

Unprecedented Simplicity

An elegant proof of the optimality of the semicircle capped Richard Tapia's talk on the isoperimetric problem in Minneapolis.

By James Case

Revisiting the isoperimetric problem in an invited address at the 2012 SIAM Annual Meeting, Richard Tapia of Rice University observed that the earliest known proofs of the “isoperimetric theorem,” including the analytic one given by Euler (in 1744) and the geometric one offered by Jakob Steiner (in 1838), were incomplete for having assumed without proof that a solution exists.

The roots of the problem, Tapia said, are lost in antiquity. Pythagoras seems to have been aware—before 500 BCE—that of all simple closed planar curves of a given length, the circle encloses the greatest area, although the remarks attributed to him on the subject are somewhat ambiguous.

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The Smart Money's on Numerical Analysts

I'd like to mention two of the biggest unsolved problems in numerical analysis. One of them, if solved affirmatively, would change the world. The other would have little practical effect but would settle a mystery that has been standing for fifty years.

The first problem is, can an $n \times n$ linear system of equations $Ax = b$ be solved in $O(n^{2+\epsilon})$ operations, where ϵ is arbitrarily small? In other words, could there be a “fast matrix inverse,” like the fast Fourier transform?

The standard algorithms, like Gaussian elimination, take $O(n^3)$ operations, and you can see that cubic exponent reflected in the history of computing. In sixty years, computer speeds have increased by 15 orders of magnitude, from flops to petaflops. With a fast matrix inverse and plenty of memory, the dimension of matrix problems we could handle would have grown from $n = 10$ to $n = 10^{8.5}$. In fact, we are nowhere near that scale.

It has been known for more than 40 years that, in theory, the exponent of 3 can be beaten. Strassen reduced it to 2.81 in 1969, and Coppersmith and Winograd reduced it further in 1990, to 2.376. Despite much conceptual progress since then, however, especially in the past few years, the exponent has improved only to 2.373. And the algorithms implicit in this highly theoretical work are complicated,

too complicated to have much promise in practice. It is an article of faith for some of us that if $O(n^{2+\epsilon})$ is ever achieved, the big idea that achieves it will correspond to an algorithm that is really practical.

My own faith has been strong for years. Back in 1985, I made a \$100 bet with Peter Alfeld that a fast matrix inverse would be found by 1995. It wasn't, so I paid him \$100 and renewed the bet for another decade. It still hadn't been found by 2005, so I paid him a further \$100 and we renewed once more. One day I will win!—or my heirs?

If a fast matrix inverse is found, everything in computational science will be shaken up. That's what happened with the FFT after 1965, and the fast matrix inverse would be equally epochal. I believe it is in the same category of importance as the celebrated $P = NP$?

The second big unsolved problem is also in the area of linear algebra. Why is Gaussian elimination numerically stable in practice, even though it's unstable in the worst case? In other words, why does Gaussian elimination work?

For a brief period in the 1940s, it was believed that Gaussian elimination would not work, that it would be undone by rounding errors on a computer. Experiments soon showed, however, that it was utterly reliable in

practice, and Jim Wilkinson became famous by developing a theory that went partway to explaining this. Wilkinson showed that an algorithm will have all the accuracy properties one could reasonably ask for if it is “backward stable,” delivering the exact answer to a slightly perturbed problem. It was a beautiful and powerful observation that has been a centerpiece of numerical analysis ever since.

The trouble is, though most algorithms of numerical linear algebra are backward stable, Gaussian elimination is not. (Throughout this discussion I am speaking of the standard variant of Gaussian elimination, with row or “partial” pivoting.) Wilkinson showed that its stability can be quantified by a number known as the “growth factor,” ρ , the ratio of the largest entry in the final upper-triangular matrix U to the largest entry in the original matrix A . Unfortunately, although ρ is usually small, it can be as large as 2^{n-1} if you pick A diabolically. All this was already known and published by Wilkinson in a landmark paper in 1961.

Given the existence of such matrices, why doesn't Gaussian elimination fail in practice? If you look in the textbooks, you will find that they do not confront this question mathematically but make empirical statements like “In practice such growth is very rare,” or “This bound is much too pessimistic in most cases.” My favourite analysis is the one attributed to Wilkinson himself:

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Uncertainty Quantification 2012

Uncertainty Quantification for Environmental Models

By Mary C. Hill, Dmitri Kavetski, Martyn Clark, Ming Ye, and Dan Lu

Environmental models are used to evaluate the fate of fertilizers in agricultural settings (including soil denitrification), the degradation of hydrocarbons at spill sites, and water supply for people and ecosystems in small to large basins and cities—to mention but a few applications of these models. They also play a role in understanding and diagnosing potential environmental impacts of global climate change. The models are typically mildly to extremely nonlinear. The persistent demand for enhanced dynamics and resolution to improve model realism [17] means that lengthy individual model execution times will remain common, notwithstanding continued enhancements in computer power. In addition, high-dimensional parameter spaces are often defined, which increases the number of model runs required to quantify uncertainty [2]. Some environmental modeling projects have access to extensive funding and computational resources; many do not.

The many recent studies of uncertainty quantification in environmental model predictions have focused on uncertainties related to data error and sparsity of data, expert judgment expressed mathematically through prior information, poorly known parameter values, and model structure (see, for example, [1,7,9,10,13,18]). Approaches for quantifying uncertainty include frequentist (potentially with prior information [7,9]), Bayesian [13,18,19], and likelihood-based. A few of the numerous methods, including some sensitivity and inverse methods with consequences for understanding and quantifying uncertainty, are as follows: Bayesian hierarchical modeling and

Bayesian model averaging; single-objective optimization with error-based weighting [7] and multi-objective optimization [3]; methods based on local derivatives [2,7,10]; screening methods like OAT (one at a time) and the method of Morris [14]; FAST (Fourier amplitude sensitivity testing) [14]; the Sobol' method [14]; randomized maximum likelihood [10]; Markov chain Monte Carlo (MCMC) [10]. There are also bootstrapping and cross-validation approaches. Sometimes analyses are conducted using surrogate models [12].

The availability of so many options can be confusing. Categorizing methods based on fundamental questions assists in communicating the essential results of uncertainty analyses to stakeholders. Such questions can focus on model adequacy (e.g., How well does the model reproduce observed system characteristics and dynamics?) and sensitivity analysis (e.g., What parameters can be estimated with available data? What observations are important to parameters and predictions? What parameters are

important to predictions?), as well as on the uncertainty quantification (e.g., How accurate and precise are the predictions?).

The methods can also be classified by the number of model runs required: few (10s to 1000s) or many (10,000s to 1,000,000s). Of the methods listed above, the most computationally frugal are generally those based on local derivatives; MCMC methods tend to be among the most computationally demanding. Surrogate models (emulators) do not necessarily produce computational frugality because many runs of the full model are generally needed to create a meaningful surrogate model. With this categorization, we can, in general, address all the fundamental questions mentioned above using either computationally frugal or demanding methods. Model development and analysis can thus be conducted consistently using either computationally frugal or demanding methods; alternatively, different fundamental questions can be addressed using methods that require different levels of effort.

Based on this perspective, we pose the question: Can computationally frugal methods be useful companions to computationally demanding methods? The reliability of computationally frugal methods generally depends on the model being reasonably lin-

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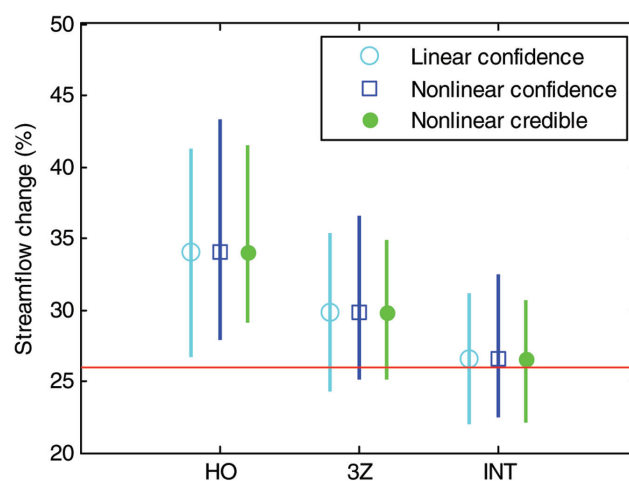


Figure 1. Linear and nonlinear confidence intervals and nonlinear credible intervals (using INT as an example; 106, 1594, and 420,000 model runs, respectively) on predicted change in streamflow caused by pumpage for three alternative models. The horizontal line defines the true value of the prediction, which is known for this synthetic problem. The nonlinear credible intervals are calculated by MCMC with a DREAM algorithm. (After [9].)

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1 Unprecedented Simplicity

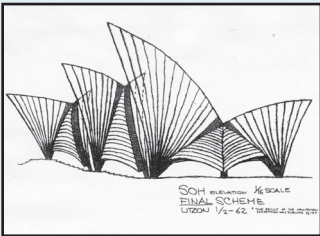
1 The Smart Money’s on Numerical Analysts

1 Uncertainty Quantification for Environmental Models

5 SIAM Explores Modeling for STEM Pipeline

6 Mathematics: Handmaiden to Architecture

Drawing on “a vast and eclectic store of knowledge,” reviewer Philip Davis writes, mathematician/author Alexander Hahn surveys some of the world’s great buildings. The “eyebrow-raising book filled with pictures and diagrams” can be seen as “a celebration of mathematics in its infinite variety.”



6 Physics and Computation

Leading off with up-to-date instances of “computer technology bumping up against fundamental physical constants,” Ernest Davis reviews a book on physics-based limits on computation. Most impressed by the chapter on quantum computing, he cites its fair-minded discussion of different interpretations of quantum theory while lamenting the meager discussion of what has been accomplished.

12 A Leading Role for Mathematics in the Study of Ionic Solutions

Hoping for “an army of mathematicians” to take on the challenges of ionic solutions, Bob Eisenberg surveys contributions and limitations of the Poisson–Boltzmann and Poisson–Nernst–Planck equations. “Work on PB–PNP sets the stage on which the moving dance of biology can be studied, as it is actually lived,” he says, pointing to promising approaches now awaiting application.

9 Professional Opportunities

Mathematicians in the Shark Tank!

By Fadil Santosa
and Richard Sowers

We’re all aware of careers in industrial mathematics, but what about a career in entrepreneurial mathematics? Because the majority of new jobs are in small businesses, the Institute for Mathematics and its Applications at the University of Minnesota decided to run an experiment, which took the form of a workshop, Fostering Mathematical Entrepreneurship: Creating New Businesses for Wealth and Impact. Held August 2 and 3 at the IMA, the workshop was designed to expose mathematics grad students to the notion of starting their own businesses. John Dexheimer (Lightwave Advisors and First Analysis Private Equity), Doug Johnson (University of Minnesota Venture Center), Fadil Santosa (IMA), and Richard Sowers (University of Illinois at Urbana–Champaign) organized the workshop; 20 graduate students attended.

Kicking off the workshop was Jeff Hoffstein of Brown University, who is co-founder of NTRU, a company focused on cryptography. His talk, in which he recounted his journey as an entrepreneur (see accompanying interview), was followed by two panel discussions. One panel was made up of people from companies built on technologies in which mathematics is an important component; the other featured members of the venture capital community in discussions of the types of companies they fund.

In the afternoon, after a crash course on creating a business plan, the students were divided into groups and given assignments. The assignments were formed around technologies that the organizers had come up with; all required mathematics in order to be realized and all were assumed to exist. A team’s task was to develop a business plan based on the assigned technology. Some of the technologies are:

- Algorithms for reconstructing documents that have been shredded (based on the DARPA challenge at <http://archive.darpa.mil/shredderchallenge/>).
- Simulation of diamond cutting and visualization of cut diamonds.
- Noise cancellation technology for homes.
- OCR for hand-written mathematics.

Each group was to come up with a 10- to 15-minute presentation (to be given the following morning) with the aim of attracting venture or angel funding. In other words, they had to project what the size of the market would be, how their product would compare with others, and so forth (thank goodness for the web). None of these projects were centered around the students’ actual research; they were essentially case studies and thought experiments.

The organizers were amazed by the quality of the presentations. The thought and the



Student team members (from left) Elizabeth Lam (Toronto), Drew Swartz (Purdue), and Lei Ge (Central Florida) make a business pitch.

hard work that went into the business plans were noticeable. Moreover, the delivery was in general polished and convincing. It was clear that the students were enthusiastic and genuinely excited about the exercise. As organizers, our modest goal was to ask the students to step briefly outside their comfort zones. They exceeded our goals by immersing themselves in an unfamiliar world and functioning as budding entrepreneurs.

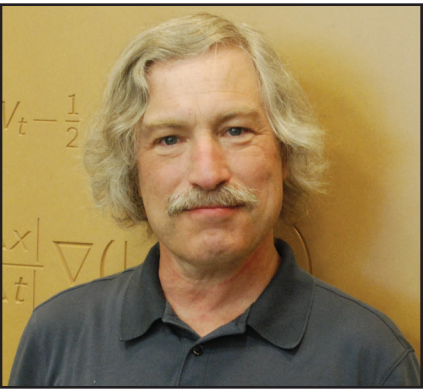
One student remarked that she did not realize until she participated in the workshop how much fun it was to put together a business plan. Another said, “I now have a better idea of what opportunities are out there for me, and hearing the personal experiences of individuals with similar backgrounds, their successes and failures, is invaluable.” In many ways, mathematics is a good preparation for entrepreneurship. It

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An Interview with Jeff Hoffstein

Fadil Santosa: *You were trained as a number theorist and you are a successful academic. What made you decide to work on something applied?*

Jeff Hoffstein: I started out as the purest of the pure mathematicians. If there was an application, I wasn’t interested. About 1992, though, I had a child, and I realized that applications that led to a lot of money could have their point. I looked around for problems to solve. In 1994, I heard a talk by Dorian Goldfeld that connected a previous result of ours to cryptography. I realized that if these ideas could be used to create a public-key cryptosystem, the resulting system would be far more efficient and lightweight than public-



Jeff Hoffstein, an outsider to the cryptography community, describes the rocky path of the company he and two Brown University colleagues built around their public-key cryptosystem.

key cryptosystems based on factoring large integers or the discrete log problem.

FS: *The cryptosystem you created, NTRU, based on lattices in high dimensions, is very original. As an “outsider” to the crypto community, was it difficult to convince people that you had something new?*

JH: It wasn’t hard to convince people that it was new. It was hard to convince them that it was secure. NTRU is a collaboration with two Brown colleagues: Jill Pipher (now director of ICERM) and Joe Silverman. We were all pure mathematicians with little connection to the crypto community. When we tried to introduce NTRU, all we got was pushback and outright hostility. In fact, I would say it wasn’t until a few years ago that the crypto community finally began to accept the fact that NTRU might be secure.

FS: *What were the steps you took to get NTRU off the ground?*

JH: The main idea for NTRU was in place around 1995. Joe Silverman and I went to Bell Labs in 1996 and presented it to Andrew Odlyzko. The next step was to present a talk in the “rump session” (2- to 6-minute talks) at Crypto 1996. The response was rather hostile. There were several reasons for this. One is that we were outside the crypto network and were viewed with suspicion. The key misunderstanding is that the community thought that there was an easy solution to the hard problem the system was based on. What we did next was to incorporate. We had already filed a provisional patent on the technology. An early investor was Sony. Shortly afterward, we hired a CEO and raised investor capital. We grew the company. In 2000 we had 2 key employees, by 2001 we had over 20. Unfortunately, it turned out to be harder to sell lightweight public-key cryptography than we had expected.

FS: *During the start-up phase, how much of your effort was devoted to NTRU?*

JH: Joe, Jill, and I were on leave from Brown for a good part of the first few years. Speaking of which, I would advise anyone starting a company: “Don’t quit your day job.”

FS: *What were the hiccups during this period?*

JH: First, we contracted the software development to a company that was not able to deliver. We had to recover from that. More seriously, business pressures pushed us to develop a digital signature scheme. We did this, but we sent it out the door too soon, and major flaws were quickly discovered by the crypto community. While we did fix these, our credibility (already

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Isoperimetric Problem

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ous. Euclid (330–260 BCE) proved that the equilateral triangle maximizes the enclosed area among all triangles of given perimeter, and that the square does likewise among all such rectangles. In a book titled *On Isoperimetric Figures*, Zenodorus (200–140 BCE) reportedly gave proofs of the following two theorems:

Among all polygons of equal perimeters and equally many sides, the regular polygon contains the greatest area.

The circle encloses a greater area than any regular polygon of equal perimeter.

The book itself has been lost. We know of it only from partially preserved contents in the works of Pappus (290–350 CE) and Theon (335–405 CE) of Alexandria.

Despite the lack of a formal proof, the validity of the isoperimetric theorem was widely accepted in the ancient world. Virgil's *Aeneid* recounts the story of Queen Dido's clever application of the theorem. When the ship in which she was travelling washed up in a storm on a foreign shore, she persuaded the local monarch to grant her as much land as she could cover with the hide of a bull. Dido instructed her servants to cut the hide into a single long thong (best accomplished by starting on the perimeter and spiraling inward), and then to string it out in the shape of a semicircle stretching inland from the seashore. Though surprised by the result, the monarch stood by his bargain, and Dido founded within the ensuing land grant what eventually became the thriving city of Carthage. Tapia exhibited pictures of several medieval cities, including Paris, whose protective walls formed semicircles bounded on the open side by unfordable rivers.

Nothing more of mathematical consequence was said on the isoperimetric problem until 1744, when Euler cast it in a form essentially equivalent to the following “Queen Dido” problem:

$$\begin{aligned} &\text{maximize } \int_{-a}^a y(x) dx \\ &\text{subject to } \int_{-a}^a \sqrt{1 + [y'(x)]^2} dx = a\pi; \\ &y(-a) = y(a) = 0, \end{aligned}$$

and concluded that the solution—which he tacitly assumed to exist—can only be the

semicircle $y_0(x) = \sqrt{a^2 - x^2}$, $-a \leq x \leq a$. In 1755, at the end of a brief letter to Euler, the then 19-year-old Lagrange attached an appendix describing his revolutionary method of “variations,” whereby he could readily deduce “Euler’s equation” along with the rudimentary “multiplier rule” used by the master to obtain his solution. So taken was Euler with this new method that he abandoned his own geometric techniques, adopted those of Lagrange, coined the term “calculus of variations,” and referred thereafter to multiplier theory as “Lagrange multiplier theory.” Tapia noted, in a technical aside, that the arc length integral for the semicircle does in fact exist as an improper integral.

The next significant development came from Steiner (1796–1867), a Swiss geometer who disliked analysis and doubted that anything proved with it couldn’t be proved with traditional geometry. To strengthen his case, he offered (in 1838) a novel geometric proof of the isoperimetric theorem. Analysts of the time, however, led by Dirichlet, were quick to point out that the proof was incomplete, as it rested on the assumption that a solution exists. What would be required, they wondered, to “complete Steiner’s proof”?

The question remained open until 1879, when Weierstrass developed his famous sufficiency theory and applied it to the isoperimetric problem. Over the next forty odd years, a substantial series of papers by a who’s who of prominent analysts offered alternative proofs of the optimality of the semicircle $y_0(x)$.

Tapia argues, however, that all the early sufficiency proofs were unnecessarily complicated: The authors had failed to recognize and exploit the underlying concavity of the problem. Indeed, he noted, it was not until Johan Jensen (in 1905) and Herman Minkowski (circa 1907) that modern mathematics began to recognize the importance of functional convexity, despite the fact that both Archimedes and Fermat had defined and exploited the property of convexity for geometric curves.

Tapia’s first sufficiency proof involves the functional

$$J(y) = \int_{-a}^a \left\{ y(x) - a \sqrt{1 + [y'(x)]^2} \right\} dx;$$

the semicircle $y_0(x) = \sqrt{a^2 - x^2}$, $-a \leq x \leq a$; and a concave alternative $y(x) \neq y_0(x)$ satisfying the boundary condition $y(-a) = y(a) = 0$. Defining $\eta = \eta(x) = y(x) - y_0(x)$ and $\phi(t) = J(y_0 + t\eta)$, he combines the facts that $\phi'(0) = 0$ and $\phi''(0) < 0$ with Taylor’s

Emulating Queen Dido’s application: Medieval Paris, like many other cities of the age, was enclosed in semicircular walls, with the openings closed off by a river.



theorem in the form $\phi(1) = \phi(0) + \phi'(0) + \frac{1}{2}\phi''(\theta)$ for some $\theta \in (0,1)$ to conclude that $J(y) < J(y_0)$ and, hence, that among functions of the same arc length, y_0 is indeed the desired solution of the isoperimetric problem.

Hard though it is to imagine a simpler proof of this or any other significant result, Tapia offered a variety of comparably elementary variations, all of which are independent of the means by which one arrives—as did the ancient Greeks—at the hypothesis that the semicircle solves Dido’s problem. Even Peter Lax’s clever proof [1] of the isoperimetric theorem seems—as Tapia emphasized with a set of patently photoshopped slides depicting Lax and himself as matadors competing mano à mano for the title of author of the simplest proof—unduly complicated in comparison.

Why, Tapia wondered aloud, did neither Euler nor Lagrange, nor any other 19th-century analyst, think to use Taylor’s theorem as a means of proving the isoperimetric theorem? Euler was certainly familiar with Taylor’s theorem, if not with the particular

form of the remainder used by Tapia in the proof presented here. On the other hand, the form in question is the work of Lagrange, and virtually every subsequent analyst has employed it on occasion.

In conclusion, Tapia voiced his belief that the isoperimetric problem has been the most impactful of all the problems of antiquity on the development of modern mathematics. Few if any questions have occupied the attention of so many giants in the field, or inspired them to greater heights of creativity, he said. Though cases could be made for any of the ancient construction problems (doubling the cube, trisecting the angle, squaring the circle, and perhaps a few others), Tapia’s candidate seems as worthy as any.

References

[1] P.D. Lax, *A short path to the shortest path*, Amer. Math. Monthly, 102:2 (1995), 158–159.

James Case writes from Baltimore, Maryland.

Hoffstein

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iffy) was seriously impacted. In 2003, investors pulled out and we had to lay off 70% of our employees. But we adapted, diversified our business, developed new products, and we survived. Then in 2005 we discovered that our books were not quite right. We just did not pay enough attention to our records and finances, and a sufficient system of checks and balances was not in place. This was a near-death experience, but we found money to keep things going and employees took pay cuts. We were doing well until the Great Recession of 2008. We started to head downward and needed to do something.

FS: *So what did you do?*

JH: I didn’t like the idea of letting people go. So we sought an exit. We got ourselves acquired by Security Innovation in 2009. This turned out to be a great marriage. SI is doing well, and the future looks bright.

FS: *Your journey was quite a roller coaster ride. What kept you going?*

JH: I seriously believed that there was a need for the efficient public-key cryptography that NTRU provided, and that it would be accepted someday. I also don’t like losing.

FS: *What wisdom can you impart to a mathematical scientist who wants to start a company?*

JH: I do have a few messages: (1) Find the right problem to attack with what you already know. (2) Scale your financial expectations. (3) Trust your gut instincts; know when to take professional advice (and when not to). (4) Be alert for business pressures that drive “solutions” that are not ready. (5) Networks are vital. (6) Find the “killer app” if possible.

FS: *The title of your talk at the IMA workshop was “Math for ‘fun’ and ‘profit.’” Was the whole experience fun and profitable?*

JH: Well, the experience was in many ways surreal. I would say that it was fun and it was profitable, but you have to stretch the standard definitions of the words “fun” and “profitable.”

NSF Solicits Proposals for New Quantitative Explorations of Data Program

The National Science Foundation recently issued a solicitation for its Expeditions in Training, Research, and Education for Mathematics and Statistics through Quantitative Explorations of Data (EXTREEMS–QED) program. Details about the newly created program can be found at <http://www.nsf.gov/pubs/2012/nsf12606/nsf12606.htm>.

A long-range goal of EXTREEMS–QED is to support efforts to educate the next generation of mathematics and statistics undergraduates, who will confront new challenges in computational and data-enabled science and engineering.

The deadlines for full proposals are January 31, 2013, November 6, 2013, and the first Wednesday in November annually thereafter.

Gene Golub
G²S³ 2014
SIAM Summer School

Call for Proposals: Gene Golub SIAM Summer School 2014

SIAM is calling for Letters of Intent for possible proposals of topics and organizers for the Gene Golub SIAM Summer School (G²S³) for approximately 45 graduate students in 2014.

Deadline for the Letters of Intent: January 31, 2013.

Information about the summer school in 2013, Matrix Functions and Matrix Equations, an archive of prior summer schools, and the call for proposals for the 2014 G²S³ can be found at

<http://www.siam.org/students/g2s3/>

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Uncertainty

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ear, which usually means smooth nonlinearities and the assumption of Gaussian errors; both tend to be more valid with more linear models. The reliability of computationally demanding methods depends on wise choice of parameter-value ranges and on a sufficient number and proper distribution of parameter samples. Many theoretical and empirical comparisons suggest that frugal computational methods often produce results similar to those for computationally demanding methods [9], indicating that in many circumstances nonlinearities may not be as problematic as sometimes feared. Figure 1 compares uncertainty intervals calculated with computationally frugal linear and nonlinear confidence intervals, and with demanding MCMC credible intervals. The problem is synthetic, which means that the true value of the prediction is known. For this problem, it appears that difficulties caused by model inadequacy are more serious than the approximations made in order to use computationally frugal instead of computationally demanding UQ methods. This suggests that at times, a wise approach may be to use mainly computationally frugal UQ methods and to focus resources on exploring alternative models.

Recent investigations of model nonlinearity have suggested that models can be more nonlinear than the systems they attempt to replicate. In [8] and references cited therein, thresholds are discussed as a source of unrealistic nonlinearity. Commonly, below a threshold value for simulated results, a variable is held constant, while above the threshold linear variations occur. Thresholds may be consistent with small-scale results, yet averaging mechanisms in complex environments may justify a smoother function. Using a smoother curve profoundly affects the reliability of frugal methods based on local derivatives. Similarly, erratic performance of time-stepping routines can produce dramatic, and unrealistic, model nonlinearities that deteriorate the reliability of computationally frugal methods of uncertainty evaluation. Making models more robust by eliminating false nonlinearities and numerical artifacts makes it easier to understand real system nonlinearities. The greater understanding is derived in part because the frugality of the computations allows analyses at multiple sets of parameter values. For example, graphs produced for different sets of parameter values (see Figure 2) showed that though the same parameters remained important, the dominant observation types changed. Such insight can be important to data-monitoring decisions and can be obscured by false linearities.

The results shown in Figures 2 and 3 address two of the fundamental questions posed earlier. Figure 2 offers insight into the questions: What parameters can be estimated with available data? What observations are important to parameters? These questions can be answered with computationally demanding methods, such as MCMC and FAST, as well as computationally frugal methods, one of which is shown here [2,7]. The key to reliable results for the statistic shown is careful scaling, as discussed in [7].

The composite scaled sensitivity (CSS) and parameter correlation coefficient (PCC) are calculated as follows [7]:

$$CSS_k = \{\sum_{i=1,n} [\sum_{j=1,n} (\partial y'_k / \partial b_j) b_j (\omega_{ki}^{1/2})^2]\}^{1/2}, \quad k = 1, np; \quad (1)$$

$$PCC_{k,j} = V_{k,j}(\mathbf{b}) / [V_{j,j}(\mathbf{b})^{1/2} V_{k,k}(\mathbf{b})^{1/2}] \\ V_{k,j}(\mathbf{b}) = [s^2(\mathbf{X}^T \mathbf{X})^{-1}]_{k,j}, \quad k = 1, np; \quad j = 1, np. \quad (2)$$

For the results presented in this work, n is the number of observations; $(\partial y'_k / \partial b_j)$ the sensitivity of the k th simulated value y'_k to the j th parameter b_j ; and np the number of parameters. Sensitivities were calculated by

MODFLOW-2000 [5] with the sensitivity-equation method in $np + 1$ model runs, or by perturbation with central differences in $(2 \times np) + 1$ model runs using UCODE_2005 [11]. $V_{i,j}(\mathbf{b})$ is the entry in the parameter variance-covariance matrix for parameters i and j ; this is a variance for $i = j$, a covariance for $i \neq j$. \mathbf{X} is a matrix of sensitivities with entries equal to $(\partial y'_k / \partial b_j)$, ω is the weight matrix, and s^2 is the unbiased regression variance. PCC for extremely correlated parameters can be calculated through creative use of round-off error [6,7].

Figure 3 addresses the question: What observations are important to predictions? The importance of existing old observations and potential new observations is considered. For both, the importance of different observations depends on choices made in model construction, and results shown in Figure 3 reveal consequences of such decisions. The computationally frugal observation-prediction (OPR) statistic used is defined as how much a calculated confidence interval would increase if existing observations were removed and how much it would decrease if new observations were added [16]. The equations are:

$$OPR_i = 100 \times (s_{z(i)} - s_z) / s_z \quad (3a)$$

$$s_{z(i)} = [(\partial z / \partial \mathbf{b})^T [s^2(\mathbf{X}_{(i)}^T \boldsymbol{\omega}_{(i)} \mathbf{X}_{(i)})^{-1}] (\partial z / \partial \mathbf{b})]^{1/2} \quad (3b)$$

$$s_z = [(\partial z / \partial \mathbf{b})^T [s^2(\mathbf{X}^T \boldsymbol{\omega} \mathbf{X})^{-1}] (\partial z / \partial \mathbf{b})]^{1/2}, \quad (3c)$$

where i identifies the observation, and $\mathbf{X}_{(i)}$ and $\boldsymbol{\omega}_{(i)}$ indicate that the sensitivity matrix \mathbf{X} and weight matrix $\boldsymbol{\omega}$ have been modified by the addition of rows and columns related to new observation i . The importance of existing observations is evaluated by the removal of rows and columns of \mathbf{X} and $\boldsymbol{\omega}$, as indicated by $(-i)$; in practice, entries in the weight matrix are set to zero. The weight matrix is determined through an analysis of errors, as required to obtain minimum variance parameter estimates ([7], Appendix C). The use of a standard deviation in equation (3) instead of a confidence-interval width is consistent with an assumed Gaussian distribution.

The brief analysis and references presented here suggest that increasingly, as models become more robust, a full uncertainty toolbox that includes computationally frugal methods, such as methods based on local derivatives, along with computationally demanding methods, such as MCMC, and presentation of results in the context of fundamental questions in ways that facilitate comparisons between different models and hypotheses, will best serve the needs of environmental modeling.

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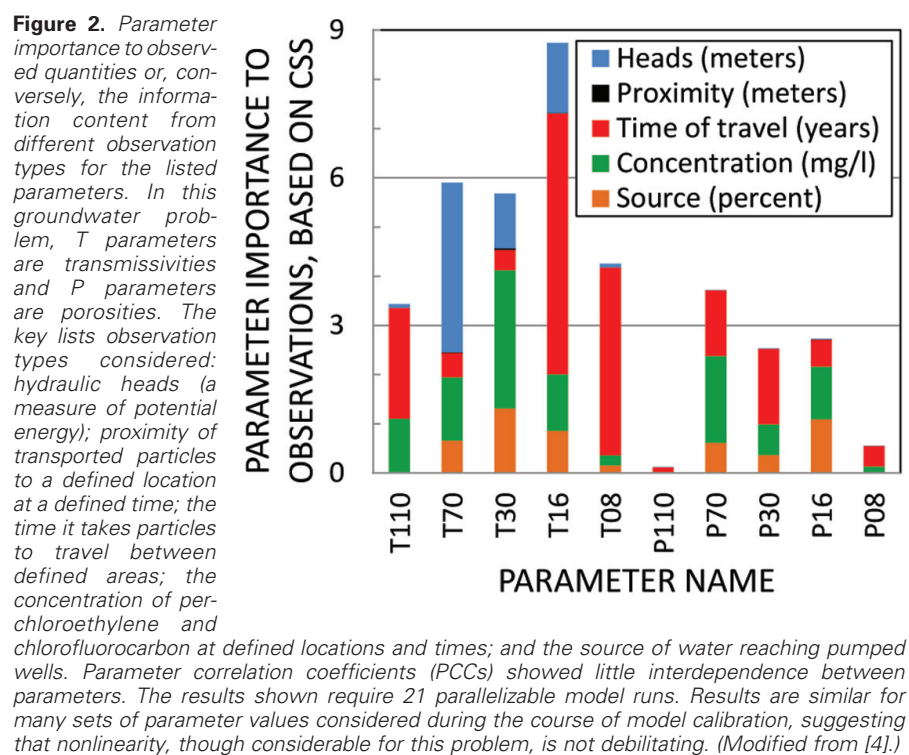


Figure 2. Parameter importance to observed quantities or, conversely, the information content from different observation types for the listed parameters. In this groundwater problem, T parameters are transmissivities and P parameters are porosities. The key lists observation types considered: hydraulic heads (a measure of potential energy); proximity to transported particles to a defined location at a defined time; the time it takes particles to travel between defined areas; the concentration of perchloroethylene and chlorofluorocarbon at defined locations and times; and the source of water reaching pumped wells. Parameter correlation coefficients (PCCs) showed little interdependence between parameters. The results shown require 21 parallelizable model runs. Results are similar for many sets of parameter values considered during the course of model calibration, suggesting that nonlinearity, though considerable for this problem, is not debilitating. (Modified from [4].)

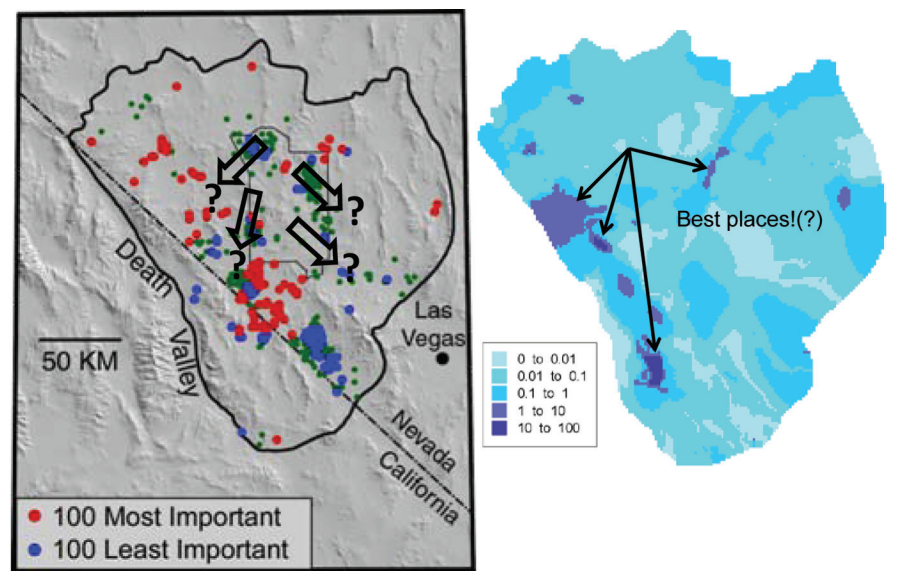


Figure 3. Importance of observations to predictions of transport within the Nevada National Security Site (NNSS). Left, the NNSS is outlined in gray and the model boundary in black, and the transport locations are represented schematically. The observation-prediction (OPR) statistic is used to measure observation importance [16]. The existing old 501 hydraulic head observations are ranked. Right, evaluation of one potential new head measurement anywhere in model layer 1. The most important observations in the southwestern part of the model occur largely because the rocks there are defined in the model as hydraulically similar to the rocks in the NNSS, but their occurrence here under steep head gradients facilitates estimation of the parameter value. Each of these results required 49 parallelizable model runs. (Modified from [7] and [15].)

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Acknowledgments

The references were selected from areas of environmental modeling to form an introduction for interested readers. A comprehensive list would be inordinately long for this publication; additional information can be found in works cited in some of the references listed.

The authors thank Jeremy White of the U.S. Geological Survey and Luis Tenorio of the Colorado School of Mines for their reviews of this article.

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SIAM Explores Modeling for STEM Pipeline

On the last two days in August, Peter Turner, SIAM's vice president for education, led a workshop at the National Science Foundation titled Modeling across the Curriculum. The 53 participants—members of the SIAM community, representatives from NSF, ASA, and MAA, as well as some high school teachers—spent the two days discussing ways to increase the presence of mathematical modeling and computational applied mathematics in high school and early college curricula.

Why SIAM? Why are we involved in high school and early college education? Aren't we a research organization? SIAM's mission is to promote applied mathematics and computational science, especially at the research level. But this primary mission has educational implications. The pipeline of scientists and engineers, including applied mathematicians and computational scientists, depends on appropriate education at lower levels. SIAM has an education committee, which Turner chairs, for this reason.

In fact, the preparation and motivation of students in high school and early college have become hot discussion topics even at the U.S. national level. Readers may remember the February 2012 report from PCAST, the President's Council of Advisors on Science and Technology: *Engage to Excel: Producing One Million Additional College Graduates with Degrees in Science, Technology, Engineering, and Mathematics*. SIAM was among several societies to respond to the report, supporting some recommendations, objecting (in some

cases) to others. SIAM's letter, written jointly by our education and science policy committees, encouraged interdisciplinary collaborations and increased connections among the STEM disciplines, deeming it "essential that modeling and applications be emphasized early in students' math education. . . ."

Participants in the Modeling across the Curriculum workshop explored these ideas, breaking into three working groups, each with a well-defined focus: K–12 STEM Education; Modeling across the Curriculum: A Model for Undergraduate STEM Degree Programs; and Evaluation/Assessment and College Readiness. Each working group is preparing a draft for a report that will be issued by the end of the year.

With leaders among K–12 and early college educators as participants, Turner points out, the workshop should lead to ideas that can be implemented on a large scale. The next step is release of the draft report, which will be presented during SIAM's Education Minisymposium at the Joint Math Meetings in San Diego (January 9–12, 2013). Further ahead, an expanded follow-up workshop will be held to explore the main recommendations of the three working groups.

In the K–12 arena, most states have adopted new Common Core State Standards for mathematics, which call, like the PCAST report, for increased emphasis on modeling and applications. The working group on K–12 education will have specific recommendations as to how this can be achieved, either through new courses

or through supplementary project-based materials for existing math and science courses.

Among options under discussion at the undergraduate level are coordinated approaches to early STEM courses that can help make clear the relevance of early college mathematics to the real world. This, Turner says, will necessarily involve elements of modeling, computation, and applied mathematics within the context of meaningful applications. New degree programs and new minors emphasizing such approaches are possible longer-term developments.

A key issue identified in the PCAST report is the "math gap." Addressing the difficulties associated with this problem requires attention not only to the content of early college courses, but also to the background of incoming students, especially in mathematics. Assessment of students' college readiness is a complex statistical and educational problem. The third working group focused on this issue.

The report should provide a starting point for future studies and proposals that will have a far-reaching impact on the state of applied mathematics, and STEM education as a whole, in the U.S. Again, why SIAM? From a self-serving viewpoint, Turner points out, SIAM's involvement directly impacts the pipeline of future members and leaders of SIAM and our profession. By happy coincidence, these activities also respond to an important national need. Applied mathematics, and SIAM, need to be the essential core of STEM if it is not simply to regress to the four S, T, E, and M silos.—JMC

Money

continued from page 1

"Anyone that unlucky has already been run over by a bus!"

So what is going on? It is clear from experiments that the fraction of matrices with dangerously large growth factors ρ is extraordinarily small. One might imagine various ways to make this idea precise, and I believe that a good approach is this: For random matrices with independent normally distributed entries, how fast does the probability of encountering a growth factor $>\rho$ decrease as a function of ρ ? Experiments show that it decreases exponentially, or at least faster than any inverse power of $\rho/n^{1/2}$ —see Fig. 22.2 in my textbook with Bau. But nobody has managed to prove this. Years ago I proved it for the bottom-right entry of U , but I was never able to extend the proof to the other entries, all of which enter into the definition of ρ .

Like the problem of the fast matrix inverse, the problem of the stability of Gaussian elimination has seen conceptual advances in recent years. Spielman, Teng, and Sankar have developed smoothed analysis, which gives a new probabilistic twist to algorithmic questions (*SIAM Journal on Matrix Analysis and Applications*, 2006; also Sankar's 2004 thesis at MIT). Spielman was recently named one of this year's MacArthur Fellows, partly for this work. Smoothed analysis hasn't yet solved the

Gaussian elimination problem, however, and in fact, its best known results don't distinguish between pivoted elimination, whose striking stability we are trying to explain, and the unpivoted variant, which is unstable.

Precisely posed unsolved problems are one of the glories of mathematics. Even in applied mathematics, for all our close connections to practical applications, they can motivate and inspire us. I will give \$1000 for a proof that Gaussian elimination with partial pivoting is stable in the probabilistic sense specified above.

Shark Tank

continued from page 2

is a competitive field that requires logical thought processes, careful analysis, the ability to convince, and the desire to solve problems.

Douglas Ulmer, chair of the School of Mathematics at Georgia Tech, attended as an observer. He noted at the end that the workshop was very different from the typical mathematics workshop: "This was a valuable experience that more mathematicians should be exposed to. Not everyone will end up starting a company after they go to a workshop like this, but this kind of activity really broadens their perspective and informs them of opportunities for mathematicians. The IMA should run workshops like this for faculty also."

At this clearly nonstandard mathematics workshop, the students seemed to find immense enjoyment in the challenge of connecting (admittedly fictional) mathematical ideas to something that could be commercialized. The IMA is planning another such workshop for the future; stay tuned.

Students interested in seeing potentially viable ideas for business might want to check out the following:

- www.kaggle.com (a big data competition site)
- www.innocentive.com (a technology crowd-sourcing site)
- www.xprize.org (the Xprize foundation challenges site)
- www.topcoder.com (another competition site)
- www.kickstarter.com (crowd-source funding site).

Fadil Santosa is director of the Institute for Mathematics and its Applications at the University of Minnesota. Richard Sowers is a professor in the Department of Mathematics at the University of Illinois at Urbana-Champaign.

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Mathematics: Handmaiden to Architecture

Mathematical Excursions to the World’s Great Buildings. By Alexander J. Hahn, Princeton University Press, Princeton, New Jersey, 2012, 317 pages, \$49.50.

Some years ago, while my son and his family were living in St. Louis, I visited the city and its Gateway Arch for the first time. The Arch was then already a great tourist attraction. (Its construction was begun in 1963 and completed in 1965.) On a later trip, which was professional, I was shown around the city by Professor ABC, a local mathematician. He naturally took me to see the Gateway Arch, and we went inside. Later, standing outside and looking up at the Arch, I asked my companion about the mathematics of the Arch:

What mathematics do you see in the Arch, or what mathematics does it make you think of?
I see a parabola, he replied. No, I think it must be a catenary.
Nothing else?
Nothing. Should there be something else?

I answered in a non-committal fashion, but in my mind I did not give Professor ABC a passing grade.
I return to the Gateway Arch and its mathematics below.
Alexander Hahn, a professor of mathematics at the University of Notre Dame

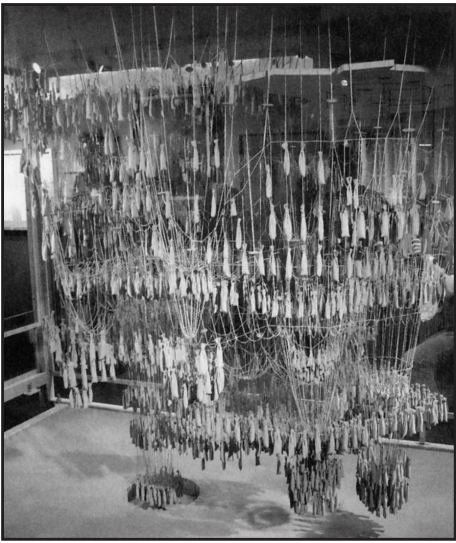
and a prolific writer, has drawn on a vast and eclectic store of knowledge to produce an eyebrow-raising book filled with pictures and diagrams, including two dozen images in full color. In fact, Hahn has produced a half dozen books rolled into one. What we have here is a potpourri, a gallimaufry, a salad bar, or perhaps a celebration of mathematics in its infinite variety. Taking a cue from Stephen Leacock’s Lord Ronald, Hahn flung himself upon his mathematical horse and rode madly off in all directions.

Allow me to detail some of the directions. *Excursions* is of “coffee table” size and quality. You can dip into its pages and view with enjoyment the many fine reproductions of famous buildings and then read how the author has linked them to mathematics. You may very well have visited some of these buildings: St. Peter’s in Rome, the U.S. Capitol Building, the Guggenheim Museum in Bilbao, La Sagrada Familia in Barcelona. . . . I’m surprised that he skipped Frank Lloyd Wright’s helical Guggenheim on Fifth Avenue in New York City. Alternatively, you may consider giving *Excursions* to a young mathematical aspirant of junior high school age. He or she will find in it a *Gradus ad Parnassum*, so to speak, to the rudiments of Euclidean geometry, to elementary calculus, to statics, and even to a bit of numerical analysis. This textbook aspect is rounded out by the inclu-

sion of many problems that the aspirant could work through.
If you are familiar with three-dimensional analytic geometry or with computer graphics, you will find considerable elucidation and delight within these theories. Thus, the “sails” or the “waves” of the famous Sydney Opera House are composed of a sequence of spherical triangles of varying sizes.
If you are interested in Russian ecclesiastical history, you will be intrigued by the story of how Peter the Great and Charles-Augustin de Coulomb of electric charge fame (1736–1806), years apart, were involved in the design of St. Isaac’s Cathedral in St. Petersburg. Hahn devotes five pages to a discussion of Coulomb’s *Essay on Problems of Statics* (1773).

You may have read conjectures as to how the huge and mysterious heads on Easter Island in the middle of the Pacific Ocean were lifted into position. If so, you will be interested to know that the obelisk in front of St. Peter’s Basilica in Rome, standing 80 feet high and weighing more than 700,000 pounds, was moved in 1586 to its present location—a distance of 260 yards. “Five hundred mathematicians, engineers and others came to present proposals about how best to move the obelisk,” Hahn writes. The accompanying image from the book shows the scaffolding and suggests how the work was done.
In another illustration, you will see how the square roots of the successive integers can be arranged in a spiral that this reviewer dubbed the “spiral of Theodorus.”* How this is relevant to architecture is not explained. Nor is the inclusion of Gauss’s list of the regular polygons that can be constructed with ruler and compass.
“Use a word three times and it is yours” was a daily feature years ago in my city’s newspaper. In the glossary to *Excursions* you will come across the following words: squinch, groin, pendentive, and voussoir; propose to colleagues that they use these words and watch them blanch.
As promised, I return to the Gateway Arch. The author gives it short shrift, pay-

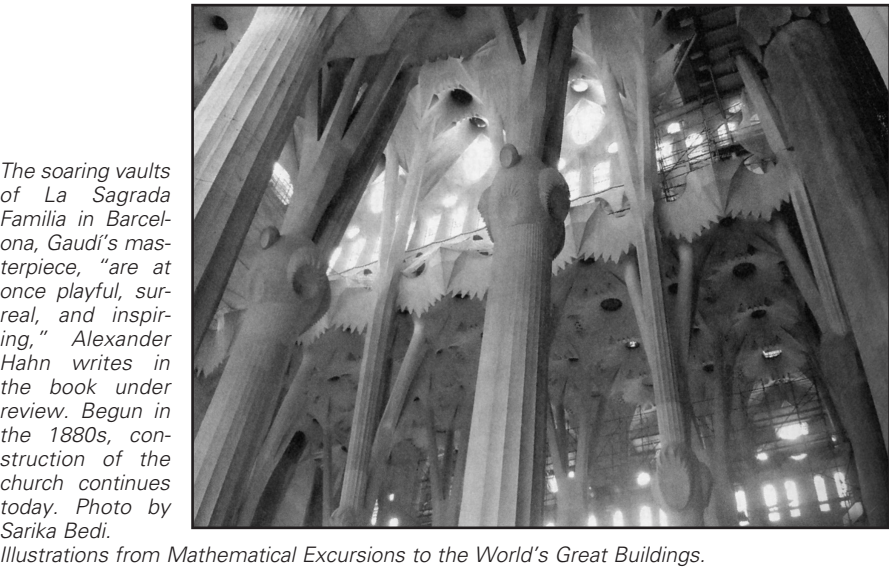
*Spirals: From Theodorus to Chaos, Philip J. Davis, A.K. Peters, 1993.



Gaudi’s designs for La Sagrada Familia, Hahn says, “relied on careful and elaborate studies of complex systems of loaded strings.” One of his models is shown here. Photo by Cleftref.

ing much more attention to other famous buildings, e.g., the Hagia Sophia in Istanbul or the Colosseum in Rome. He describes the Gateway Arch as a “compressed catenary” and lets it go with the formula $-A \cosh(Bx/b) + (h + A)$. Now that’s a formula for a plane curve. But the Arch is a solid, or rather a hollow shell large enough to house a tram that carries visitors. The cross sections of the shell are equilateral triangles tapering from 54 feet at the two bases to 17 feet at the top. Should Professor ABC have known all this? Should the author of *Excursions* have coined a special name for a 3-D squashed catenary with equilateral cross sections?
To complete the story of the mathematics employed to describe the Arch in its full scope, we should really add the hundreds, perhaps thousands, of informal computations, now hidden from view, that were performed during the design and structural stages in the offices of Eero Saarinen and Hannskarl Bandel. All this was done in the late 1970s, I tell my students, assuring them that there was mathematical life before the advent of MATLAB or computer graphics.

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.



The soaring vaults of La Sagrada Familia in Barcelona, Gaudi’s masterpiece, “are at once playful, surreal, and inspiring,” Alexander Hahn writes in the book under review. Begun in the 1880s, construction of the church continues today. Photo by Sarika Bedi. Illustrations from Mathematical Excursions to the World’s Great Buildings.

Physics and Computation

Computation and its Limits. By Paul Cockshott, Lewis M. Mackenzie, and Greg Michaelson, Oxford University Press, Oxford, UK, and New York, 2012, vi + 239 pages, \$63.00.

In the past few months, I have twice read newspaper reports of computer technology bumping up against fundamental physical constants. The first was an announcement that an international team, led by Michelle Simmons of the University of New South Wales, had constructed a transistor consisting of a single atom. The second was an offhand remark, in an article about the Knight Capital fiasco, that because of the speed of light, 1foot per nanosecond, stock trading companies now need to locate their offices close to the trading floor. If your office is a mile from Wall Street, and you are running a 10-GHz machine, then by the time you receive the latest market news and respond, you have fallen 100,000 machine cycles behind your competition; in these days of high-speed trading, when gigabucks are made and lost in nanoseconds, you might as well send in your orders by foot messenger. One hundred seventy-five years ago, the electric telegraph made the world small; the electronic computer has made it large again. As it happens, the scales of the atom and elementary particles play large roles in the

analyses in the book under review; the speed of light is a very minor player.
Computation and its Limits is partly a discussion of the limits that physics places on computation, partly a more general discussion of the relation between physics and computation. The most important and informative chapters of the book are the later ones. Chapter 5, a discussion of thermodynamics and computation, is centered around Rolf Landauer’s (1961) argument about the entropy generated with each use of an AND or an OR gate in a computer. Chapter 6 is an extended discussion of the principles of quantum computing. Chapter 8 reviews and refutes a number of proposals that have been made for constructing computers that violate the Church–Turing thesis.
Chapters 5 and 6 contain extensive, self-contained introductions to thermodynamics and quantum theory, respectively. Unfortunately, like many self-contained introductions, these are largely unnecessary for readers who know the subject matter and largely over the heads of readers who do not. I found myself in the first category for the thermodynamics and in the second for the quantum mechanics, despite having taken a semester course in quantum mechanics a quarter century ago. Moreover, after the thermodynamic preliminaries of chapter 5, the actual presentation

of Landauer’s argument is unsatisfying. The argument, in brief, is that, because an AND gate takes two bits as input and produces one bit as output, one bit of information is lost; one bit of information corresponds to $k_B \cdot \log 2$ of thermodynamic entropy. Two obvious questions arise: First, how do you know that every physical implementation of a calculational bit has this thermodynamic equivalent? Second, since the inputs are still present at the input ports, in what sense are they lost? Neither question, particularly the second, is adequately discussed.
A much clearer presentation can be found in the paper “Physical Limits of Computing” by Michael Frank (*IEEE Computing in Science and Engineering*, May 2002), which is not cited here. That paper, incidentally, also discusses some physical limits of computation not included by Cockshott et al., such as the maximum density of information per unit volume. Proposals for getting around the Landauer limit by using reversible computations that do not lose information date back to work of C.H. Bennett in the early 1970s. Cockshott et al. discuss and reject one rather far-fetched design by Fredkin and Toffoli that achieved this aim using elastic collisions among billiard balls. They do not, however, discuss or even cite any of the more recent work in the area.
Despite the gaps in my understanding, I found the chapter on quantum computing the most interesting and informative in the book. In particular, the discussion of the various interpretations of quantum theory—the Copenhagen interpretation, the many-worlds

interpretation, and so on—seemed to me remarkably well-written and fair-minded; the difficulties involved in each theory are clearly explained and acknowledged. The description of the general theory of quantum computing and of the methods that have been considered for its physical implementation is extensive and detailed. Curiously, though, there is little discussion of what has actually been accomplished. The implementations of Shor’s algorithm, which to date have succeeded in factoring 15, are not mentioned. The D-Wave machine is mentioned in passing as “controversial,” but few details are given about either the machine or the controversy.
Chapter 8 deals with a number of proposals for constructing machines that succeed in computing “non-computable” functions. Some of these were clearly not meant as practical suggestions. In the plan by Etesi and Nemeti, for example, the solution to a halting problem would be learned by a computer an instant before it passed the Schwarzschild radius of a black hole. Beggs and Tucker propose a computer that uses infinitely long rigid rods. Others rely on mechanisms that carry out infinite-precision arithmetic on real-valued quantities. Cockshott et al. knock all of them down without breaking much of a sweat.
The chapter and the book end, however, in a serious misstatement. A machine that solved an uncomputable problem, the authors write, would be of no use because its answer could not be checked for correctness, and

Computation

continued from page 6

it would not be a general-purpose machine because it would not be able to solve its own halting problem; rather, it would be a special-purpose measuring device. None of this seems right to me.

Suppose that friendly space aliens arrive tomorrow in their UFO and make us a gift of a laptop that runs Java programs; the F11 key can solve the halting problem for any Java program that is inputless and that does not make a system call to the F11 key itself. This machine is perfectly consistent with Turing’s proof; indeed, it is simply an oracle machine, much studied in computation theory. We are naturally skeptical, so we test it with a few hundred difficult programs for which we happen to know the answer—the search for a solution to Fermat’s last theorem, say. (We might write a program that systematically searches through all tuples of integers $x, y, z, n > 2$, for a counterexample to Fermat’s last theorem. Since Wiles’s proof, we know that this program does not terminate; but that is not obvious just from an examination of the code.) The machine gives the right answer for all the test problems. Then it seems to me that (a) we are entitled to say that we “know” that this computer solves the halting problem, in the sense in which we “know” pretty much anything else; and (b) this is a general-purpose computer, in the same sense that an ordinary computer is a general-purpose computer. I don’t expect that this will happen, but it is not logically impossible.

The remainder of the book seems to me less interesting, with substantial philosophizing of a kind not appealing to me. An early chapter begins with a discussion of Wigner’s article “The Unreasonable Effectiveness of Mathematics in the Natural Sciences.” On the second page of that discussion, “mathematics” is reinterpreted as “computation,” a manoeuvre that in my opinion throws away Wigner’s point. To take Wigner’s first example, Newton’s law of gravity

$$m_i \cdot \frac{d^2 \vec{x}_i}{dt^2} = \sum_{j \neq i} \frac{G m_i m_j}{|\vec{x}_j - \vec{x}_i|^2} \cdot \frac{\vec{x}_j - \vec{x}_i}{|\vec{x}_j - \vec{x}_i|}$$

is elegant mathematically but unpleasant computationally, particularly when $n > 2$. If the planets moved along paths composed of straight-line segments parallel to the coordinate axes with integer-valued vertices at constant reciprocal integer speeds, we would be entitled to admire how well adapted the laws of physics are for easy computation. My view is that Wigner’s article is best read as an expression of wonderment, rather than as a question with a useful or meaningful answer.

Finally, chapter 7 has to do with the real numbers. Cockshott et al. argue, obviously correctly, that infinite-precision real numbers are not physically meaningful. I do not know that anyone has ever claimed otherwise. They conclude that computer scientists should be skeptical about arguments that involve the existence of infinite-precision real numbers, such as Cantor’s proof that there are uncountably many real numbers.

This seems to me a bad direction to pursue. Mathematicians, computer scientists, and even physicists continue to use the real number system not because they think it is a true description of physical reality at the tiniest scale, or out of a foolish Platonism, or a sentimental attachment to the paradise that Cantor, Bolzano, Weierstrass, and others built for us; rather, once you learn how the system works, it is much easier to think about than finite-precision numbers. Anyone who doubts this is invited to compare the axioms of the real number system to the IEEE standard for floating-point arithmetic.

Readers with a serious interest in the relation between physics and computation will certainly find this book worth a look. The door is open, however, for someone to write a much better book on the subject.

Ernest Davis is a professor of computer science at the Courant Institute of Mathematical Sciences, NYU.

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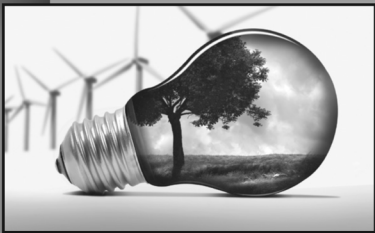
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MATERIALS FOR A SUSTAINABLE ENERGY FUTURE

September 9 – December 13, 2013

Organizing Committee

Martin Bazant (MIT), Giulia Galli (University of California at Davis), Graeme Henkelman (University of Texas at Austin), Keith Promislow (Michigan State University), Matthias Scheffler (Fritz-Haber-Institut der Max-Planck-Gesellschaft)

Scientific Overview

A secure and sustainable energy future that is not based on a fossil-fuel based infrastructure requires the design of new materials for efficient energy conversion, transport, and storage. Indeed, materials development is a rate limiting step in many potential new energy conversion strategies, impacting the efficiency of photovoltaic solar cells, the storage capacity and power density of batteries for automobile applications, the synthesis of liquid fuels, and the catalysis and durability of energy conversion in fuel cells. A key bottleneck in this historic transition is the wide range of length scales present in the morphology and time scales in the transport phenomena. Serious progress in the development of new materials requires predicative modeling which surmounts the particle-continuum divide. Recent developments in macro-micro modeling, incorporating machine and manifold learning, combined with new classes of continuum models and increases in computational resources, provide a new framework with which to develop a fundamental understanding of complex materials.

Workshop Schedule

- Tutorials: September 9 - 13, 2013
- Workshop I: Solar Cells, September 23 - 27, 2013
- Workshop II: Fuels from Sunlight, October 14 - 18, 2013
- Workshop III: Batteries and Fuel Cells, November 4 - 8, 2013
- Workshop IV: Energy Conservation and Waste Heat Recovery, Nov. 18 - 22, 2013

Participation

Creating interactions between people with different expertise and a common goal will facilitate breakthroughs in predictive materials design. This program will bring together researchers from mathematics, physics, materials science, engineering, chemistry, biology, computer sciences, and other sciences with the goal to understand the mathematical structure of continuum models governing material properties as well as the electronic, atomic, and molecular structure of such new materials.

Full and partial support for long-term participants is available. We are especially interested in applicants who intend to participate in the entire program, but will consider applications for shorter periods. Funding is available to participants at all academic levels, though recent PhDs, graduate students, and researchers in the early stages of their careers are especially encouraged to apply. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM’s mission and we welcome their applications. More information and a link to an application are available online.

This program is part of the “Mathematics for Planet Earth” project which involves dozens of scientific societies universities, research institutes, and foundations from around the world.



www.ipam.ucla.edu/programs/mse2013



Mathematical Biosciences Institute

Emphasis Year 2012-2013 Mathematical Neuroscience

Mathematics describes key dynamical mechanisms for patterns of neural activity and quantifies levels of information in these patterns. At the same time, new mathematics, that often bridges information theory, dynamical systems, and statistical mechanics, has been inspired by the complexity of the underlying networks and the computations they perform. Over the past decade, mathematics has entered different subfields of neuroscience, and has suggested unexpected parallels among others, please visit: <http://www.mbi.osu.edu/2012/scientific2012.html>

Future Emphasis Programs

Fall 2013 Ecosystem Dynamics & Management: <http://www.mbi.osu.edu/2013/scientific2013.html>

Spring 2014 Frontiers in Imaging, Mathematics, and the Life Sciences:
<http://www.mbi.osu.edu/2014/scientific2014.html>

Visitor and Postdoctoral Fellowship Opportunities

- **Now accepting Long-term Visitor applications for the Ecosystem Dynamics & Management year:**
http://www.mbi.osu.edu/visitors/visit_mbi.html
- Three-Year Postdoctoral Fellowships (deadline 12/13/12):
http://www.mbi.osu.edu/postdoctoral/three_year.html
- Early Career Awards (deadline 12/3/12): http://www.mbi.osu.edu/postdoctoral/early_career.html
- Participate in MBI workshops (due 2 months before workshop):
<http://www.mbi.osu.edu/forms/applyworkshop.html>

MBI Associate Director

MBI has an opening for a 2-3 year rotator as Associate Director. The position will be 25% research and 75% administrative. The Associate Director will have primary responsibility for program organization. Other responsibilities could include postdoctoral fellow mentoring, outreach, and educational programs, among other possibilities, depending on the interests of the candidate. For details see: http://www.mbi.osu.edu/assoc_director.html

Organize an MBI Emphasis Program

MBI seeks researchers to organize semester or yearlong emphasis programs at MBI for Fall 2015 and beyond. Emphasis programs consist of either three or six weeklong workshops and related activities. For details see: http://www.mbi.osu.edu/organize_ey.html

Become an Institute Partner

MBI welcomes the participation of other academic and industrial institutions and invites those interested to join the MBI Institute Partner Program. The Program subsidizes travel and local expenses of IP researchers including member faculty, postdoctoral fellows, and students, to allow their participation in research and education programs at MBI. For more details, contact MBI Director Marty Golubitsky at mg@mbi.osu.edu.

www.mbi.osu.edu



*MBI receives major funding from the National Science Foundation Division of Mathematical Sciences and is supported by The Ohio State University.
MBI adheres to the AA/EOE guidelines.*



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 \$2.70 per word (minimum \$325.00). Display advertising rates are available on request.
Advertising copy must be received at least four weeks before publication (e.g., the deadline for the January/February 2013 issue is December 14, 2012).
Advertisements with application deadlines falling within the month of publication will not be accepted (e.g., an advertisement published in the January/February issue must show an application deadline of March 1 or later).

Clarkson University Department of Mathematics

The Department of Mathematics at Clarkson University (<http://www.clarkson.edu/math>) invites applications for a tenure-track assistant professor position in applied mathematics (Pos. #312), starting in August 2013. The department is especially interested in candidates with expertise in computational areas of applied mathematics, including statistics or dynamical systems; however, those working in all areas of applied mathematics will be considered. Responsibilities will include teaching undergraduate- and graduate-level mathematics courses, and directing graduate students. Minimum requirements are a PhD in mathematics by the date of appointment, demonstrated excellence in both research potential and teaching ability, and fluency in English. In addition, the successful candidate should be able to interact with other faculty in the department and the university.

Applications, including a vita and three reference letters, should be submitted to: <https://clarkson.peopleadmin.com/>. Completed applications will be reviewed starting immediately.

Clarkson University is an affirmative action/equal opportunity employer. Women and minorities are urged to apply.

University of Michigan Department of Mathematics

The Department of Mathematics anticipates an opening at the tenure-track or tenured level, pending authorization, beginning in September 2013. Candidates should hold a PhD in mathematics or a related field (e.g., statistics) and should show outstanding promise and/or accomplishments in both research and teaching. A joint position with the Department of Statistics is available; however, truly exceptional candidates from any area of pure, applied, computational, or interdisciplinary mathematics will be considered. Salaries are competitive and are based on credentials.

More detailed information regarding the department can be found on its website at <http://www.math.lsa.umich.edu>.

Junior candidates should furnish a placement dossier consisting of a letter of application, curriculum vitae, and three letters of recommendation; senior candidates should send a letter of application, curriculum vitae, and the names of three suggested references. In all cases, applicants should provide a statement of teaching philosophy and experience, evidence of teaching excellence, and a statement of current and future research plans. Application materials should preferably be submitted electronically through the AMS MathJobs website: <http://www.mathjobs.org>. Alternatively, applications can be sent to: Personnel Committee, University of Michigan, Department of Mathematics, 2074 East Hall, 530 Church Street, Ann Arbor, MI 48109-1043. Applications are considered on a continuing basis; however, applicants were urged to apply by November 1, 2012. Inquiries can be made via e-mail to: math-fac-search@umich.edu.

The University of Michigan is an affirmative action/equal opportunity employer and is supportive of the needs of dual career couples. Women and minority candidates are encouraged to apply.

University of Michigan Department of Mathematics

The Department of Mathematics invites applications for a Lecturer III position in mathematics, pending authorization, to begin in September

2013. This is not a tenure-track position; however, it can be renewed annually for up to the first four years, and thereafter, for intervals of three to five years. Criteria for selection and for renewal are excellence in classroom teaching and participation in administration of the department's program in Actuarial and Financial Mathematics. Interest and activity in pedagogical research is encouraged but not essential for reappointment. The successful candidate is likely to have either a doctorate or equivalent credentials in actuarial mathematics and substantial experience in teaching mathematics.

More detailed information regarding the department can be found on its website at <http://www.math.lsa.umich.edu>.

Applicants should submit a curriculum vitae, a statement of teaching philosophy and experience, evidence of teaching excellence, and the names of at least three references. Application materials should preferably be submitted electronically through the AMS MathJobs website: <http://www.mathjobs.org>. Alternatively, applications can be sent to: Personnel Committee, University of Michigan, Department of Mathematics, 2074 East Hall, 530 Church Street, Ann Arbor, MI, 48109-1043. Applications are considered on a continuing basis; however, applicants were urged to apply by November 1, 2012. Inquiries can be made via e-mail to math-fac-search@umich.edu.

The University of Michigan is an affirmative action/equal opportunity employer. Women and minority candidates are encouraged to apply.

University of Connecticut– Avery Point Regional Campus

Department of Mathematics

The department invites applications for a nine-month, tenure-track, assistant professor position, starting in the fall of 2013. The fields of the search are numerical solutions of PDEs and optimization, with interest in mathematical modeling (in meteorology, oceanography, fluid dynamics, or marine ecology). Qualifications include a PhD or an equivalent foreign degree in mathematics or a closely related area, demonstrated evidence of excellent teaching, and outstanding research experience and potential.

Applicants should apply online at: <http://www.mathjobs.org/jobs>. Applicants who have questions or requests for additional information can e-mail the Hiring Committee at averypointhiring@math.uconn.edu.

The University of Connecticut is an affirmative action/equal employment opportunity employer and actively solicits applications from minorities, women, and people with disabilities.

University of Illinois at Urbana-Champaign

College of Engineering
Department of Industrial
and Enterprise Systems Engineering

The Department of Industrial and Enterprise Systems Engineering at the University of Illinois at Urbana-Champaign invites applications for two full-time tenured or tenure-track faculty positions at all levels in the areas of engineering systems design and operations research/financial engineering, to begin August 16, 2013. Applicants at all ranks will be considered. All candidates must have a doctoral degree by the appointment start date.

For a complete position announcement and application form, applicants should go to: <http://jobs.illinois.edu>. The review of applications began November 1, 2012, and will continue until

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

the positions are filled. Questions should be referred to Amy Summers, (217) 244-5703; arsummer@illinois.edu.

Illinois is an affirmative action/equal opportunity employer (see <http://www.inclusiveillinois.illinois.edu>).

Colorado State University

Department of Mathematics

The Department of Mathematics at Colorado State University invites applications for a tenure-track assistant professor position in the area of mathematics education. A full job description, including minimum qualifications, can be viewed at <http://www.natsci.colostate.edu/employment/EDU/>.

Applicants should apply online at the College of Natural Sciences website: <https://cns.natsci.colostate.edu/employment/MathEd/>. Complete applications include the submission of an AMS cover sheet; a curriculum vitae; a statement of interest in the mathematics education position specifically, including a one-paragraph summaries of dissertation topic and plans for future scholarly activities; a research statement; a teaching statement; and at least three letters of recommendation. For full consideration, applications must be completed by December 9, 2012. Complete applications of the semi-finalist candidates will be available to department faculty for review. Colorado State University conducts background checks on the final candidates.

Colorado State University is an affirmative action/equal opportunity/equal access employer.

Arizona State University–West Campus

School of Mathematical and Natural Sciences

The School of Mathematical and Natural Sciences at Arizona State University's West Campus invites applications for a tenure-track assistant professor position, to begin in August 2013. Applicants must have a PhD or an equivalent degree in mathematics, applied mathematics, or a related field, with demonstrated expertise in numerical analysis, optimization, numerical methods, or a related area. Duties involve teaching at the undergraduate level, engaging in research and scholarly activity, and providing service to the school and the profession.

Applicants should send a letter of application, statements describing their research program, teaching philosophy, and commitment to diversity; curriculum vitae, unofficial graduate transcripts, and the names of three references electronically to: Jamie Howell, newcollegejobs@asu.edu, and mention reference number #10191 in the subject line. Applicants must arrange for three letters of reference be sent to newcollegejobs@asu.edu. Applicants should see <http://newcollege.asu.edu/jobs> for complete information on qualifications and the application process. The deadline for applications is January 7, 2013.

Arizona State University is an affirmative action/equal opportunity employer. Women and minorities are encouraged to apply; more information can be found at <https://www.asu.edu/titleIX/>.

University of California Merced

School of Natural Sciences

The School of Natural Sciences at UC Merced (<http://naturalsciences.ucmerced.edu>) invites applications in the area of applied mathematics (<http://appliedmath.ucmerced.edu>) at the levels of full/associate professor (tenured) and assistant professor (tenure-track), starting July 1, 2013. The school is seeking exceptionally qualified candidates with expertise in modeling, applied analysis, scientific computing, or related areas.

Special attention will be paid to applicants who participate in interdisciplinary research and will contribute to developing the applied mathematics curriculum and to one or more of the campus research initiatives in the natural sciences, engineering, and/or social sciences.

More information and application procedures can be found at: <http://jobs.ucmerced.edu/n/academic/position.jsf?positionId=4246>.

UC Merced is an affirmative action/equal opportunity employer.

San Jose State University

Department of Mathematics

The SJSU Department of Mathematics has one opening for a tenure-track assistant professor position in applied mathematics, starting in August 2013. The successful candidate is expected to maintain an active research program, supervise student research, teach undergraduate and graduate applied mathematics courses, and work on curriculum development. The candidate must possess a PhD in applied mathematics or a related area at the time of appointment. An interest in mathematical biology, combinatorics/graph theory, numerical analysis, or financial math/actuarial science would be desirable.

The department houses a BS program in Applied Mathematics and concentrations in Applied and Computational Mathematics, Economics, and Actuarial Science, as well as CAMCOS, a center that organizes industrial research projects for students.

Applicants can see a complete position description at: http://www.sjsu.edu/math/employment/Faculty_position_2013/index.html.

Washington State University

Department of Mathematics

Applications are invited for a tenure-track assistant professor position in computational mathematics in the Department of Mathematics at Washington State University in Pullman, Washington, to begin August 16, 2013. Minimum required qualifications are a PhD in mathematics or a related field by the position start date; a demonstrated record of research accomplishment or potential for research accomplishment; an ability to communicate effectively with both students and colleagues; and expertise in computational mathematics, with applications in computational finance. Job duties of the successful candidate for this position will include teaching undergraduate and graduate courses in computational mathematics, conducting a vigorous research program supported by extramural funding, and participating in committee services at the department, college, and/or university level. Two years of postdoctoral experience are preferred. This position will emphasize quality research, curriculum development, and effective teaching. The ability to participate in collaborative and interdisciplinary activities is expected. Salary is commensurate with training and experience.

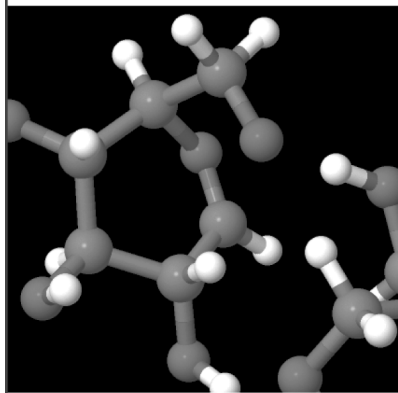
Applicants should provide a vita, research and teaching statements, and at least three letters of recommendation. Applicants should submit all application materials and arrange to have letters of recommendation uploaded to: <http://www.wsujobs.com>. The review of applications begins December 3, 2012. Applicants can see a complete Notice of Vacancy at <http://www.math.wsu.edu/math/positions/welcome.php> or by e-mailing gilchrist@math.wsu.edu.

WSU is an affirmative action/equal opportunity educator and employer. A complete AA/EEO statement can be viewed at <http://www.wsujobs.com>.

See Opportunities on page 10

DEPARTMENT OF ENERGY

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Opportunities

continued from page 9

Washington State University

Department of Mathematics

Applications are invited for a tenure-track assistant professor position in nonlinear or stochastic optimization in the Department of Mathematics at Washington State University, in Pullman, Washington, to begin August 16, 2013. Minimum qualifications are a PhD in mathematics or a related field by the position start date; a demonstrated record of research accomplishment or potential for research accomplishment; an ability to communicate effectively with both students and colleagues; and expertise in algorithms for nonlinear or stochastic optimization. Job duties of the successful candidate for this position will include teaching undergraduate and graduate courses in mathematics, conducting a vigorous research program supported by extramural funding, and participating in committee services at the department, college, and/or university level. Two years of postdoctoral experience are preferred. This position will emphasize quality research, curriculum development, and effective teaching. The ability to participate in collaborative and interdisciplinary activities is expected. Salary is commensurate with training and experience.

Applicants should provide a vita, research and teaching statements, and at least three letters of recommendation. Applicants should submit all application materials and arrange to have letters of recommendation uploaded to: <http://www.wsujobs.com>. Applicants can see a complete Notice of Vacancy at <http://www.math.wsu.edu/math/positions/welcome.php> or by e-mailing gilchrist@math.wsu.edu.

WSU is an affirmative action/equal opportunity educator and employer. A complete AA/EEO statement can be viewed at <http://www.wsujobs.com>.

Massachusetts Institute of Technology

Department of Mathematics

The Department of Mathematics at MIT is seeking to fill positions in pure and applied mathematics, and statistics, at the level of instructor, assistant professor, or higher, beginning in September 2013. The department also seeks candidates for a Schramm Postdoctoral Fellowship. Appointments are based primarily on exceptional research qualifications. Appointees will be expected to fulfill teaching duties and to pursue their own research program. A PhD is required by the employment start date.

For more information and application procedures, applicants should visit: <http://www.mathjobs.org>. For full consideration, applications should be submitted by December 1, 2012.

MIT is an affirmative action, equal opportunity employer.

California State University, Fullerton

Department of Mathematics

The Department of Mathematics invites applications for two tenure-track positions in applied mathematics. Candidates for these positions should be applied mathematicians with a background in computation and mathematical modeling (deterministic and/or stochastic); the appointment date is August 19, 2013. A PhD in applied mathematics or a related field must be completed by the starting date. Salary is competitive and will be commensurate with rank, experience, and qualifications.

Applicants should send a cover letter; a teaching statement (including commitment to excellence in teaching a diverse student population), a research statement (including a five-year research plan), a curriculum vitae, and three letters of recommendation that address teaching and research potential, as well as his/her potential to be a productive department member. Applicants who received their degree within the last five years should include graduate transcripts. Applicants must submit their materials to: <http://www.mathjobs.org>. A complete ad can also be found at <http://www.mathjobs.org>. The review of completed applications will begin on November 30, 2012, and will continue until the positions are filled.

Texas Tech University

Department of Mathematics and Statistics

The Department of Mathematics and Statistics at Texas Tech University invites applications for three tenure-track assistant professor positions, to begin in the fall of 2013. A PhD degree at the time of appointment is required. The department is seeking candidates who will be engaged in nationally visible scholarship, establish externally funded research programs, interact with the existing research groups in the department, involve graduate students in their research, and show excellence in teaching at the undergraduate and graduate levels. It is anticipated that one of the positions will be in statistics, one in numerical analysis, and one in another area compatible with the department's existing research programs. Candidates with very strong records who will bring externally sponsored research to Texas Tech will be considered for associate or full professor ranks.

The department has active research groups in both pure and applied mathematics (see <http://www.math.ttu.edu/FacultyStaff/research.shtml>). The department fosters a spirit of interdisciplinary collaboration across areas of mathematics as well as with engineering and the physical and biological sciences.

Applicants should apply for position numbers T96800 for statistics, T96232 for numerical

analysis, and T96376 for all other areas at: <http://jobs.texasastech.edu>. Applications should include a completed AMS standard cover sheet and a vita. Three letters of reference and any material in addition to that completed online should be sent to: Alex Wang, Hiring Committee Chair, Department of Mathematics and Statistics, Texas Tech University, Lubbock, TX 79409–1042. The review of applications will begin immediately.

Texas Tech University is an affirmative action/equal opportunity employer. Texas Tech University is committed to diversity among its faculty. The university strongly encourages applications from women, minorities, persons with disabilities, and veterans, and will consider the needs of dual-career couples.

Indiana University Bloomington

Department of Mathematics

The Department of Mathematics seeks applications for a tenure-track position, with appointment beginning in the fall of 2013. Exceptionally well-qualified applicants may also be considered at the tenured level. Outstanding candidates with a PhD in any area of pure or applied mathematics and with postdoctoral or faculty-level experience are encouraged to apply, with particular emphasis in the areas of algebra and pure and applied analysis. A minimum requirement is a PhD in mathematics. Salary will be commensurate with qualifications and the level at which the position is filled. The base teaching load for research-active faculty is three courses per year.

The department maintains strong research groups in all of the principal fields of mathematics. Bloomington is located in the forested hills of southern Indiana and offers a rich variety of musical and cultural attractions.

Applicants should submit an AMS cover sheet, curriculum vitae, a research statement, and a teaching statement, using the online service provided by the AMS at <http://www.mathjobs.org>. Applicants should arrange for four letters of recommendation, including one evaluating teaching experience. Where applicable, applicants should ask reference writers to submit their letters electronically through <http://www.mathjobs.org>. If applicants or letter writers are unable to submit materials online, they can submit them to: Search Committee, Department of Mathematics, Indiana University, 831 East 3rd Street, Rawles Hall, Bloomington, IN 47405–7106. Applications received by November 1, 2012, will receive full consideration; however, applications will continue to be accepted until the search is filled.

Indiana University is an affirmative action/equal opportunity employer and is supportive of the needs of dual-career couples.

Indiana University Bloomington

Department of Mathematics

The Department of Mathematics seeks applications for two Zorn Research Postdoctoral Fellowships, beginning in the fall of 2013. These are three-year, non-tenure-track positions with reduced teaching loads. Outstanding candidates with a recent PhD in any area of pure or applied mathematics are encouraged to apply; a minimum requirement is a PhD in mathematics. Zorn fellows are paired with mentors with whom they have compatible research interests.

The department maintains strong research groups in all of the principal fields of mathematics. Bloomington is located in the forested hills of southern Indiana and offers a rich variety of musical and cultural attractions.

Applicants should submit an AMS cover sheet, a curriculum vitae, a research statement, and a teaching statement, using the online service provided by the AMS at <http://www.mathjobs.org>. If unable to do so, applicants can send application materials to: Zorn Postdoctoral Fellowships Search Committee, Department of Mathematics, Indiana University, 831 East 3rd Street, Rawles Hall, Bloomington, IN 47405–7106. Applicants should arrange for four letters of recommendation, including one evaluating teaching experience. Applicants should ask reference writers to submit their letters electronically through <http://www.mathjobs.org>. If they are unable to do so, they can also send their letters to the previous address. Applications should be received by December 15, 2012.

Indiana University is an affirmative action/equal opportunity employer.

National University of Singapore

Department of Mathematics

The Department of Mathematics at the National University of Singapore invites applications for tenured, tenure-track, and visiting positions at all levels, beginning in August 2013. The department seeks promising scholars and established mathematicians with outstanding track records in any field of pure and applied mathematics. The department, housed in a newly renovated building equipped with state-of-the-art facilities, offers internationally competitive salaries with start-up research grants, as well as an environment conducive to active research with ample opportunities for career development. The teaching load for junior faculty is kept especially light. The department is particularly interested in, but not restricted to, considering applicants specializing in any of the following areas: analysis and Ergodic theory; number theory and arithmetic geometry; computational science, especially biomedical imaging and computational material sciences; probability, stochastic processes, and financial mathematics; and combinatorics and discrete mathematics.

NUS is a research-intensive university that provides quality undergraduate and graduate

education. The Department of Mathematics has about 65 faculty members and teaching staff whose expertise cover major areas of contemporary mathematical research. For further information about the department, applicants should visit <http://www.math.nus.edu.sg>.

Application materials should be sent via e-mail (as PDF files) to the Search Committee at: search@math.nus.edu.sg. Applicants should include the following supporting documentation in an application: (1) an American Mathematical Society Standard Cover Sheet; (2) a detailed CV, including a list of publications; (3) a statement (maximum of three pages) of research accomplishments and plans; and (4) a statement (maximum of two pages) of teaching philosophy and methodology. Applicants should attach evaluations of teaching from faculty members or students at their current institution, where applicable, and arrange for at least three letters of recommendation, including one that indicates effectiveness in and commitment to teaching. Applicants should ask their referees to send their letters directly to: search@math.nus.edu.sg; enquiries can also be sent to this e-mail address. The review process began on October 15, 2012, and will continue until the positions are filled.

Brown University

Division of Applied Mathematics

The Division of Applied Mathematics at Brown University invites applications for two Research Training Group postdoctoral fellowships. The area of emphasis is dynamical systems, differential equations, probability, or stochastic processes.

For a full posting, applicants should see the division's website: <http://www.dam.brown.edu>.

Dartmouth College

Department of Mathematics

The Department of Mathematics anticipates a tenure-track opening, with initial appointment at the assistant professor level in the 2013–14 academic year. The successful applicant will have a research profile with a concentration in computational or applied mathematics.

Applicants should apply online at <http://www.mathjobs.org>, Position ID: APACM #3874. Applications received by December 15, 2012, will receive first consideration. For more information about this position, applicants should visit the department's website: <http://www.math.dartmouth.edu/activities/recruiting/>.

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

Dartmouth College

Department of Mathematics

The Department of Mathematics anticipates a senior opening, with initial appointment in the 2013–14 academic year. The successful applicant will have a research profile with a concentration in computational or applied mathematics, will be appointed at the level of full professor, and is expected to have an overall record of achievement and leadership consonant with such an appointment.

Applicants should apply online at <http://www.mathjobs.org>, Position ID: PACM #3873. Applications received by December 15, 2012, will receive first consideration. For more information about this position, applicants should visit the department's website: <http://www.math.dartmouth.edu/activities/recruiting/>.

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Dartmouth College

Department of Mathematics

The Department of Mathematics anticipates a tenure-track opening for a mathematician working in either topology or number theory, with initial appointment in the 2013–14 academic year. The appointment is for candidates at any rank.

Applicants should apply online at: <http://www.mathjobs.org>, Position ID: TTPTNT #3875. Applications received by December 15, 2012, will receive first consideration. For more infor-

mation about this position, applicants should visit the department's website: <http://www.math.dartmouth.edu/activities/recruiting/>.

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

Georgia Institute of Technology

School of Mathematics

The School of Mathematics is accepting applications for faculty positions at all ranks and in all areas of pure and applied mathematics and statistics. Applications from highly qualified candidates, especially those from groups underrepresented in the mathematical sciences, are particularly encouraged.

For more details and application instructions, applicants should see: <http://www.math.gatech.edu/resources/employment>.

Institute for Advanced Study

School of Mathematics

The School of Mathematics has a limited number of memberships with financial support for research in mathematics and computer science at the institute during the 2013–14 academic year. The school frequently sponsors special programs; however, these programs comprise no more than one-third of the membership so that a wide range of mathematics can be supported each year. “Non-equilibrium Dynamics and Random Matrices” will be the topic of the special program in 2013–14. Horng-Tzer Yau of Harvard and Thomas Spencer of the institute will lead the program. Juerg Froehlich of ETH and Herbert Spohn of Zentrum Mathematik will be among the senior participants. More information about the special program for the year can be found on the school's homepage (<http://www.math.ias.edu/>).

Several years ago the School of Mathematics established the von Neumann Fellowships. Up to eight of these fellowships will be available for each academic year. To be eligible for a von Neumann Fellowship, applicants should be at least five, but no more than 15, years after receipt of a PhD.

Veblen Research Instructorships are three-year position that were established in partnership with the Department of Mathematics at Princeton University in 1998. Three-year instructorships will be offered each year to candidates in pure and applied mathematics who have received a PhD within the last three years. The first and third years of an instructorship are usually spent at Princeton University and will carry regular teaching responsibilities. The second year is spent at the institute and dedicated to independent research of the instructor's choice.

Candidates must have given evidence of ability in research comparable with at least that expected for a PhD degree. Postdoctoral computer science and discrete mathematics applicants may be interested in applying for a joint (two-year) position with one of the following: Department of Computer Science at Princeton University, <http://www.cs.princeton.edu>; DIMACS at Rutgers, The State University of New Jersey, <http://www.dimacs.rutgers.edu>; or the Intractability Center, <http://intractability.princeton.edu>. For a joint appointment, applicants should apply to the School of Mathematics, as well as to one of the listed departments or centers, noting their interest in a joint appointment.

Applicants can request application materials from: Applications, School of Mathematics, Institute for Advanced Study, Einstein Drive, Princeton, NJ 08540; applications@math.ias.edu. Applications can be made online at: <https://applications.ias.edu>. The deadline for all applications is December 1, 2012.

The Institute for Advanced Study is committed to diversity and strongly encourages applications from women and minorities.

See Opportunities on page 11



THE UNIVERSITY OF TEXAS AT AUSTIN

ICES POSTDOCTORAL FELLOWSHIP

The Institute for Computational Engineering and Sciences at The University of Texas at Austin is now accepting applications for the 2013 – 2014 ICES Postdoctoral Fellowship

The ICES Postdoctoral Fellowship Program offers fellowship awards for exceptional computational scientists, mathematicians, and engineers who have recently completed doctoral studies in areas relevant to research conducted at the Institute.

Fellowship stipends are \$60,000 per year. Fellows will receive UT employee benefits and relocation expenses. U.S. citizens are especially sought, however, foreign scholars may also be considered. Applications must be received by December 1, 2012

For further details and instructions for application submission, see: <https://www.ices.utexas.edu/programs/postdoc/>

Ionic Solutions

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Third, *without flows, biological systems are dead*. We cannot expect dead biological systems, whether corpses or crystals, to be the same as live systems. Gradients and flows create the devices and machines of engineering. Engineering devices are hardly worth studying when their power supplies are turned off and simple device laws no longer hold true.

Finally, mathematics must describe *biological reality and experiments as they are actually done*. Scientists cope with complex systems by simplifying the systems and then adding back components or fields, one by one. It is difficult to describe the resulting hierarchy of systems if each one is considered individually, without interactions, in the ideal tradition of chemistry. A hierarchy of inconsistent models is a challenge to the scientific process. It is understandable, nearly inevitable in such circumstances, that theories of mixtures of electrolytes (e.g., equations of

state) should include many vaguely defined parameters, of little use beyond the conditions in which they were measured.

Scientists have been crippled by their lack of consistent mathematics. Different laboratories use different models of systems and make different choices of parameters. A recent magnificent treatise ([5]: 664 pages and 2406 references) shows how difficult it is even to define the properties of a single ion in a system in which everything interacts with everything else without a consistent mathematics of interactions. Consistency is an enormous help in focusing attention, and decreasing distracting discord, as has been the case in computational electronics.

A Promising Approach

Scientists need to replace their idealized noninteracting models of ionic solutions with a consistent framework in which everything can interact with everything else. Mathematicians working on ionic solutions [7,12] are well aware that varia-

tional methods allow components and fields to be added or subtracted in functionals, from which differential equations are derived by the Euler–Lagrange process. Mathematicians need to spread their knowledge of variational methods to the physical chemists, physiologists, and molecular biologists of the world. Mathematicians need to help scientists deal with the solutions of life. I prefer energy variational methods because they embody physics. Energy variational methods aspire [1,6] to be a natural extension of thermodynamics, joining free energy and dissipation functionals, as envisioned by the Nobel prize-winning physical chemist Lars Onsager (1903–1976) and followers. These methods combine [1,4,8,9] the least action principle of mechanics with the maximum dissipation principle of Rayleigh, later applied by Onsager, including eventual time-dependent relaxation to the steady state. The derivation of the Navier–Stokes equations for incompressible flow [6] illustrates the approach.

I hope that an army of mathematicians will take up the challenge of applying their tools and skills to biological reality. Mathematicians can use consistent theories of complex fluids to allow systematic analysis and improvement of models of the plasmas of life. Computations needed include current–voltage relations in complex mixtures of bio-ions. Theories of complex fluids need to be applied to classical unsolved problems of chemistry and biology, involving plasmas containing bio-ions, organic compounds, proteins, and nucleic acids. Theories of simple fluids are not adequate.

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Bob Eisenberg is chair of the Department of Molecular Biophysics and Physiology at Rush University Medical Center in Chicago. He has posted a longer version of this note, with more complete discussion and citations, at <http://arxiv.org/abs/1207.4737>.

Opportunities

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Pomona College

Department of Mathematics

Pomona College, in Claremont, California, seeks applicants for a tenure-track position in the Department of Mathematics, to begin in the fall semester of 2013–14. The department seeks candidates in applied mathematics, and the position is targeted at the rank of assistant professor. The department is looking for candidates who have demonstrated excellence in research and teaching, and who are interested in mentoring students and in directing students in independent work. The strongest candidates will have postdoctoral experience, have a strong research agenda, and show significant progress in their research. It is a priority of Pomona College and its Department of Mathematics to have faculty who have experience working with students from diverse backgrounds and a demonstrated commitment to improving access to and success in higher education for underrepresented students.

Pomona College is a highly selective liberal arts college with 1500 students (<http://www.pomona.edu>), located at the eastern edge of Los Angeles. Pomona is the founding member of the Claremont Colleges, a consortium of seven institutions with over 40 active mathematicians. The teaching load at Pomona College is 2–2.

Pomona College strongly prefers online applications submitted at: MathJobs.org (<http://www.mathjobs.org>). Applicants can also send applications via electronic mail to: mathsrch@pomona.edu or to: Search Committee, Department of Mathematics, Pomona College, 610 North College Avenue, Claremont, CA 91711–6348. A complete application will include a letter of application, curriculum vitae, graduate transcripts, at least three letters of recommendation (at least one of which evaluates teaching), a description (for the non-specialist) of research accomplishments and plans, and a statement of teaching phi-

losophy. Applications completed by December 1, 2012, will receive full consideration.

Pomona College is an equal opportunity employer and especially invites applications from women and members of underrepresented groups.

Statistical and Applied Mathematical Sciences Institute

Postdoctoral Fellowships for 2013–14

Postdoctoral fellowships (up to 6) are available at the Statistical and Applied Mathematical Sciences Institute for either of the two SAMSI Research Programs for 2013–14: Computational Methods in the Social Sciences and Low-Dimensional Structure in High-Dimensional Systems. Appointments will begin in August 2013 and will typically be for two years. Appointments are made jointly between SAMSI and one of its partner universities, where teaching is a possibility. Extremely competitive salaries, travel stipends, and health insurance will be offered.

Further information can be found at <http://www.samsi.info>.

Applicants should go to: <http://mathjobs.org>, SAMSIDP2013 Job #3759 to apply.

University of Texas at San Antonio

Department of Mathematics

The University of Texas at San Antonio invites applications for one tenure-track position at the rank of assistant professor in mathematics, pending budget approval, starting in the fall of 2013. The successful candidate will be expected to have a PhD degree in mathematics by the time of appointment, a strong research record, and demonstrated evidence of excellent teaching ability. Applicants who are selected for interviews must be able to show proof that they will be eligible and qualified to work in the U.S. by the time of hire.

Information on the mathematics program, a full version of the job announcement, and details on what to include in an application can be viewed at: <http://math.utsa.edu>.

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Stony Brook University's Department of Applied Mathematics and Statistics is soliciting applications for the Frey Family Endowed Chair of Quantitative Finance, a tenured professorship. Candidates must have a distinguished reputation for research and graduate training in mathematics, statistics or operations research and its application to the theory and practice of quantitative finance. The endowed chair will direct the department's growing quantitative finance program (currently 60 master's and PhD students) and must articulate a strong vision for the development of a quantitative finance program and outreach to the leaders in the investment community.

The department is ranked among the top 10 applied mathematics departments in the U.S. Its 22 full-time and 15 adjunct faculty have a broad array of research interests and collaborations in applied mathematical sciences. It has access to several high-performance computers, including a 100Tf Blue Gene system. The department graduates about 18 PhD, 55 MS and 110 BS degrees annually. The University is located 60 miles from Manhattan and one mile from the headquarters of Renaissance Technologies. Review of applications will begin in Fall 2012 and will continue until the position is filled.

For a full position description, application procedures or to apply online, visit www.stonybrook.edu/jobs (Ref. #: F-7442-12-08-S) or submit a New York State employment application, cover letter, curriculum vitae and statement of research by mail to: Professor W. Brent Lindquist, Chair, Department of Applied Mathematics & Statistics, Stony Brook University, Stony Brook, NY 11794-3600; or by email to b.lindquist@stonybrook.edu. In addition, please arrange for three letters of professional reference to be sent directly to Prof. Lindquist.



Stony Brook University

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A Leading Role for Mathematics in the Study of Ionic Solutions

By Bob Eisenberg

It is hard to see big things from up close, in math and science, as in the world. Many mathematicians approach biology for interesting problems, but sometimes the biggest problems, which offer the greatest opportunities, are too close to see. The study of ionic solutions as they occur in life is one such problem.

Biology occurs in saltwater solutions—biological plasmas—that evolved from primitive oceans of the earth [2,3]. Biological plasmas contain large concentrations of the bio-ions sodium (Na⁺), potassium (K⁺), and chloride (Cl⁻), variable concentrations of calcium (Ca²⁺), and much lower concentrations of organic acids and bases of many types. Without proper ions, water is lethal to cells and proteins.

Bio-ions control a wide variety of biological processes. The Hodgkin–Huxley equations couple atomic changes in proteins (ion channels) and macroscopic flows of ions in nerves. Propagating signals called action potentials are the result. Ions, proteins, macroscopic flows, and gradients are coupled in many of life’s essential processes.

Calcium ions and complex organic molecules (e.g., hormones) control many processes. Calcium signals organize heart muscle to pump blood and prompt cells to release other chemical signals. Calcium means one thing in one place, something else in another place, rather as voltages in different places in a computer mean quite different things.

We have viewed these bio-ions as nearly hard spheres, with different diameters and permanent charge, independent of the local electric field, surrounded by water. Because ions are strongly coupled by electrical and steric forces, I believe that the mathematics of ionic solutions needs to be the mathematics of complex fluids. Ionic solutions are not simple fluids.

Chemical/Mathematical Traditions

Physical chemists and physiologists have studied mixtures of bio-ions for more than a century. Early scientists had to cope with ionic solutions without mathematical tools that deal with interactions consistently. Theoretical chemistry exploited the idea of ideal solutions at chemical equilibrium in a most imaginative and powerful way. These idealizations allowed the study of atoms even when their existence was still being debated. Experimental measurements included current–voltage relations that allow detailed tests of theories of ionic solutions.

The chemical tradition succeeded because it focused on idealized systems without interactions. Its paradigm was the infinitely dilute, uncharged, perfect gas, without

boundary conditions or untidy interactions. Chemists have treated ions separately, one type at a time, in solutions at equilibrium. Interactions, flows, and boundary conditions have not been treated consistently. Without modern mathematical and computational methods, the chemical tradition achieved remarkable success by restricting its gaze, but the chemical tradition deals with idealized simple fluids—and chemical reactions—as if they occurred without spatial gradients.

The mathematical tradition used the Poisson–Boltzmann (PB) and Poisson–Nernst–Planck (PNP) equations to describe interactions of point charges. PB–PNP is widely used even today to model transistors and semiconductor devices. It was only natural to hope that PB–PNP would do as well with ionic solutions. Mathematicians understandably were more interested in solutions of equations than in solutions of ions, particularly the messy nonideal properties produced by finite-size interacting particles.

PB–PNP succeeds in certain isolated cases—for example, those with vanishing

I believe that daunting interactions of ions, microelements, and the macroscopic world can be handled automatically and consistently by the theory of complex fluids.

concentrations of monovalent ions of one type. Although these cases can be significant, natural biological function almost always occurs in physiological solutions beyond the reach of PB–PNP equations. As Torrie and Valleau [10] put it: “It is immediately apparent that classical theory [Poisson–Boltzmann] has broken down completely. It . . . fails to show [the] qualitative behavior [and] is seriously in error for quite low concentrations.”

PB–PNP theories fail because they treat ions as points. In reality, the size, shape, and microdynamics of ions are important in almost all solutions. In 1M solutions, ions of diameter 2Å are roughly 8Å apart. The electric field and entropy of such a system are not those of point particles. (In the classical chemical units of number density: 1M = 1Molar = 6.02 × 10²³ particles per liter = 6.02 × 10²⁶ particles per cubic meter.)

The difficulties with PB–PNP theories acquire startling importance near DNA, ion channels, and enzymes, and in electrodes of batteries, where ions are crowded together in mixtures with divalents at number densities higher than 10M. (For comparison, solid NaCl is 37M.) Indeed, PB–PNP theories fail most dramatically where ions are

most important, near structures that use ions to perform macroscopic functions.

Devices—whether ion channels or enzymes, or batteries—concentrate ions in some regions (to maximize flow) and deplete them in others (to maximize control). A theory must deal seamlessly with large ranges of concentration if it is to deal with the devices of engineering or biology.

An Army of Mathematicians Is Needed

A review of the numerical analysis of PB in *SIAM Review* [11] motivated this article, which was catalyzed by valuable discussions with Chun Liu and Wei Cai. Analysis of the PB equations provides the initial iterates for the development of numerical procedures needed to solve the big problem (with all interactions). Work on PB–PNP sets the stage on which the moving dance of biology can be studied, as it is actually lived.

Work on the living problem, however, requires mathematics that describes interacting ions in devices. The mathematics can start with bio-ions described as hard

spheres diffusing in a uniform dielectric. Such analysis is beginning. These solutions of bio-ions can be studied with the existing theory of complex fluids. More realistic descriptions of ions and water can be used later if needed.

It will take an army of mathematicians to study the ionic solutions of physical chemistry and biology as complex fluids. Mathematicians will need to learn the experimental traditions of physical chemistry and physiology before they can address longstanding unsolved problems. They will have to rework their tools to deal with the realities of ions in solutions and near channels, proteins, and electrodes. I believe that daunting interactions of ions, microelements, and the macroscopic world can be handled automatically and consistently by the theory of complex fluids.

Beyond the bio-ions, additional components of extra- and intra-cellular solutions—organic ions, amino acids, even nucleic acids and proteins—can be added as microelements as needed. Reduced models of some of these components are already known. Organic and biochemists have been making reduced models of these components and their chemical reactions for 150 years. I suspect that their reduced models could be improved by appropriate extensions of the theory of inverse problems. Chemical reactions could be treated by the theory of complex fluids, as interactions of microelements (reactants), bio-ions, and

water, involving rearrangements of internal (electronic) structures of reactants, according to Schrödinger’s wave equation for the electron.

Simulations are an alternative approach, favored by computer scientists. But simulations of biological plasmas present formidable challenges: They must deal simultaneously with mixtures and flows over some 10 orders of magnitude in size, time, and concentration [3]. They must couple atomic-level motions of proteins to macroscopic electric fields if they are to compute action potentials of nerves. Simulations so far have not included divalents, mixtures, large concentrations, flow, or macroscopic boundary conditions. Calibration remains in the future. Simulations may eventually reach these goals with the help of more powerful computers. Meanwhile, simulations can serve as models of microelements in multiscale theories of complex fluids.

But first the community of scientists who know the theory of complex fluids will need to study real-world electrolytes. If they limit themselves to uncalibrated simulations of tiny systems, to Poisson–Boltzmann equations and point particles, their work will have limited value. It will not apply to most living systems. It will set the stage of life, but it will not account for the action on the stage.

Math and Biological Reality

Biological reality determines mathematical treatment in several ways:

First, real biological solutions are characterized by *interactions on all scales*: Everything interacts with everything else in ionic solutions. PB–PNP theories and simulations have not plumbed the biological realities of divalents, mixtures, or molar concentrations. The free energy of one type of ion depends on the concentration of all other types of ions. The thermodynamic driving force for a single ion depends not only on the concentration of that ion—as assumed tacitly in much of chemistry and biophysics—but rather on all ions present. Even in bulk solutions, flow of any one ion depends importantly on all other ions. Classical treatments often attribute complexities of the ions themselves entirely to enzymes, channels, or chemistry.

Second, biological reality means that *non-equilibrium can be easier*. Simplifying biological (or engineering) devices can inadvertently make them difficult to study. Biological devices (like nerve membranes) have evolved to follow simple robust laws in physiological conditions, where gradients of concentration and potential are always present to drive flows. Devices at equilibrium, without gradients of electrical or electrochemical potential, no longer are devices at all. They follow no particular laws and are hard to study, analogous to the study of amplifiers when disconnected from power supplies.

See **Ionic Solutions** on page 11

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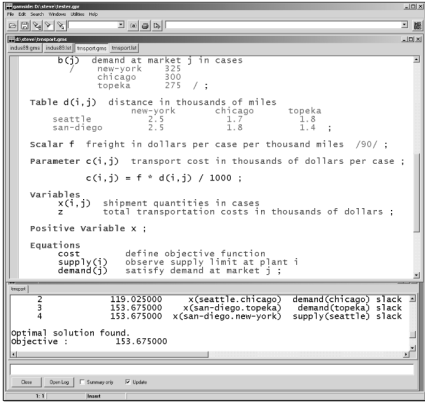
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