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Spotlight on UQ

During a recent visit to KAUST and its Center for Uncertainty Quantification, SIAM president Irene Fonseca met with the KAUST student chapter of SIAM. Shown here, standing, from left: Noha Alharthi, Han Liu, Luiz Faria, Lulu Liu, Irene Fonseca, Zehor Belkhatir, Gustavo Ivan Chavez Chavez, Tareq Malas, Fadi Eleiwi, and Ayman Karam; kneeling: Yiannis Hadjimichael and Mohammed Al Farhan.

KAUST's Center for UQ was created two years ago in an international competition for Strategic Research Initiatives. Raul Tempone, director of SRI-UQ, offers a brief look at the center and its activities on page 4. Research in UQ, he points out, is fundamentally interdisciplinary and strongly grounded in application areas—and hence a good fit for KAUST.

Tempone is also active in the SIAM Activity Group on UQ, which held its second conference in Savannah, Georgia, March 31 to April 3. Reflecting the reach of the field, the conference was held in cooperation with the American Statistical Association, the GAMM Activity Group on UQ, and the American Geophysical Union. Each organization was represented by one of the organizing committee co-chairs: Michael Griebel (GAMM), Max Gunzburger (chair, SIAG/UQ), Marcia McNutt (AGU), and Philip Stark (ASA).

Among the outstanding invited talks at the conference was "Uncertainty Quantification in Bayesian Inversion," by Andrew Stuart of the University of Warwick. Stuart and coauthor Marco Iglesias responded to a request from SIAM News *for an article based on the talk with the article that begins below.*

Richard Tapia Receives NSB Vannevar Bush Award

Richard Tapia of Rice University has received the National Science Board's 2014 Vannevar Bush Award. Honored at a banquet and award ceremony at the State Department on May 6, Tapia was cited for "his extraordinary leadership, inspiration, and advocacy to increase opportunities for underrepresented minorities in science; distinguished public service leadership in science and engineering; and exceptional contributions to mathematics in the area of computational optimization."

Accompanied by Jean Tapia, his wife of 55 years, and their two children, Tapia gave an acceptance speech to an audience made up of current and former NSB members, science leaders, family, and friends. He recalled his role as an outspoken critic of the long-delayed inclusion in the US of "Latinos in upper levels of administration in academia and the National Science Foundation." Nonetheless, he pointed out, for the first time in history, the director of NSF, France Cordova, the chair of NSB, Dan Arvizu, and the recipient of the Vannevar Bush Award are all Mexican–Americans. "Awards of this magnitude and prestige," Tapia said, are important in that they add credibility to work on behalf of underrepresented minorities "and facilitate its implementation."

Mexican–Americans all: NSB chair Dan Arvizu, Richard Tapia, and NSF director France Cordova. Photos courtesy of the National Science Foundation/Sandy Schaeffer Photography.

Attending a ceremony at the State Department in honor of a longtime member of SIAM was an inspiring and thrilling moment for me. To convey the significance of this award to readers of *SIAM News*, I asked a set of national and SIAM leaders in applied mathematics and education to offer personal thoughts on Tapia's contributions.

"What makes Richard so remarkable is that he continues to show us what's possible—that this nation has thousands of children from all backgrounds who can become productive mathematicians and scientists," said Freeman Hrabowski, president

See **Richard Tapia** *on page 8*

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UQ and a Model Inverse Problem: *CO_2 Capture/Storage*

By Marco Iglesias and Andrew M. Stuart

Quantifying uncertainty in the solution of inverse problems is an exciting area of research in the mathematical sciences, one that raises significant challenges at the interfaces between analysis, computation, probability, and statistics. The reach in terms of applicability is enormous, with diverse problems arising in the physical, biological, and social sciences, such as weather prediction, epidemiology, and traffic flow.

Loosely speaking, inverse problems confront mathematical models with data so that we can deduce the inputs needed to run the models; knowledge of these inputs can then be used to make predictions, and even to devise control strategies based on the predictions. Both the models and the data are typically uncertain, as are the resulting deductions and predictions; as a consequence, any decisions or control strategies based on the predictions will be greatly improved if the uncertainty is made quantitative.

Bayesian Approach to Inverse Problems

A mathematical model of an experiment is a set of equations relating inputs u to outputs y. Inputs represent physical variables that can be adjusted before the experiment takes place; outputs represent quantities that can be measured as a result of the experiment. For the *forward problem* the mathematical model G is used to predict the outputs y of an experiment from given inputs u. For the *inverse problem* the mathematical model is used to make inferences about inputs u that would result in given measured outputs y [6,11]; in practice, many inverse problems are *ill-posed* in the sense of Hadamard: They fail to satisfy at least one of the criteria for well-posedness—existence, uniqueness, and continuous dependence of the solution on data. When the measured data is subject to noise, and/or when the mathematical model is imperfect, it is important to quantify the uncertainty inherent in any inferences and predictions made as part of the solution to the inverse problem. The Bayesian approach to inverse problems allows us to undertake this task in a principled fashion. When properly applied, this formulation of inverse problems can simultaneously regularize any ill-posedness present.

In the Bayesian approach the pair (u,y) is considered a random variable, and the solution of the inverse problem is the conditional probability distribution of the random variable u given y, denoted $u|y$. A formula for this conditional probability distribution is given by *Bayes' rule*, which states that

$$\mathbb{P}(u|y) \propto \mathbb{P}(y|u)\ \mathbb{P}(u).$$

In words: The *posterior* $\mathbb{P}(u|y)$, which is what we know about the unknown u given the data y, is proportional to the *likelihood* $\mathbb{P}(y|u)$, which measures how likely the observed data is for given inputs u, multiplied by the *prior* $\mathbb{P}(u)$, which describes our knowledge of the unknown prior to the acquisition of data. We describe a concrete application below, and the reader may wish to revisit our overarching mathematical presentation with that example in mind.

Bayes' rule, and its application, are illustrated schematically in Figure 1. The *prior* is denoted by the black dotted curve in the INPUT space, with MODEL G defining its likelihood; data y is then used to obtain the *posterior*, denoted by the red curve in the INPUT space.

What does this update in probability distributions, from the prior to the posterior, do for us? Our answer is found in the predictions of uncertainty in the QUANTITY OF INTEREST q: Without data (under the *prior*), we make the prediction denoted by the black dotted curve; with data (under

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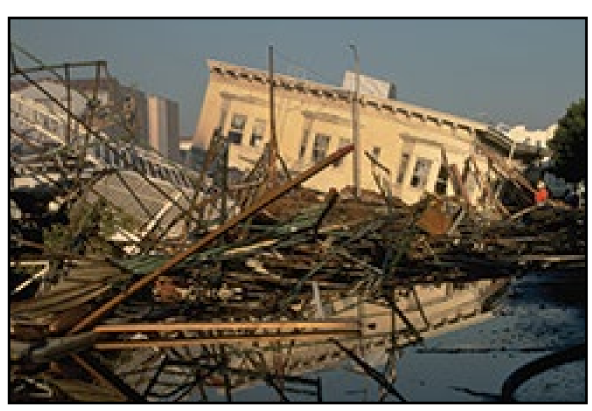
Modeling the Tohoku Earthquake

Challenges and Rewards

Coinciding with the third anniversary of the Tohoku earthquake and tsunami in northern Japan, Jeremy Kozdon, an assistant professor of applied mathematics at the Naval Postgraduate School in Monterey, California, narrated a video about his collaborative work in earthquake modeling with Eric Dunham (an assistant professor of geophysics at Stanford University). Periodically, written questions appear in the video; they were posed by interviewer Margot Gerritsen of Stanford, where Kozdon was a postdoc in geophysics before moving to NPS. Kozdon's story of the unexpected, and gratifying, use of his group's code and models by other scientists should be inspiring to applied and computational mathematicians, especially young people in search of an application area in which they can put their knowledge and interests to good use. This article presents highlights from the video.*

Kozdon, who grew up in the Bay Area, came by his interest in earthquakes naturally: He was in elementary school at the time of the 1989 Loma Prieta Earthquake, which he remembers as occurring during the baseball World Series then under way, and as a cause of widespread devastation, including collapse of the Bay Bridge. Years later, on receiving his PhD, he realized that the geosciences are a rich area for computational and applied mathematicians: "You can have a real impact in that field" by applying many of the techniques in wide use among applied and computational mathematicians.



Loma Prieta Earthquake, California, 1989.

Dunham and Kozdon's team studies earthquakes by means of dynamic rupture modeling. Kozdon describes the complexity of the approach with relish: The group models the fault response, as well as the waves propagating away from the fault, carrying perturbations, velocity, and stress; the waves then feed back into the interface, which is governed by highly nonlinear friction laws, related to the velocities, stresses, and discontinuities at the fault. "We want to model what happens at that level," he says.

The group's modeling has been informed by high-friction lab experiments performed elsewhere, in which rocks slide past each other at displacement velocities on the order of meters/second. A major modeling challenge arises in linking lab results to real-world events. Kozdon is now beginning to explore the use of adaptive mesh refinement techniques to study what happens in moving up from the lab scale (centimeter) to the field scale (where the dimensions of faults can be in hundreds of kilometers).

The Tohoku earthquake and tsunami occurred along a subduction zone. Subduction zones, in which one plate goes under another, tend to be the sites of the largest earthquakes and the greatest tsunami hazards. "One thing we've been exploring with our model," Kozdon says, is "Why did the tsunami occur?" In answer, he mentions the large amount of sea floor uplift caused by the large amount of slip; estimates of the displacement of the fault are as high as 80 meters, with a consensus that it was in the tens of meters.

This was surprising to earthquake scientists, who had not believed that the top section of the fault would slip during a large earthquake—that the energy wasn't there. "What we were able to show with our models," Kozdon says, is that—even with the assumption that energy is not there to release on that segment of the fault, and neglecting the dynamics of what's going on—wave energy released from deep slip on the fault comes up and is reflected from the sea floor and channeled onto that top portion of the fault, driving the rupture through that region.

He identifies the heart of the modeling challenge: "How do you set up initial conditions? You can't take measurements of the state of stress of the Earth kilometers under the surface." The group proceeded by doing an ensemble of simulations to try to understand how the uncertainties and their understanding of the physics and the initial conditions affect the final result.

The group first got involved in modeling the Tohoku earthquake soon after the event. At the time, they didn't see their codes as set up for large-scale simulations: "We had a big parallel code, but had only used it on simplified geometries."

In the midst of these feelings of doubt, another scientist (Emily Brodsky, a professor at UC Santa Cruz) approached them, wanting to drill across the fault so that they could take measurements. The Japan Trench Fast Drilling Project (JFAST) scientists thought that the methods developed by Dunham and Kozdon could help, answering such questions as, What do we expect to see? If we see various things, what does that mean?

The Japan Trench Fast Drilling Project.

This was a proud moment for him and the team. "Seeing our code do simulations, putting in extremely challenging and complicated geometries, with extremely small angles, which make it a difficult problem to simulate, seeing the geoscience community get excited about your results—I've had only a few moments like that in my career."

At this point in the video, Gerritsen brings Kozdon down to earth with a question about his "most embarrassing moment" in his work on earthquakes. He's ready with an answer: "One of the silliest things I did was in bringing the model into our code. We took some published data, to give us the geometry, the angles at which the fault is dipping and where the various material layers are. I had misread the caption, didn't realize that there was a 1.5 scaling in the vertical direction."

The misstep led him to a deeper appreciation of working as part of a team. "Fortunately, my colleagues were forgiving." . . . "Being part of a collaborative team is great; having someone who understands things looking at them alongside me" is invaluable.

"Three years ago," Kozdon says, "I didn't know that much about earthquake modeling." What he did have was "a deep understanding of the numerics and computing, and also good physical intuition." His advice to people wishing to get involved in the field is to master the fundamentals, "to get down in the trenches with physicists."

"There's a big push right now in geoscience to use computation," he says. "That community is extremely welcoming to computational folks; they know that you can offer them something."

*The video is posted at http://y2u.be/3Z-GBqWOnmo.

For Further Reading

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Levin Honored for Work on Sustainable Complex Ecosystems

On April 25, at a ceremony held at the Four Seasons Hotel in Beverly Hills, Simon A. Levin of Princeton University received the 41st Tyler Prize for Environmental Achievement. The international prize, established by John and Alice Tyler in 1973, recognizes individuals who have "made outstanding contributions to scientific knowledge and public leadership to preserve and enhance the environment of the world."

I had the opportunity to attend this event, as well as the extraordinary lecture, "Obstacles and Opportunities in Environmental Management," delivered by Levin at the University of Southern California on April 24. In the course of these commemorative events, attended by family, friends, and collaborators of Levin, I collected a plethora of statements that vividly illustrate why Levin has joined the class of Tyler laureates, a prestigious group that includes May R. Berenbaum, Paul R. Ehrlich and Anne H. Ehrlich, Jane Goodall, Thomas Eisner and Jerrold Meinwald, Edward O. Wilson, Mario J. Molina, Eugene P. Odum, and G. Evelyn Hutchinson, to name but a few.

"Simon Levin has uniquely captured the importance of complexity theory and expanded our ability to think and to act positively in ways that will sustain global biodiversity and ecosystem services," said Alan Covich, a member of the Tyler Prize Executive Committee. Levin's research and mentoring of students and colleagues, Covich continued, have had "international impacts and provided greater understanding of self-organizing, complex adaptive systems. The ability to integrate models of natural and social systems provides new perspectives on meeting the many challenges of understanding nonlinear systems, especially those 'insurmountable opportunities' created by socio-economic dynamics."

Citing Levin's contributions in science and in science for policy, and his talent for communicating with general audiences, Don Saari stressed that these were gifts that Levin "has used effectively for advancing public awareness." In particular, addressing Levin, Saari applauded his accomplishments in "science for policy" that have been directed toward making lasting changes. "This ranges from the practical—serving on the board of directors of the New Jersey Nature Conservancy—to your work with the Beijer Institute, along with your leadership roles in several organizations, including the Santa Fe Institute and, as chair of the Council, the International Institute for Applied Systems Analysis in Vienna."

Levin's contributions to our understanding of ecological systems have certainly been impressive, Mimi Koehl of UC Berkeley added, but "what makes him really special is the incredible job he has done of mentoring and educating such a diverse and distinguished group of students and postdocs . . . . Simon has made his mark on ecology not only through his own work, but also through his influence on his students and collaborators, both as a teacher and as a friend."

As a former postdoctoral fellow of Levin, I take this opportunity not only to congratulate him on this honor but also to thank him for the myriad of contributions that he has made to the mathematical community through his work with societies like SIAM; for his editorial work on a myriad of journals and book series that have highlighted and expanded the role of mathematics at the interface of the computational, life, and social sciences; and for the impact that he has had on placing mathematics at the heart of the study of critical environmental sciences, of health disparities, and of science policy questions that have a direct impact on the quality of our lives and the future of society.

The Tyler Prize committee recognized Simon Levin "for his research revealing the complexity of, and relationships between, species and ecosystems. His work has been fundamental in the crafting of environmental policies and advancing the study of complex ecosystems—the myriad relationships and interactions in nature." USC Photo/Steve Cohn.

On a personal note: I met Simon Levin through his articles and books in the mathematics library of the University of Wisconsin–Madison. The recommendations of the late James F. Crow, Fred Brauer (my PhD adviser), and the ecologist Dan Waller convinced him, somehow, that I had a future in mathematical biology. After we met at UCLA in January 1985, Simon opened doors for me not only at Cornell University but also at his home; soon afterward, like every one of his students and postdocs, I became a member of the Levin family. He introduced me to the study of disease dynamics and evolution, and under his leadership we studied the dynamics of influenza under cross-immunity and the impact of social dynamics on the spread of HIV.—*Carlos Castillo-Chavez, Arizona State University.*

Further information about the prize can be found at http://www.tylerprize.usc.edu/.

Key to a Fruitful Biological/Mathematical Collaboration

Letters to a Young Scientist. *By E.O. Wilson, Liveright, New York, 2013, 256 pages, $21.95.*

BOOK REVIEW
By Alan Hastings

E.O. Wilson's *Letters to a Young Scientist* is part memoir, part advice to young scientists. Much of the advice really does apply broadly and would be of interest to many young members of the SIAM community, with, of course, appropriate correspondences between the biological examples in the book and the interests of applied mathematicians. One of Wilson's ideas, however, generated controversy, at least within the mathematical community, when he expressed it in an op-ed piece in *The Wall Street Journal.** He seemed to be saying that scientists do not need to know mathematics. A response to Wilson's piece appeared a few days later in *Slate.*† Before getting to the issue of the role and importance of mathematics, it is important to consider other parts of the book.

What comes through in the entire volume is a sense of the importance of passion in scientific research, and of the necessity for scientists to immerse themselves in the problem at hand. These and other lessons come through clearly, in a series of specific examples from Wilson's long life and career as an influential scientist. The advice, of course, is easily applicable to anyone who is planning on a career in research in any area of science, including applied mathematics.

Some of the more specific advice is equally applicable to scientists in a broad range of fields, and to applied mathematicians in particular. All young scientists, for example, would do well to consider the recommendation, together with specifics on how to carry it out, that they try to achieve something truly novel (called "entrepreneurship" by Wilson, as discussed in chapter 6). Doing something that is not just a publishable extension of an existing result, but rather is really new, will be more rewarding in almost all ways.

The advice about what Wilson calls "quick, easily performed experiments" applies equally to applied mathematics. Too often, the literature directed to young applied mathematicians seems to imply that results come as flashes of insight, like lightning bolts. What young readers need to understand instead is the importance of experimenting, of trying to prove a variety of conjectures—essentially, of doing precisely the mathematical equivalent of what Wilson suggests—as a way to develop really new ideas and results.

As another example, his emphasis on the importance of sustained effort comes through clearly and applies broadly. Doing research is hard work and requires looking at a problem in many different ways, just as Wilson suggests.

Now to the controversy. How does the apparent universality of Wilson's lessons square with the part of the book in which he states that a biologist does not need to know mathematics? First, we need to look at what he actually wrote. What Wilson says is that learning mathematics was unnecessary for him because he always had someone to collaborate with. And he has made substantial contributions, as a collaborator, to theoretical advances in ecology that did involve mathematics. His suggestion is that young scientists could follow the same path and bring in the mathematics needed through collaboration. The question is, does this recipe for success still hold? Is it the best advice?

Without a recording of the interactions between Wilson and his mathematical collaborators, it is impossible to say exactly what the interactions were like. But Wilson does identify one of the most challenging and important aspects of using mathematical approaches in ecology as the formulation of the biological problem in mathematical terms, and then the interpretation of the mathematical results in the language of the biologist. This clearly requires that the biologist and the mathematician have a common language. And that is really possible only if the biologist knows at least some mathematics, and the mathematician knows some biology.

Wilson writes that the analysis of mathematical models by his mathematical collaborator did not require his input and that he did not, therefore, need to learn mathematics. I would argue, based on the need for a common language, that at least some mathematical knowledge was necessary. It might be reasonable to conclude that the greater the mathematical knowledge of the biologist, and the greater the biological knowledge of the mathematician, the more fruitful the collaboration will be. A collaboration is fruitful, after all, only when the combined knowledge of the collaborators is greater than the knowledge of any single participant. As problems become more and more complex—including, for example, those that have been the focus of Mathematics of Planet Earth—progress will require truly collaborative efforts driven by approaches across mathematics and a range of sciences. Some areas of ecology, in particular, because of the emphasis on numbers of individuals, have long required the genuine involvement of mathematicians.

"These collaborations succeed only when there is a common language, which means that all participants must work to learn as much as possible about all the fields involved."

A more useful rephrasing of Wilson's advice to biologists about mathematics (and a converse statement for applied mathematicians) would be: Biologists should not be afraid to seek out mathematically adept collaborators, as advances may require novel mathematical approaches. The equally valid converse: Because advances in biology require deep biological insights, applied mathematicians should be well served by collaborations with quantitatively oriented biologists. Yet these collaborations succeed only when there is a common language, which means that all participants must work to learn as much as possible about all the fields involved.

Why is mathematics so essential for understanding biological questions? This and other challenging issues come up naturally in Wilson's interesting memoir. I would argue that—barring distraction by the single headline-grabbing (at least for a SIAM audience) comment that studying mathematics is not important—all young scientists would greatly profit from reading and thinking about his book. And those who develop a deep understanding as to why the statement about the unimportance of mathematics is not only wrong, but essentially not supported by the arguments in the book, will find the book both more interesting and more useful.

I leave readers with a final challenge to take up after reading Wilson's book. What would letters to a young applied mathematician (in the 21st century) look like?

Alan Hastings is a professor in the Department of Environmental Science and Policy at UC Davis.

*"Great Scientist ≠ Good at Math," April 5, 2013.

†Edward Frenkel, "Don't Listen to E.O. Wilson," April 9, 2013.

The Mathematization of America's National Sport

The Sabermetric Revolution: Assessing the Growth of Analytics in Baseball. *By Benjamin Baumer and Andrew Zimbalist, University of Pennsylvania Press, Philadelphia, 2014, 240 pages, $26.50.*

BOOK REVIEW
By Philip J. Davis

The peak of my involvement (if I may call it that) with baseball occurred when I was eleven. I went to all the high school games (25 cents for a season ticket), I was an ardent Red Sox fan, I listened to Fred Hoey's radio broadcasts of the games from Fenway Park, I collected baseball cards of the famous players: Lefty Grove, Wes Ferrell, Joe Cronin, et al. This involvement vanished when I entered high school, and over the years I've hardly followed Major League Baseball at all. Still, baseball is the one sport I watch on TV—but only for five or ten minutes. I am bored by all the slo-mo replays.

Baseball has a discrete structure, as opposed to the semi-continuous structure of basketball or hockey, and is therefore very amenable to mathematization. Some baseball statistics may have been around since the 1800s, and their number had grown by the time I was eleven. But more recently the mathematization of the sport has grown exponentially (as people say), and this is what *The Sabermetric Revolution* is all about. The "saber" in sabermetric, which derives from the acronym for the Society for American Baseball Research, refers to "the use of statistical methods to analyze player performance and game strategy."

The authors know their stuff. Both are professors at Smith College; Benjamin Baumer used to be a statistical analyst for the New York Mets, and Andrew Zimbalist is an economist who has written about labor and economic policies in baseball. Their book is an in-depth successor to the best-selling 2003 *Moneyball: The Art of Winning an Unfair Game*, which morphed into the 2011 movie.

Acronyms a-plenty populate the pages. BABIP, DER, DIPS, ERA, HITf/x, OPB, PECOTA, and SAFE are just a sampling of the specific types of data collected and analyzed. (BABIP, for example, means batting average on balls in play.) Pythagoras makes a star appearance with the formula

$$WPCT = RS^2/(RS^2 + RA^2),$$

where $WPCT$ = expected winning percentage, RS = runs scored, RA = runs allowed (whatever that means). The book contains scatter diagrams, tree structures, rules of thumb. It even alludes to partial derivatives.

The increasing mathematization of baseball is indeed a revolution. "More than half of the thirty clubs have more than one person who is primarily working on analytics," the authors write. . . . "The challenge in today's front offices is to find enough employees who are capable of extracting meaningful information from what is quickly becoming a torrent of data." An individual player is reduced to a vector of numbers and a league to an 8×3 matrix. ID compactification galore!

Watching a recent Red Sox–Minnesota Twins game, I was annoyed by the constant display of the batters' vectors—along with such associated features as the velocity and the arrival location of the pitches. All these pop-ups or ancillary goodies reduce the pristine purity and simplicity of the game. Under mathematization, baseball has undergone a serious metamorphosis.

One last and somber thought. Do games like baseball and football constitute "a moral equivalent of war," to use William James's expression? Printed opinion seems to agree with him: They are instances of war carried out by other means. But I doubt that fans would buy into this harsh evaluation. "Play ball!" is what the umpire shouts out to start things rolling. Plainly and simply, baseball is a game.

Philip J. Davis, professor emeritus of applied mathematics at Brown University, is an independent writer, scholar, and lecturer. He lives in Providence, Rhode Island, and can be reached at philip_davis@brown.edu.

International Agenda for KAUST's UQ Center

The two-year-old Center for Uncertainty Quantification at the King Abdullah University of Science and Technology exemplifies the connections forged by KAUST with universities, professional societies, and industry worldwide. KAUST established the center in mid-2012, following a worldwide competition for Strategic Research Initiatives.

In its short existence, SRI-UQ has held two international workshops and hosted more than 40 world-class scientific visitors. SRI-UQ is actively mentoring a thriving cohort of graduate students and postdoctoral fellows, and several new UQ-related graduate courses have been created. As part of its mission, SRI-UQ also interacts with industry not only in Saudi Arabia and the region, but throughout the world.

SRI-UQ and SIAM. Clockwise from front left: Ben Mansour Dia, Alvaro Moraes, Pedro Vilanova, Hamidou Tembine, Hakon Hoel, SRI-UQ director Raul Tempone, SIAM president Irene Fonseca, Kody Law, and Bilal Saad.

UQ methods are essential to an understanding of complex systems, in which varying levels of uncertainty in different components can affect system behavior. Researchers in the area seek to quantify and eventually reduce the impact of those uncertainties in decision-making, risk assessment, and forecasting. As a consequence, UQ is particularly well suited to interdisciplinary research. Progress in the area requires combinations of advanced mathematical, statistical, and computational methods, as well as deep insight into application domains. Accordingly, SRI-UQ fosters a rich interdisciplinary research environment, in which more than 30 researchers interact with experimentalists at KAUST. Within this unique setting, SRI-UQ works to advance the state of the art in both theory and algorithms, while focusing on high-impact applications that include green wireless communications, complex

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the *posterior*), we can make a more refined prediction, denoted by the red curve.

Notice that all predictions are equipped with uncertainty. Furthermore, in this illustration, the Bayesian approach to the inverse problem has reduced the uncertainty, as manifest in the spread of the posterior probability distribution for the quantity of interest, reflecting the extra information obtained from the data. The reader will immediately see the benefits of this reduced uncertainty in any number of applications, including the examples of weather prediction, epidemiology, and traffic flow mentioned earlier, as well as in the increasingly vast numbers of application domains in which quantitative models and noisy data are available.

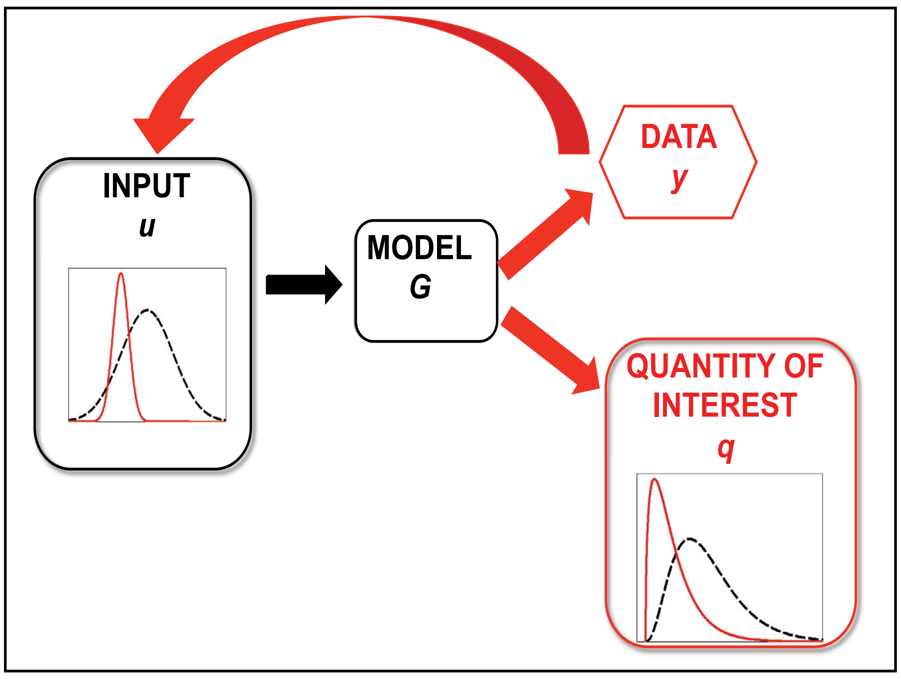

Figure 1. *Uncertainty quantification in Bayesian inversion.*

Practical Problem: CO_2 Capture and Storage

What, then, are the challenges for applied mathematics? To get some insight into where the challenges emerge, we consider the use of carbon capture and storage to facilitate global mitigation of the greenhouse effect [3]. Suppose, for example, that we are interested in assessing the economic viability and environmental impact of injecting CO_2 into the subsurface.

A typical CO_2 storage site could be a depleted oil/gas field or a deep saline aquifer (see Figure 2). The mathematical model in this case consists of the partial differential equations that describe the plume of injected CO_2 in the subsurface. Important inputs to the model are the permeability of the storage site, along with other geologic features, such as existing faults and fractures. Natural outputs comprise the measurements of bottom-hole pressure from the injection well and, possibly, of surface deformation from satellite data and GPS devices. Because the subsurface is not directly observable, the problem of inferring its properties (inputs) from measurements (outputs) is particularly important: With accurate inference, decisions can be made on the basis of a variety of quantities of interest, concerning both the safety and the financial feasibility of the storage site; for example, one might wish to assess the potential groundwater contamination from leakage of CO_2.

The challenges inherent in this application become apparent when we consider what is hidden in the deceptively simple Bayes' law stated above. In this example, the likelihood itself is defined through solution of the forward model, which is a coupled set of conservation laws (PDEs) describing the physics of multi-phase flow in a porous medium. The probability distribution on the input space of permeabilities lives on a space of functions; in practice, this means that we will be representing probabilities on very high-dimensional spaces. To probe the posterior probability distribution, then, we need to take on the challenge of solving complex PDEs over an enormous space of input permeabilities. Similar daunting challenges emerge in a vast range of applications. Nonetheless, the last decade has seen considerable advances in the Bayesian approach to inverse problems, and the book [10] has played a major role in establishing the viability of the approach on today's computers.

Because our subject is in its infancy, with growing numbers of applications and a range of methodologies, considerable long-term challenges remain. A key modelling question, which will be very application-specific, concerns the choice of prior for the unknown. A key computational question concerns ways to probe the posterior distribution with sufficient accuracy that we can compute the posterior probability distribution on quantities of interest. Furthermore, these modelling and computational questions interact.

The subject is in need of sustained input from applied mathematicians who can help to guide the development of algorithms, through analysis of their complexity and through computational innovation. This work needs to be done in the context of classes of application-specific prior models. Success in this area requires an appreciation for analysis (e.g., of PDE-based forward models), computation (e.g., high-dimensional integration), probability (e.g., in specifying random field priors), and statistics (e.g., in exploiting data in the design of algorithms to explore the posterior). In each case the work needs to be guided by application-specific modelling considerations.

Returning to the example of CO_2 storage, we consider priors for the subsurface permeability that deliver different "typical" functions, as displayed in Figure 3, left and centre. On the left, the permeability is piecewise-constant, and the unknown parameters define the position of the layers of different materials that constitute the subsurface, together with the position of the fault and the permeability values within each layer. In the centre image, the permeability is defined through the location of a single interface; the considerable variability above and below the interface is represented by a function, and not just a single value. Prior models for which these two different permeabilities are "typical" will be quite different and will lead to different computational considerations; moreover, if prior knowledge is scarce, the prior might need to incorporate both permeabilities as "typical," possibly along with those of other types, such as that displayed in Figure 3 (right). Details of the mathematical formulation of such problems, and references to the engineering literature in which these models were originally developed, can be found in [9].

Once the prior and forward model are specified, the posterior is defined via Bayes' rule, and we then move on to the computational task of exploring the posterior and computing expectations with respect to it. Monte Carlo–Markov Chain, or MCMC, is a natural methodology for studying these problems, and the last decade has seen considerable progress in the theory and practice of these methods in high dimensions [5]. Nevertheless, vanilla Monte Carlo-based methods, whilst enormously flexible, are hampered by their $N^{-1/2}$ convergence rate [2], meaning that computational complexity (cost per unit error) can be rather excessive. As a consequence, we are likely to see the development of multi-level Monte Carlo [8] and quasi-Monte Carlo [2] methods in the context of inverse problems. In addition, the use of generalized polynomial chaos methodologies and their relatives [1,4,7,12] is likely to be transferred into the context of inverse problems, as exemplified in [13]; again, these methods hold the possibility of improving on the complexity of Monte Carlo methods. Interested readers can find further details in the articles [14,15] and the references therein.

In this burgeoning field, the numerous opportunities for research in applied mathematics are driven by both the enormous numbers and types of applications, together with the wide range of areas in the mathematical sciences from which contributions are needed. The subject is at a tipping point, where computational power is starting to allow the exploration of quite complex Bayesian models, and the opportunity for impact is high. In summary, this is an excellent area for applied mathematicians who are looking for new research challenges.

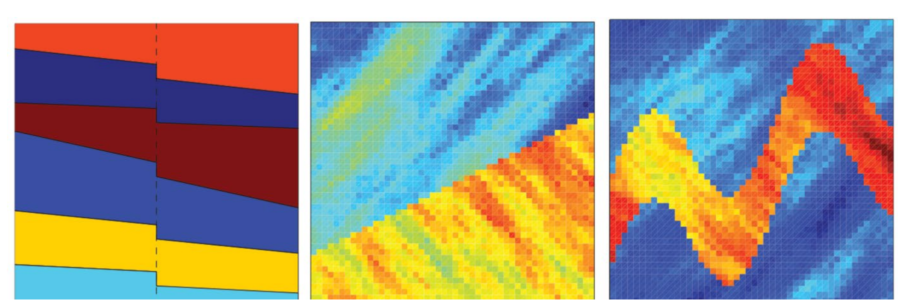

Figure 3. *Draws from various permeability priors: piecewise-constant layer model with fault (left), piecewise-continuous layer model (centre), and piecewise-continuous channel model (right).*

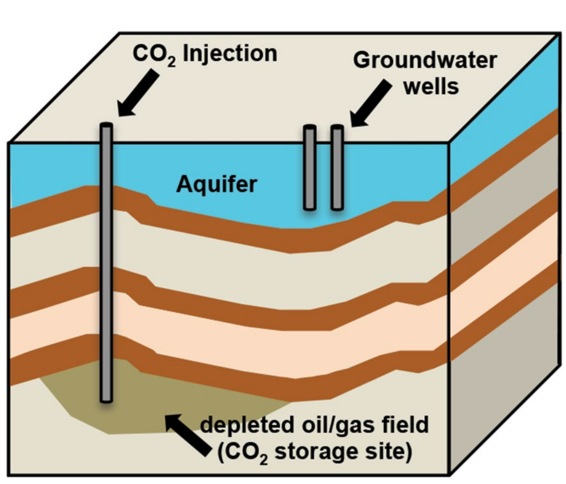

Figure 2. *Geologic storage of CO_2.*

Acknowledgments

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Marco Iglesias is an assistant professor in the School of Mathematical Sciences, Nottingham University, UK. Andrew Stuart is a professor of mathematics at the Mathematics Institute, Warwick University, UK. This article is based, in part, on a lecture delivered by Stuart at the 2014 SIAM Conference on Uncertainty Quantification, held in Savannah, Georgia.

KAUST

continued from page 4

multiscale electromagnetic systems, and reactive computational fluid dynamics.

A constant in the evolution of SRI-UQ has been close ties with SIAM: SRI-UQ director Raul Tempone is the current technical director of the SIAM Activity Group on Uncertainty Quantification, and several SRI-UQ members, including deputy director Omar Knio, serve on the editorial boards of SIAM journals. Visits to KAUST are something of a tradition for SIAM presidents; following in the footsteps of several of her predecessors, Irene Fonseca visited SRI-UQ in March 2014. As shown in the photo on page 1, she also took the opportunity to meet with members of KAUST's student chapter of SIAM.

KAUST officially opened in 2009 as an international, graduate-level research university in Thuwal, Saudi Arabia. KAUST integrates research and education, leveraging the interconnectedness of science and engineering, and works to catalyze the diversification of the Saudi economy through economic and technology development. KAUST faculty now number about 130, and 600 graduate students are enrolled in MS and PhD programs.

Additional information about the structure and activities of SRI-UQ, along with job openings and a list of publications, can be found at http://sri-uq.kaust.edu.sa/.

—Raul Tempone, Director, Strategic Research Center for Uncertainty Quantification, KAUST.

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Applications should include a statement of research interest (that also explains an applicant's suitability for this position), a CV, and contact information for three references. Applications should be sent to: Thuy Nguyen, ttnguyen@stanford.edu.

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Applications must be submitted online through: http://www.anl.gov/careers/apply-job. Correspondence and supporting letters of recommendation should be submitted to Named-Postdoc@anl.gov. For more information, applicants should visit the Argonne Postdoc Blog at https://blogs.anl.gov/postdoc/ or contact the postdoctoral program coordinator, Kristene Henne, at khenne@anl.gov.

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The Center for Systems Biology Dresden invites applications for several open postdoctoral positions in computer science, computational science, and applied mathematics within the prestigious ELBE Postdoctoral Fellowship Program. The center seeks outstanding candidates who have a strong computational background and interest in working in a multidisciplinary environment to develop data analysis, computer vision, bioimage analysis, high-performance computing, and numerical simulation algorithms and theories to establish computational biology as an integral part of the life sciences. ELBE fellowships are awarded on a competitive basis to outstanding young researchers with a doctoral degree. To foster collaboration, fellows are usually affiliated with two hosting groups working in different disciplines.

The Center for Systems Biology Dresden focuses on developing and using computational methods to address key questions in biology and to transform data into knowledge. The center is a joint activity by the Max Planck Institute of Molecular Cell Biology and Genetics and the Max Planck Institute of the Physics of Complex Systems. The center is a highly interactive and collaborative workplace with an international atmosphere in which English is the working language and there is a strong commitment to interdisciplinary training and career development. The center provides access to cutting-edge computer infrastructure and laboratory facilities. The MPI–CBG was named one of the Best Places to Work for Postdocs in 2011.

Dresden was awarded City of Science in 2006 and is one of the leading scientific centers in Europe with three Max Planck and 13 other research institutes, and the Dresden University of Technology as one of 11 Universities of Excellence in Germany. Dresden has half a million inhabitants and is considered one of the most beautiful cities in Germany, located two hours from Berlin and Prague.

The deadline for applications is September 5, 2014. For details about the application procedure, applicants should visit: http://mpg-sysbio.de/index.php?id=jobs.

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Smale Problem
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distinct zeros of $z^4 - 1$. There may even be points of the complex plane that do not belong to any basin of attraction, as is the case for the quadratic polynomial $z^2 + 1$. Launching Newton's method from any real starting point yields a sequence of real "approximations" incapable of approaching either imaginary zero.

In order to take advantage of Bezout's theorem on the number of zeros of a system of complex homogeneous polynomials, we begin by letting $d_1, \cdots, d_n$ be the degrees of $f_1, \cdots, f_n$, and homogenizing each f_i by multiplying each constituent monomial by whatever power of an auxiliary variable z_0 is needed to increase its degree to d_i. The result will be a system of n homogeneous polynomials of degrees $d = (d_1, \cdots, d_n)$ in the $n + 1$ variables $z_0, \cdots, z_n$. A variant of Newton's method, known as the projective Newton's method, applies to such systems.

If $\mathbb{H}_{(d)}$ is the vector space of all homogenous systems f of degree d, then $dim\mathbb{H}_{(d)}$ can be shown to be $N = \sum_{i=1}^{n} C_n^{n+d_i}$, where C_n^m is a binomial coefficient, and the number of solutions $\zeta = (\zeta_0, \cdots, \zeta_n)$ is known by Bezout's (19th-century) theorem to be $B = \prod_i d_i$. In particular, if each d_i is 2, then $N \sim n^3/2$ while $B = 2^n$. The number of solutions ζ is thus exponential in n, dashing any hope for a polynomial-time algorithm to produce all solutions.

With only a few equations of high degree, the problem can be reduced via exact symbolic techniques (Gröbner bases, resultants, and the like) to that of solving a univariate polynomial of degree B in polynomial time. But that fact alone does not lead to a solution of Smale's 17th problem, even in combination with the homotopy methods employed by Smale in his early work on single polynomials, much of it [5,6] in collaboration with Shub.

Homotopy Methods

In his talk, Shub described recent progress toward a complete solution of Smale's 17th problem via homotopy methods. Such methods operate by embedding a trivial system f_0 and a target system f_1 in a continuum of systems $f_t; 0 \leq t \leq 1$ in the hope that, for some partition $0 = t_0 < t_1 < \cdots < t_m = 1$ of the interval [0,1], it will prove possible to solve each intermediate system $f_{t_i} = 0$; $i = 0,1, \ldots, m$ in turn, with each intermediate approximation r_{t_i} serving as the starting point in a search for the next. Thus, Shub's algorithms α all proceed by discrete steps from an initial approximate solution r_0 of $f_0 = 0$ to . . . to a solution $r_i\, r_{t_i}$ of $f_{t_i} = 0$ . . . to the desired approximate solution r_1 of $f_1 = 0$.

A homotopy $\Gamma_t = (f_t, \zeta_t)$ is a curve in the space of all pairs (f, ζ), and an approximate homotopy is a surrounding tube so slender that Newton's method converges quadratically to ζ_τ from any starting point r_τ within the section $t = \tau$ of that tube. Nothing prevents such tubes from merging and/or bifurcating as t increases from 0 to 1.

To analyze homotopy algorithms, Shub considered the "solution variety" V of all pairs (f, ζ) such that $f(\zeta) = 0$. When appropriate norms are imposed on the (factor) spaces of systems f and arguments ζ, V becomes a smooth differentiable manifold $\mathcal{M}$ on which one can define—among other things—the length Λ of a homotopy $\Gamma_t = (f_t, \zeta_t)$ to be

$$\Lambda(\Gamma_t) = \int_0^1 \mu(f_t, \zeta_t)\, \|(\dot{f}_t, \dot{\zeta}_t)\|\, dt,$$

$\mu(f_t, \zeta_t)$ being a generalization of the usual "condition number" for a system of linear equations, defined wherever $\nabla f_t(\zeta_t) \neq 0$. The inclusion of $\mu(f_t, \zeta_t)$ within the arc-length integral causes geodesics in $\mathcal{M}$ to deviate from the straight and narrow toward regions favorable to computation, much as light rays in outer space bend toward concentrations of mass.

Shub mentioned a proof by Carlos Beltrán and Luis Miguel Pardo [2,3] that the problem Q can be solved *with high probability* in polynomial time, leading some in the field to consider Smale's problem #17 solved. After all, if such a method fails to produce a solution within a reasonable amount of time, another try can always be made from a different starting point, thereby squaring the (already small) failure probability.

Shub does not consider Smale's problem #17 solved—he is certain that Smale had in mind an algorithm α that would work for sure. After mentioning progress in this direction by Felipe Cucker and Peter Bürgisser [4], Shub ended his presentation by urging listeners to help "finish solving Smale's 17th problem."

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James Case writes from Baltimore, Maryland.

A Smale Challenge Problem Edges Toward Solution

By James Case

In 1998, Stephen Smale compiled a list of 18 challenge problems for the 21st century. Two of them—the Riemann hypothesis, at #8, and a problem concerning the topology of algebraic curves and surfaces, at #16, were held over from Hilbert's more famous list of 23 challenge problems for the 20th century. Others were unmistakably 20th century in origin, including #3, P = NP? ; #18, concerning the limits of intelligence; and #17, which asks for an algorithm capable of computing approximately, in low-order polynomial average time, a single zero of a system of n polynomial equations in n complex unknowns. Michael Shub, whose 1967 UC Berkeley thesis on dynamical systems was directed by Smale, and who is currently an adjunct professor of mathematics at the CUNY Graduate School, surveyed progress toward a solution of Smale's 17th problem in an invited talk at the 2013 SIAM Annual Meeting.*

To speak of average computation time, one must specify a class of problems to be solved, an algorithm for solving them, and a measure of the size of any problem in the given class. Smale initiated the investigation of average computational times, setting out first to discover an efficient algorithm for finding the roots of a single complex polynomial. In later work [7], he sought to explain why the simplex algorithm works as well as it does in practice, despite being NP-complete in unfavorable cases. His work on the simplex algorithm was particularly fruitful, as it answered a question many were asking and spawned a flurry of follow-up activity.

*Slides and audio for many sessions from AN13, including Shub's AMS invited lecture, can be found at siam.org/meetings/presents.php.

The class of problems the simplex algorithm is designed to solve is just the class of linear programs

$$(P) \qquad \text{minimize } \langle c,x\rangle \quad \text{subject to } Ax \le b \text{ and } x \ge 0,$$

where A is an $m \times n$ matrix of real numbers, and b, c, and x are conformable real vectors. There is a natural way to turn the set of all such problems into a manifold $\mathcal{M}$, and a natural measure of the "size" $|P|$ of any problem $P \in \mathcal{M}$, namely $|P| = \min(m,n)$. If $T(P;\alpha)$ denotes the time required for algorithm α to solve the problem $P \in \mathcal{M}$, and if there is a natural probability measure on $\mathcal{M}$, it is then possible to compute the expectation $E(T(P;\alpha))$. If $\mathcal{M}$ consists of all linear programs, if α is a certain version of the simplex algorithm, and if $T(P;\alpha)$ is proportional to the number of vertices visited by α, it is known [1] that

$$E(T(P;\alpha)) = O(|P|^2).$$

Systems of Equations

The situation with regard to the solution of systems of equations is less transparent. Relying on his experience in solving practical problems at IBM (where he was a member of the research staff from 1985 to 2004), Shub observed that methods which work for systems of polynomial equations tend to work nearly as well for equations of other types. Accordingly, it made sense to confine his attention to the following problem:

$$(Q) \qquad \text{find } \zeta = (\zeta_1, \cdots, \zeta_n) \quad \text{such that } f(\zeta) = 0,$$

where $f = (f_1, \cdots, f_n)$ is a system of (real or complex) polynomials in $z_1, \cdots, z_n$.

Whereas it is easy enough to impose a manifold structure on the set of all such systems, and to define a probability measure on the resulting $\mathcal{M}$, it is not so clear what algorithm(s) α to consider, or even how to define $T(Q;\alpha)$ for a given $Q \in \mathcal{M}$ and α. Unlike the simplex algorithm, which terminates after a finite number of steps, standard algorithms for computing the zeros of even a single polynomial do not. Standard techniques, such as Newton's method, typically produce an infinite sequence of approximations devised to converge to the desired ζ. Shub's response was to consider an algorithm to have terminated on arrival in a neighborhood throughout which Newton's method is or at least appears to be quadratically convergent. Such neighborhoods typically occupy but a small portion of the surrounding basins of attraction.

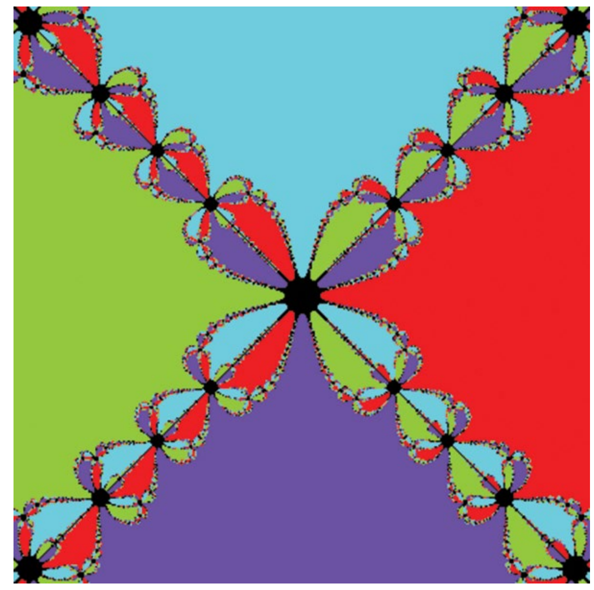

Figure 1. *Basins of attraction for Newton's method applied to $z^4 - 1$.*

Basins of attraction are notoriously complex, as shown in Figure 1, which depicts the basins of Newtonian attraction of the

See **Smale Problem** *on page 7*

Richard Tapia

continued from page 1

of UMBC. "His passion for education and his commitment to young people should inspire all of us to do more. In the words of Aristotle, 'choice not chance determines your destiny.'"

"Richard Tapia as well as his story have been a personal inspiration for me and many, many people who come from groups which have been traditionally prevented from making their unique contributions to the progress of science, technology, engineering and mathematics fields in the United States. By his success, he has demonstrated what is possible," said Sylvester James Gates, 2012 recipient of the National Medal of Science.

Among those expressing admiration for Tapia's efforts were two former SIAM presidents. "For nearly half a century," in the words of Doug Arnold, "Richard Tapia has been a tireless force for excellence and inclusion in [STEM disciplines]. . . . The face of American mathematics literally would not be the same were it not for Richard Tapia's work."

Mac Hyman focused on Tapia's passion for science and commitment to engaging others to consider careers in the mathematical sciences: "He has the rare ability to inspire and share his love for mathematics with underrepresented communities, and has given a generation of young professionals the self-confidence to embrace careers in the mathematical sciences."

Self-described "outspoken critic" of a society too slow to elevate Latinos to prominent positions, Richard Tapia graciously accepted the Vannevar Bush Award.

"Richard Tapia has been a persistent and effective teacher and mentor for the underrepresented in our society, drawing them to the beauty and value of mathematics," said Rita Colwell, who as director of NSF (1998–2004) supported dramatic increases in funding for the mathematical sciences. "He is personally responsible for a large number of new entrants to the world of mathematics, including women, a component of society rarely encouraged to enter mathematics as a professional career path. Richard deserves the recognition and accolades now coming to him."

As a fellow mathematician, Brit Kirwan, chancellor of the University System of Maryland and chair of the Board on Higher Education and Workforce of the US National Academies, considers Tapia "a personal hero for his lifelong commitment to excellence and inclusion in higher education" and for his research, which "has broadened the frontiers of knowledge in important areas of mathematics." Tapia is a previous co-chair of BHEW (of which I am a current member).

Vannevar Bush was long associated with MIT, where he was a faculty member before becoming vice president and dean of the MIT School of Engineering (in 1932). In the words of L. Rafael Reif, recently inaugurated as MIT's first Hispanic president, " . . . scholar, educator, mentor, and leader, . . . the qualities that Dr. Bush held so dear make [Richard Tapia] an excellent choice for this great honor." Wesley Harris, Charles Stark Draper Professor of Aeronautics and Astronautics at MIT, pointed to Tapia's standing among the nation's leaders in producing scholarship in mathematics and in mentoring graduate students, especially underrepresented minority graduate students who have earned PhDs under his supervision.

Having participated most recently in an advisory capacity with Tapia in MIT's initiative on faculty and race,* I take this opportunity to reiterate the great impact that he has had on my life. He has made me think hard about equity and underrepresentation, particularly about the damage and severe limitations still caused by definitions of meritocracy that fail to account for the deleterious effects of history and initial conditions even as we work to ensure that everybody has access to the promises of our democracy. This effort has been led in words and actions by the incomparable Richard Tapia.—*Carlos Castillo-Chavez, Arizona State University.*

*http://web.mit.edu/provost/raceinitiative/.