I recall Lifson proudly noting that his students took his "small ideas" and applied them to much larger systems, notably biomolecules.)

In 1969 Karplus, Levitt, and Warshel intersected in Lifson's lab at Weizmann. Karplus, on sabbatical from Harvard, sought inspiration from Lifson's mastery of polymer theory and broad thinking and hoped to marry his own interests in theoretical chemistry with biology [8]. Having been Pauling's graduate student at Caltech, Karplus already had a deep interest in the structure of biological molecules. At Weizmann, further inspiration came from Lifson's visitor Chris Anfinsen, whose experiments in protein folding prompted Karplus and David Weaver to develop, in 1975, a diffusion–collision model for protein folding calculations [8].

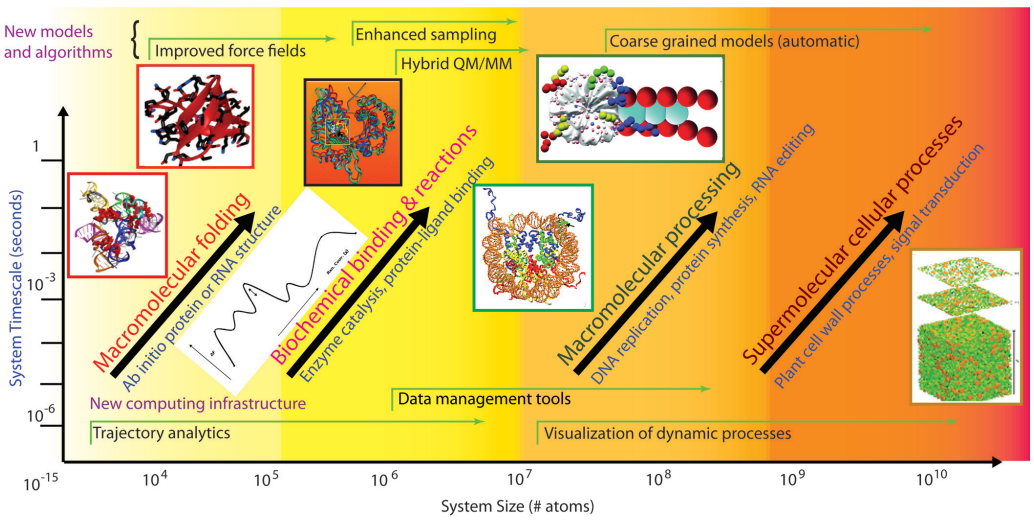

Figure 1. *Vision for the future of the field of molecular modeling. Adapted from a figure developed by the author and members of a DOE study panel [23].*

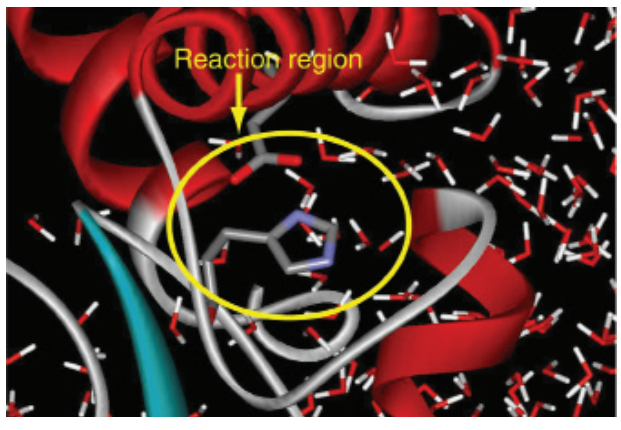

Figure 2. *With hybrid MM/QM methods, a small reaction region is treated quantum mechanically, while the surrounding solvent and remaining biomolecular system is treated classically. Figure courtesy of Arieh Warshel.*

This intersection of broad thinkers at Weizmann in the late 1960s also led to Warshel's postdoctoral position with Karplus at Harvard. Karplus had been working on reaction kinetics problems, specifically electronic absorption theory, and with students and postdocs (Barry Honig and, later, Klaus Schulten and others) calculated structural changes from electronic excitation related to the photo-isomerization reaction (e.g., retinal molecule) [8]. Warshel continued this line of work by constructing a program for computing vibrational and electronic energy states of planar molecules [25]. To achieve this, Warshel and Karplus used a novel combination: classical-mechanics approximation based on CFF with a quantum-mechanical Hamiltonian correction [25]. Four years later, Warshel and Levitt described a general hybrid classical/quantum scheme, not restricted to planar molecules for which the separation between quantum and classical degrees of freedom is clear [26] (Figure 2). The two reunited in Cambridge, UK, where Levitt received his PhD at the Medical Research Council under the tutelage of John Kendrew and Max Perutz, whose 1962 Nobel Prize in Chemistry recognized "their studies of the structures of globular proteins"; Levitt continued to pursue his interests in computational biology there [10]. These hybrid classical/quantum methods, essential for studying reactions in which bond breaking/formation occurs, use quantum mechanics to model a small active site, with classical mechanics for the larger region, beyond the reactive site (Figure 2). In this way, the overall computational time can be made manageable. Today, many innovative thinkers work in the huge area of computational/theoretical chemistry concerned with modeling details for the quantum region, and especially for the boundary between the two regions.

Activities under way at this time also led to other pioneering molecular dynamics simulations. Building on the simulation technique described in 1959 by Alder and Wainwright but applied to hard spheres [1], Rahman and Stillinger reported the first molecular dynamics work on a polar molecule, liquid water [18]. Again, computer power was not sufficient for realistic simulations, and the idea did not catch on quickly. In the late 1970s, Warshel brought his and Levitt's CFF program to the Karplus lab, where, rewritten by Karplus's graduate student Bruce Gelin, it formed the basis for second-generation programs, including CHARMM at Harvard and AMBER from Peter Kollman's group at UCSF.

A spectacular application of CHARMM was the first simulation of protein dynamics, by Andrew McCammon with Gelin and Karplus in 1977 [14]. Although modeled in a vacuum, with a crude molecular mechanics potential, and covering only 9.2 ps (tiniest "building" in Figure 3), the results emphasized the advantage of the dynamic view compared to the static, time-averaged X-ray image. Though these early simulation results stood the test of time, realistic molecular dynamics simulations generally require the inclusion of solvent (water) and ions in the physical environment. This necessitated the further creation of water force fields, which were developed by Berendsen, Jorgensen, and others in the late 1970s and early 1980s. These advances and the advent of supercomputers in the mid- to late 1980s led to molecular dynamics simulations of biomolecular systems, resulting in numerous exciting discoveries about the systems.

The vision of another giant in the field, the late Peter Kollman, led to the application of force-field methodology and computer simulation to biomedical problems, such as enzyme catalysis and protein/ligand design [24]; his group's free energy methods, combined quantum/molecular mechanics applications, and contacts with industry opened many new doors for practical pharmaceutical applications of molecular modeling.

Critical Assessment

The new field of computational structural biology faced exciting yet difficult times as it matured and expanded to many new areas of application. En route, it capitalized on the growing capabilities of high-speed computers. Initially, the pioneers were not widely supported, partly because their work could not easily be classified under a traditional label like physical or organic chemistry. At the same time, experimentalists were quite curious about the predictions produced by molecular modeling and simulations. As described in our earlier field perspective article [22] and a related *SIAM News* article [21], the new capabilities made possible by supercomputers in the late 1980s also led to inflated expectations and unrealistic predictions that temporarily harmed the field. Reports of various triumphs were followed in the media by extrapolated projections that computational tools would soon supplant experimentation and lead to novel computer-designed drugs (see quotes in [22]).

But a determined focus by modelers on two major limitations of biomolecular computations—imperfect force fields and limited conformational sampling—resulted in many improvements and refinements. In fact, in [22] we used historical facts to create a "field expectation" curve showing that, despite early exaggerated expectations, the field rebounded around 2000 and moved onto a productive trajectory, working hand-in-hand with experiment [22]. Thus, this year's Nobel Prize celebrates the ability of simulations not only to *survive* critical assessment by experimentalists, as described in 2005 [9], but to *thrive* as a field in its own right. Self-critique is also an important feature of the field: Several collective exercises, carefully distinguished from competitions—in protein structure prediction, RNA structure prediction, and other important applications—have served to assess progress and guide future developments in the field.

A Productive Present

Today, several popular biomolecular simulation packages are adapted to the latest computational platforms, as biomolecular modelers take advantage of the explosion of accessible technology and the tremendous increases in computing memory and speed. For example, the free and open-source software NAMD, developed at the University of Illinois at Urbana–Champaign by Schulten and co-workers, can be adapted to many force fields and computer architectures [16]. A specialized computer for long molecular dynamics simulations developed at D.E. Shaw Research is also available through a national supercomputer center. Such programs, along with technological advances, have led to important milestones.

See **Nobel Prize** *on page 5*

Mathematics, Management Consulting, and Emerging Markets

Careers in the Math Sciences

By Ibrahima Ba

Ibrahima Ba is a vice president at HIP Consult Inc., a Washington, DC-based management consulting firm that focuses on emerging markets. He has actively worked on infrastructure-deployment initiatives within the information and communications technology sector.

A few months ago, I was talking to a client in Johannesburg, South Africa, when we were stymied by a telecom bandwidth economics and modeling issue.

The client has a capacity- and business-planning team whose role it is to predict, given unit pricing of various bandwidth circuit types (155 mbps, 622 mbps, 2.5 Gbit/s, and 10 Gbit/s), the optimal basket of circuits that will simultaneously reduce overall cost and handle the rapidly accelerating traffic growth.

Historically, such decisions were made infrequently, they were static in nature, and calculations could be approximated manually, meaning with simple Excel formulas. But this time, the client was contemplating a major investment and needed to run various options to account for long-term traffic growth and price compression scenarios.

When I reviewed the client's model and issues, the problem and required techniques seemed to fit something I had learned years ago in a course in operations research at the Ecole des Mines in France. Back at my hotel, I took out paper and pencil and jotted down what I thought was the problem:

Minimize $F = 100*x + 300*y + 700*z + 1000*w$, where the variables x, y, z, and w are the units of capacity to purchase and the coefficients 100, 300, 700, and 1000 the given price for each capacity, subject to the constraint that x, y, z, and w are integers (you cannot purchase half circuits) satisfying the inequality $155x + 622y + 2480z + 9920w \geq T$, where T is the given traffic need. A complicating factor was that pricing changed over time and with the length of the circuit, and that traffic was growing each year.

I realized that this was a classic optimization problem, requiring use of a simplex algorithm. Indeed, this simple but powerful method helped the client's forecasting team solve the problem once and for all.

Math is powerful, even with only a fraction of its potential tools applied in business and management. This is not to say that every question should be turned into a mathematical model to solve. Quite the opposite: With intuition, basic analytical skills, and experience, we can for the most part address problems with simple calculations and logic.

Career Options for a Mathematician

Growing up in Mauritania, West Africa, I always enjoyed mathematics. The subject was logical and did not require costly tools or textbooks; moreover, the country's educational system rewarded the study of mathematics and engineering, as these skills were scarce and needed. (Mauritania was known as the country of a million poets!) Yet, because of the country's lack of resources, the math curriculum emphasized abstract mathematics.

When I ended up in France for my undergraduate studies, I discovered applied mathematics and started to develop a taste for it, which led me to a graduate program in engineering at the Ecole des Mines de Saint-Etienne. Still uncertain about my future career, I completed two master's degrees—one in engineering at the Ecole des Mines and the other, to keep my options open, in applied mathematics at the University of Lyon. Adding to the mix, I developed an interest in information technology and computational science.

Without much long-term job planning, I landed in Chicago to start my career as a scientific programmer at Argonne National Laboratory. But a few years later, influenced by friends and alumni from the Ecole des Mines, I realized that with my math skills I could pursue a nontraditional professional path that might be more rewarding. To facilitate a career switch, I enrolled in an MBA program at Northwestern University. I have to admit that with my math background, many of the analytical courses seemed straightforward; however, I began to develop a passion for the soft skills of marketing, strategy, and management.

Whereas math is an important instrument for solving problems, other disciplines can provide better tools for selling the solution—which is what is required in business! Yes, the world is not as logical or Cartesian as I thought growing up in Mauritania.

Why Management Consulting? Why Strategy?

Most of my MBA classmates already had a firm idea of the careers they wanted to pursue, having arrived with several years' experience within specific industries. I was

See **Emerging Markets** *on page 6*

Nobel Prize

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Figure 3 shows representative advances in molecular system sizes and timescales over several decades, including the early landmark simulations discussed above. In 1998 the 1-μs folding simulation of a small protein required four months of dedicated Cray computing [4]. In 2010 and again this year, the 1-ms simulation of a small protein [17] was made possible by Anton, the D.E. Shaw computer. At the same time, impressive developments in computer speed and memory have made possible simulations of extraordinary sizes, such as the 5-ns simulation of a virus system of more than 64 million atoms this year [27].

We have come a long way from the computers of the early days, Golem, CDC-1604, IBM-360, and their predecessors, with their tiny memories, low floating-point performance, limited compilers, and cumbersome physical requirements (e.g., magnetic tape, punch cards). Today, successful applications to biology and medicine are routinely reported, and mathematicians and computational scientists are the contributors of many important ideas and methods, including symplectic integrators, particle-mesh Ewald methods for electrostatic computations, and Markov state models for sampling (details can be found in [20]). Recent successes include structure predictions that precede experiment, protein folding theories, and modeling-aided drug discovery and design. Other important achievements involve successful interpretation of experimental structures, especially resolution of experimental contradictions, as well as production of new hypotheses for biological and chemical systems, which ultimately can be tested [22].

A Bright Future

Looking ahead, it is clear that multiscale modeling approaches like those devised by this year's Nobel laureates will be needed to describe biological processes on many levels (see Figure 1). The physical problems extend beyond the folding of individual biomolecules to the understanding of enzymatic reactions and binding processes, pathways that involve proteins and nucleic acids (e.g., DNA replication and RNA editing), and processes on cellular scales, like cell signaling, cellular metabolism, tumor growth, and neural circuitry. All these applications will require continuous development of methods and infrastructure support for data analysis and visualization. Ultimately, techniques for automatic coarse-graining of biological models could serve as a telescope focused on the region of interest: By adjusting both spatial and temporal domains, we might some day be able to focus the calculation on the process of interest at the desired scale, whether it occurs on the level of a single molecule or an entire organism. Needless to say, technological advances, together with a multidisciplinary community of scientists who have a broad vision, will be required to meet the important challenges in biology and medicine we now face.

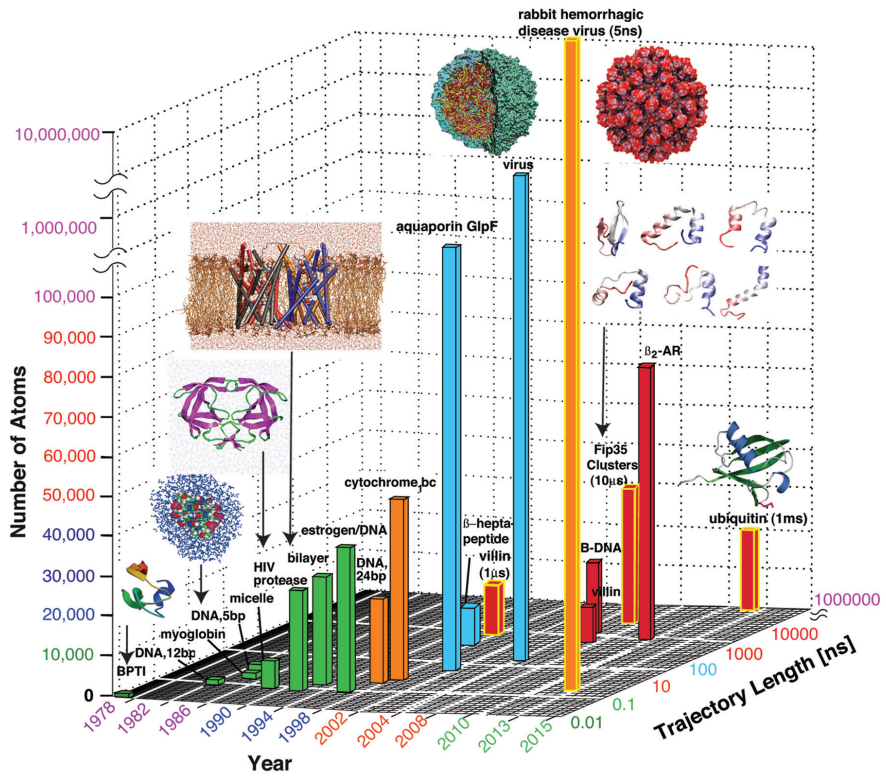

Figure 3. *The evolution of molecular dynamics simulations with respect to system sizes and simulation times. The "buildings" are colored according to simulation duration. See text and [20] for details.*

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Emerging Markets

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for a position that for many recruiters, analytical and quantitative skills are among the key criteria. Employers can teach us business, but math skills are harder to acquire on the job. One profession—management consulting—stood out for me as providing the greatest long-term flexibility.

Management consulting is the practice of helping organizations improve their performance. A relationship with an organization generally starts with a review of a specific problem the organization would like to solve. This is followed by the development of hypotheses or assertions of a possible answer, after which those hypotheses are either substantiated or disproved via rigorous data-driven analysis.

Based on their experience, management consultants are often hired to provide advice or an external industry perspective, or for benchmarking. They are sometimes viewed as neutral and external to the organization's internal politics. They can bring a fresh perspective and intellectual horsepower to tackle complicated issues.

Generally, the consulting industry hires from top programs and gives preference to candidates with strong analytical backgrounds. The recruiting interview process sometimes involves case studies that can take the form of a math or logic quiz; for example:

- Estimate the number of golf balls you can fit in a 747 plane (not that you're likely to do it);
- Estimate the number of garbage cans in New York City. Some may ask you to go further and estimate the number of rats living in New York City (do you see the correlation?); and
- Estimate the number of Wi-Fi connections in London.

Obviously, we don't expect you to know the exact answer to any of these questions. What the recruiter is looking for is your level of comfort with uncertainty, and your ability to structure a methodology, follow through with calculations, and come up with an answer that can then be debated.

Other important skills in consulting are communication (oral, written, and with PowerPoint); research, both primary (involving interviews and discussions with customers, and more) and secondary (desktop studies only); and economic modeling (mostly in Excel, but sometimes with MATLAB).

The consulting industry comprises key specialties, such as Strategy Consulting, Operational Improvement, Changing Management, Audit/Finance, and Information Technology. It can also focus on specific industries, such as consumer products, media, entertainment & communication, transportation & logistics, health care, financial services, and manufacturing, to name a few.

Strategy consulting, which tackles strategic issues of growth, expansion, divestiture, and profitability, is sometimes considered the crème de la crème of consulting. It is, however, among the most volatile segments, especially during downturns. The work is a bit more abstract—it often requires identifying business patterns and devising innovative solutions. You often need intuition (preferably backed by experience) to come up with answers. Strategy consulting is where the frontier of business modeling is pushed and where your decision can have the strongest impact (can make or break a company).

Many consulting firms have global operations with domestic or international clients. The latter segment has been growing rapidly in recent years, driven in part by the growth of emerging markets, where many infrastructure projects are in progress.

Consulting in Emerging Markets

Practically speaking, no country, company, stock, or index can grow indefinitely and deliver above-average performance. Developed markets have had a great run historically, but we cannot expect countries like the U.S., with less than 5% of the world population, to continue to command more than 20% of the total gross domestic product. This is not to suggest that the U.S. will not continue to grow, but rather that other countries are likely to develop faster in the future. This may already be the case for emerging markets, and Africa could actually be the surprising story over the next few decades.

One of the key skills you acquire as a consultant is the ability to transfer and apply knowledge across companies, industries, and countries. Having witnessed the explosion of communication, storage, and computing infrastructure and applications in the U.S., I found it natural to apply this experience to emerging markets. In most cases, the problems you address in that part of the world are classic (they have already been solved in developed markets), and the answers are known. All that is generally required is strong and disciplined execution.

Infrastructure development in emerging markets is an expanding area. Implementation of all these large projects requires skilled and experienced people—especially those with analytical skills. Consulting is not the only route, however, for someone hoping to participate in the development of infrastructure in emerging markets. Among the many other avenues are NGOs, the World Bank, international institutions, and universities. Junior mathematicians, statisticians, and computer scientists can participate and provide tremendous value in emerging markets. You need not be afraid to seek experience "far away from home"; the proliferation of phone and Internet connections has made the world a small village.

Opportunities for Mathematicians

The management consulting industry is always competing for top talent. The good news is that analytical and other hard skills are the first thing a recruiter is likely to seek in a résumé. Most companies hire at several educational levels: bachelor's, master's, and PhD. The recruiter will want to see that you have the ability to combine your analytical skills with common-sense business approaches in tackling practical problems.

You need to demonstrate that you can go beyond research papers and publications—not that these are unimportant—and can quickly grasp the problem at hand and draw from your scientific toolkit a methodology that will lead to a practical solution.

Opportunities for math and science majors have always been abundant, but I believe that they are even more so now. The needs are enormous as the world shifts to digital economies. For instance, an emerging field like Big Data, with its data sets too large and complex for analysis by standard tools, can probably absorb significant numbers of mathematicians, scientists, economists, financial modelers, statisticians, computer programmers, and others in related professions.

Conclusion: You Have the Option

Each period of development brings new types of careers, along with a reduced need for others. Some even risk extinction. With the growth of technology and communications, the cycles of change are more pronounced. It is difficult to predict where the next wave of careers will emerge, but the underlying factors that will prepare you for the future remain the same: your ability to think and solve complex problems.

Your math and science skills provide you with the option to change and adapt. They may also give you the basic building blocks for efficiently and confidently solving what may seem to be odd or unusual problems.

When I walked into my client's office in Johannesburg a few months ago, I did not expect that an old mathematical algorithm in my toolkit would save the day, let alone that it would elegantly address a real headache for the customer.

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

Professional Opportunities

Send copy for classified advertisements to: Advertising Coordinator, SIAM News*, 3600 Market Street, 6th Floor, Philadelphia, PA 19104–2688; (215) 382–9800; fax: (215) 386–7999; marketing@siam.org. The rate is $2.85 per word (minimum $350.00). Display advertising rates are available on request.*

Advertising copy must be received at least four weeks before publication (e.g., the deadline for the March 2014 issue is January 31, 2014).

Advertisements with application deadlines falling within the month of publication will not be accepted (e.g., an advertisement published in the March issue must show an application deadline of April 1 or later).

Students (and others) in search of information about careers in the mathematical sciences can click on "Careers and Jobs" at the SIAM website (www.siam.org) or proceed directly to

www.siam.org/careers

Dartmouth College

Department of Mathematics

Applications are invited for John Wesley Young Research Instructorships. These positions are for new or recent PhD recipients whose research overlaps a department member's and are available for two to three years. Instructors teach three ten-week courses spread over three terms; appointment is for 26 months, with possible renewal for 12 months. Monthly salary is $5100, including a two-month research stipend for instructors in residence during two of three summer months; for those not in residence for 11 months, salary is adjusted accordingly.

Applicants should apply online at: http://www.mathjobs.org, Position ID: JWY #4928. Applicants can also access an application through a link at http://www.math.dartmouth.edu/activities/recruiting/. General inquiries can be directed to Tracy Moloney, administrator, Department of Mathematics, tfmoloney@math.dartmouth.edu. Applications completed by January 5, 2014, will be considered first.

Dartmouth College is committed to diversity and strongly encourages applications from women and minorities.

University of Michigan–Dearborn

Department of Mathematics and Statistics

The University of Michigan–Dearborn (http://www.umd.umich.edu/math) invites applications for one tenure-track assistant professor position in applied mathematics, beginning September 1, 2014. The position requires a PhD in mathematics and a strong commitment to teaching undergraduate and graduate mathematics courses. The standard teaching load is 18 credit hours per year. Incoming assistant professors receive released time for a total of three courses (nine credit hours), to be used during the first five years of a six-year probationary period to allow more time for research. Promotion and tenure is based on a successful candidate's performance in teaching, research, and service.

Applicants should submit a cover letter, CV, three letters of recommendation, transcripts, and statements on teaching philosophy and research program to: http://mathjobs.org. The contact person for this position is Belinda Soliz, secretary, Applied Mathematics Search Committee, besoliz@umich.edu.

The University of Michigan–Dearborn is an affirmative action/equal opportunity employer.

San Diego State University

Department of Mathematics and Statistics

The Department of Mathematics and Statistics at San Diego State University invites applications for a tenure-track assistant professor position in climate mathematics, beginning in August 2014. Exceptional applicants at the associate professor level will also be considered. Applicants must have a PhD (or equivalent) in mathematics or a related field; demonstrate outstanding research potential through a record of publications and grants; demonstrate excellent skills in teaching both undergraduate and graduate courses in applied mathmatics; and show an ability to build an active interdisciplinary research program in climate mathematics, with a focus on next-generation climate models or climate data analysis. The successful candidate will join the recently founded interdisciplinary SDSU Center for Climate and Sustainability Studies and have the opportunity to participate in SDSU joint PhD programs, as well as in MA and MS programs.

Electronic or paper applications should include (1) a cover letter, (2) curriculum vitae, including a list of publications and a research summary, (3) three letters of recommendation, and (4) up to five publications. Applications should be addressed to: Climate Mathematics Search Committee, Department of Mathematics and Statistics, San Diego State University, 5500 Campanile Drive, San Diego, CA 92182–7720; dconte@mail.sdsu.edu. The review of applications will begin immediately; applications will continue to be accepted until the position is filled.

SDSU is an equal opportunity/Title IX employer.

New York University

Courant Institute of Mathematical Sciences

The Courant Institute of Mathematical Sciences anticipates a faculty position, rank open, in the Center for Atmosphere Ocean Science, a unit of the Department of Mathematics. The appointment, pending budgetary and administrative approval, is to begin in the fall of 2014. Applicants should have outstanding research accomplishments, diverse research interests, and mathematical expertise in fundamental areas of atmosphere–ocean–climate science.

Applications, consisting of a CV, a one-page research statement, and the names of three references, should be submitted to: Sylvia Mejia, Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, NY 10012; mejia@cims.nyu.edu. The closing date for applications is February 1, 2014.

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Illinois Institute of Technology

Department of Applied Mathematics

The Department of Applied Mathematics invites applications for (1) a tenure-track assistant professor position in the area of stochastics and (2) a visiting assistant professor position in an area related to departmental research, both beginning in August 2014. Successful candidates must have a PhD degree in mathematics or a closely related discipline, as well as demonstrated potential for excellence in research and teaching.

Members of the department are actively engaged in externally funded research in several areas, and the department grants BS through PhD degrees. More information can be found at http://www.iit.edu/csl/am.

Applicants should submit the following through http://www.MathJobs.org: (1) a cover letter expressing interest in one or both positions that highlights how applicants can contribute to the departmental mission, (2) curriculum vitae, and (3) succinct teaching and research statements. At least four confidential letters of reference (one addressing teaching effectiveness) should also be submitted through MathJobs. Questions can be addressed to Fred J. Hickernell, chair, Department of Applied Mathematics, (312) 567–8983, amsearch@math.iit.edu. The review of applications started in early December 2013.

IIT is an affirmative action/equal opportunity employer and especially encourages applications from women and under-represented groups.

University of Alabama

Department of Mathematics

The Department of Mathematics at the University of Alabama invites applications for two tenure-track positions at the assistant professor level. One position is in the area of numerical linear algebra in data mining, with application to any field of science and engineering; the other position is in computational statistics in data mining, with a specific focus on the area of cybersecurity. The appointments will begin on August 16, 2014. Candidates must possess a doctorate in mathematics, statistics, or a closely related field.

More information about the department and the university is available at http://math.ua.edu.

Applicants must apply online at: http://facultyjobs.ua.edu and arrange for three letters of recommendation, one of which can address teaching, to be sent to math@ua.edu. The review process started on December 1, 2013, and will continue until the positions are filled.

The University of Alabama is an affirmative action/equal opportunity employer and actively seeks diversity among its employees. Women and minority candidates are strongly encouraged to apply.

University of Colorado Denver

Department of Mathematical and Statistical Sciences

The Department of Mathematical and Statistical Sciences at the University of Colorado Denver invites applications for two tenure-track assistant professor positions, one in statistics and one in combinatorial optimization/applied combinatorics, beginning in August 2014. The department seeks candidates with excellent research potential and strong commitment to quality teaching; a typical teaching load is two courses per semester.

Located in beautiful downtown Denver, the department offers BS degrees (with several options, including one in applied mathematics), as well as MS and PhD degrees in applied mathematics.

Applications are accepted electronically at: http://www.jobsatcu.com, under job postings F00812 (applied combinatorics) and F00774 (statistics). For more information, applicants can see full job descriptions at http://jobsatcu.com, or contact stephanie.santorico@ucdenver.edu (statistics) or michael.ferrara@ucdenver.edu (applied combinatorics).

The University of Colorado Denver is committed to diversity and equality in education and employment.

Mantle Convection

continued from page 1

surface velocities by 80%, vastly reducing the non-uniqueness inherent in attempts to model mantle flow through time. MCMs have yielded key insight into the relation of mantle structure and the history of plate motion. In particular, they demonstrated that much of the large-scale structure of Earth's mantle can be attributed to the sinking of dense, old ocean floor to the CMB, and that the mantle is likely to be of uniform chemical composition at the scale of convection cells [9].

The ad hoc nature of the initial conditions assumed in MCMs is a grave limitation and has prompted an alternative approach, known as *backward advection*. Here, an estimate for present day mantle structure, commonly derived from global-scale seismic imaging, serves as the initial condition for a flow calculation, which is then integrated backward in time, neglecting thermal diffusion; such models give access to the secular variation of the mantle heterogeneity field. Backward advection exploits the immense convective vigour of the mantle—i.e., for short time periods, on the order of a few million years, thermal advection (which is time-reversible) dominates diffusion. Running mantle convection models back in time has given us a glimpse of many of the geologic phenomena affected by secular mantle variations. For instance, we have learned that motion of so-called mantle hotspots, like Hawaii, and changes in the position of Earth's rotation axis over geologic time are associated with the evolving mantle density structure (e.g., [11]). The primary reason for the failure of backward integration as a viable strategy for inferring mantle paleo-structure is simple: It leads to an accumulation of artifacts, especially near thermal boundary layers, where diffusion is, by definition, important; these are not optimal conditions for retrieving the mantle paleo-state [2].

Running mantle convection models back in time has given us a glimpse of many of the geologic phenomena affected by secular mantle variations.

For this reason, optimisation techniques are now coming to the fore as a powerful approach to the recovery of past deep Earth structure. Geophysicists seek solutions that minimise the difference between mantle heterogeneity inferred (in some form) from seismic imaging and predictions of dynamic models, subject to optimal initial conditions. This is an inverse problem for which time is a variable. Crucial to its solution is that the model derivative be found relative to the unknown initial state. Obtaining the derivative by means of classical finite differencing techniques is, of course, impractical due to the large number of parameters (in the range of 10^{12}) in modern dynamic Earth models. The adjoint method, advocated early on in meteorology [13] and seismology [14], is a mathematically elegant and computationally efficient method for obtaining the gradient information needed in the inversion. Rapidly increasing computational resources are making the adjoint approach attractive across the geosciences—in, for example, oceanography [16], seismology [5,6,15], and geodynamo simulations [7]. The adjoint equations for mantle dynamics and detailed discussions of model, data, and parameter errors can be found in [2]. Paleo-structure modeling of the Earth's mantle will provide crucial information on the history of plate-driving forces, the material properties of the deep Earth, and the temporal evolution of the CMB, as well as a deeper understanding of the development of sedimentary basins, thereby advancing us into an era of integrated investigations that will alter our view of the Earth system.

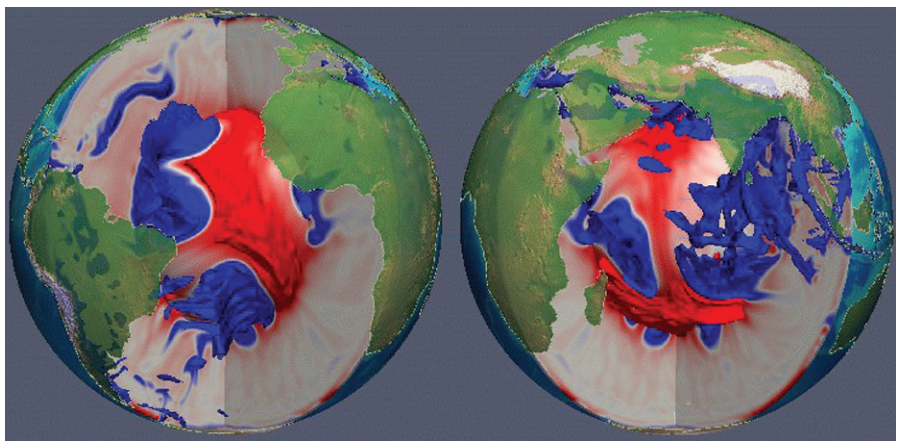

Figure 2. *Thermal structure in a mantle circulation model. The adjacent cross sections are centered on 35° (left) and 305° (right) longitude, and the color scale is saturated at –400 K and +400 K. Continents with color-coded topography are superimposed for geographic reference. Isosurfaces of temperature are displayed for –600 K and +400 K, with the +400 K isosurface clipped in the uppermost 500 km to allow views into the mantle underneath the mid-ocean ridge system. The reduced thermal heterogeneity in the upper mantle is a consequence of the low viscosity and high mobility of the flow there. Notice the prominent and hot deep mantle upwellings, in particular beneath the African continent.*

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