SOCIETY for INDUSTRIAL and APPLIED MATHEMATICS<br>3600 Market Street, 6th Floor<br>Philadelphia, PA 19104-2688 USA SOCIETY for INDUSTRIAL and APPLIED MATHEMATICS Philadelphia, PA 19104-2688 USA 3600 Market Street, 6th Floor



Volume 50/ Issue 10 December 2017

Nonprofit Org U.S. Postage Nonprofit Org<br>U.S. Postage<br>PAID<br>Permit No 360<br>Bellmawr, NJ Permit No 360 Bellmawr, NJ

# **Surprises Regarding the Hall Effect: An Extraordinary Story Involving an Artist, Mathematicians, and Physicists**

*By Marc Briane, Muamer Kadic, Christian Kern, Graeme Milton, Martin Wegener, and Dylon Whyte*

In February 2017, the front cover of *Physics Today* featured a beautiful *Physics Today* featured a beautiful microstructure of interlocking rings that, for the first time in history, reversed the sign of the Hall coefficient in a material with electrons (rather than holes) as the predominant charge carrier. The Hall effect, initially observed by Edwin Hall in 1879, predates the discovery of electrons. If one applies a magnetic field perpendicular to a conducting material—such as a copper plate—and a voltage across the plate's length, current flows. But an additional voltage develops across the width of the plate, transverse to the current flow; this is called the Hall voltage. It develops because the electrons sense a force (the Lorentz force) perpendicular to both the magnetic field and the electron velocity that needs to be balanced by something — in this case, by the force due to the electric field generated by the Hall voltage (electrons move to one side of the plate until the required voltage develops). For small fields, the

electric field induced by the Hall voltage is then linearly related to the product of the applied current and the applied magnetic field through a proportionality constant known as the Hall coefficient. Assuming that the electrons travel at constant velocity in parallel straight lines, this observation leads to the textbook statement claiming that the sign of the Hall coefficient reveals the charge carrier's sign in classical physics. However, the standard argument's weakness is the assumption that electrons travel in (approximately) parallel straight

SIZIML NYIIIS

lines, which is certainly not the case in materials with microstructure.

Development of the counterexample to the textbook claim—that the sign of the Hall voltage determines the sign of the Hall coefficient—is an interesting story in its own right. The combined efforts of many, including mathematicians, physicists, and even an artist, yielded the example that overturned classical beliefs. The story begins with a seemingly unrelated question. In a twodimensional periodic conducting composite (where the electrical potential *V* satisfies

 $\nabla \cdot \sigma \nabla V = 0$ ,  $\sigma(\mathbf{x})$  is a smooth scalarvalued periodic electrical conductivity that is positive and finite everywhere, and  $\nabla V$ is periodic with a nonzero average), one does not expect the vector-valued electric field  $-\nabla V$  to vanish inside the medium. Going further, one can think of a  $2 \times 2$ matrix-valued electric field  $E(x)$  with elements  $E_{ij} = -\partial V_j / \partial x_i$ —where each  $V_j$ solves the conductivity equations—but with an average value over  $-\nabla V_i$ 's unit cell

**M** y first encounter with the pairing of numerical analysis and uncertainty quantification goes back three decades. There was not yet a name to define the latter, and only few numerical analysts ventured into the world of probability. As a graduate student in the mid-1980s, I took some courses in statistics and intended to focus my Ph.D. thesis on the mathematics of experimental design, only to find my potential advisor leaving the institution. The search for a new topic and advisor ended successfully when Peter Henrici suggested that I examine the effect of round-off error on the computation of the fast Fourier transform using a probabilistic formulation. Round-off errors and the problems associated with finite precision arithmetic introduce a significant level of uncertainty in results of scientific computations. In the days before IEEE arithmetic, different computers followed different standards when it came to representing numbers in finite precision arithmetic, and



**Figure 1.** *Semiconductor metamaterials: from art to physics via mathematics.* **1a.** *Photograph of two-layer chain mail, courtesy of Dylon Whyte.*  **1b.** *Original blueprint of the three-constituent metamaterial suitable for reversing the sign of the Hall coefficient according to [6]. The black spheres correspond to a semiconductor constituent, the gray tori are made of ideal metal, and the homogeneous background is a weakly conducting material. Image courtesy of Christian Kern.* **1c.** *Experimental test series composed of different single-constituent, microstructured metamaterial samples.* **1d.** *Photograph of a fully functional Hall-effect metamaterial sample in the measurement probe station. 1c and 1d are courtesy of [11].*

*See* **Hall Effect** *on page 3*

## **Quantifying Uncertainty in Numerical Analysis**

#### *By Daniela Calvetti*

Figure 1. True and recovered figures. 1a. The original image. 1b. A blurred and noisy version is proportional to the product of the prior<br>of the original. 1c. MAP estimate of the hyperparameter. 1d. MAP estimate with condi *Gaussian prior with inverse gamma hyperprior.* **1e.** *MAP estimate with second-order smoothness prior.* **1f.** *MAP estimate with white noise prior. Image credit: Daniela Calvetti. See* **Numerical Analysis** *on page 4*

it was normal for the same code to produce significantly dissimilar results when run on two different machines. The literature on probabilistic analysis of error in numerical algorithms at the time was rather limited, and definitely not considered part of mainstream numerical analysis.

My probabilistic foray ended shortly after the completion of my Ph.D., and I spent the next decade and a half working in numerical linear algebra, particularly on iterative solvers for large-scale inverse problems. Although probability did not play an active role in my research, the thought that it may be key to understanding the variability of the solution as a function of the random starting vector or the random perturbation of the data kept buzzing in my head. My initial encounter with Bayesian methodology for solving inverse problems was simultaneously exciting and frustrating: not only did it look like Bayesian methodology was the natural language to describe variability in the computed results, but it seemed that one could also use the Bayesian framework to make numerical algorithms take advantage of qualitative

or partial information, or belief about the quantity to be computed. It would have been a *Eureka!* moment, except that I had no idea how to interface state-of-the-art numerical analysis and Bayesian inference. The challenge of designing computational tools for quantifying uncertainties in numerical analysis—and leveraging them to improve the computational algorithm—has since become the central theme of my research.

Fortunately, when beginning to recast numerical analysis in a probabilistic setting, it suffices to have a few basic notions of probability and an open mind. The first step towards embedding numerical algorithms into a probabilistic framework is to model all quantities whose values are unknown as random variables, where the randomness is a way of admitting our ignorance about their values rather than a statement about the variables themselves. For example, when solving a linear system  $Ax = b$ , where we assume that *A* is a known matrix and vector *b* is corrupted by some additive noise  $\epsilon$ , we model *x* and *b* as random variables because we are unsure of their values. On the other hand, we probably know something about the nature of the noise and have at least some vague ideas regarding the properties of the vector  $x$  — it is very hard to know absolutely nothing! Using Gaussian distributions  $x \sim \mathcal{N}(\bar{x}, \Gamma)$ ,  $\epsilon \sim \mathcal{N}(0, \Sigma)$  to express what we know about *x* and  $\epsilon$  is a natural entry point. Since the additive noise model implies  $\epsilon = b - Ax$ , if we know the value of *x*, then *b* inherits the uncertainty coming from the noise contribution and can be described by a shifted Gaussian  $b \sim \mathcal{N}(Ax, \Sigma)$ , called the likelihood. Once we consider the data *b*, the idea or belief about *x* that we had a priori is likely to change in light of our observation; this leads to the posterior distribution of *x*, which is the solution of the linear system in probabilistic terms. Bayes formula states that the posterior distribution is proportional to the product of the prior



# Volume 50/ Issue 10/ December 2017

#### **4 Mitigating Bias in Science and Engineering** The effects of implicit bias—the unconscious attitudes, stereotypes, and associations regarding certain groups—against women and underrepresented minorities in STEM fields are often hard to identify and quantify. Robin Andreasen explains that while it may not be possible to eliminate implicit bias altogether, steps can be taken to reduce these inclinations.

#### **7 The Clever Mathematics Behind Wall Street Intrigue** Richard Burkhart reviews *The Money Formula: Dodgy Finance, Pseudo Science, and How Mathematicians Took Over the Market*, a book by Paul Wilmott and David Orrell that explores the mathematical abuses behind the trillion-dollar swindles in London and on Wall Street. The authors delve into the mathematical models and algorithms that helped hide risk and shift it to consumers, baiting both investors and the public.

**10 Persistent Homology Analysis of Biomolecular Data** Geometric modeling is critical to understanding biomolecular structure-function relationships, but is often computationally intractable. Guo-Wei Wei demonstrates the advantages of persistent homology—a new branch of algebraic topology—which embeds multiscale geometric information into topological invariants, thus simplifying the analysis of biomolecular data.



**12 Direct Current Transmission and the Future of Electricity**

A growing number of countries are beginning to transport electricity through direct current rather than alternating current transmission lines, saving both money and energy. The United States will soon join them. James Case outlines the merits, challenges, operational complexities, and implications of high-voltage direct current systems for power distribution.

#### **11 Professional Opportunities and Announcements**

ISSN 1557–9573. Copyright 2017, all rights reserved, by the Society for Industrial and Applied Mathematics, SIAM, 3600 Market Street, 6th Floor, Philadelphia, PA 19104-2688; (215) 382-9800; siam@ siam.org. To be published ten times in 2017: January/ February, March, April, May, June, July/August, September, October, November, and December. The material published herein is not endorsed by SIAM, nor is it intended to reflect SIAM's opinion. The editors reserve the right to select and edit all material submitted for publication.

**Advertisers:** For display advertising rates and information, contact Kristin O'Neill at marketing@siam.org.

It has been called the world's most fun-<br>damental matrix equation (WMFME), If thas been called the world's most funbut it is just the associative law  $A(BC) = (AB)C$  for matrix multiplication. This simple equation directly yields many less obvious formulas and has important implications for computation.

Consider the symmetric form of the WMFME in which  $C = A$ , so that if *A* is  $m \times n$  then *B* is  $n \times m$ . The WMFME is then equivalent to  $(I_m + AB)A = A(I_n + BA)$ , which yields

#### $(I_m + AB)^{-1} = I_m - A(I_n + BA)^{-1}B$

**One-year subscription (nonmembers):** Electroniconly subscription is free. \$73.00 subscription rate worldwide for print copies. SIAM members and subscribers should allow 8 weeks for an address change to be effected. Change of address notice should include old and new addresses with zip codes. Please request address change only if it will last 6 months or more.

(to see the connection, just multiply both sides on the left by  $I_m + AB$ ). This is sometimes called the matrix inversion lemma and while it can be proved in many ways, it is really just a manifestation of the WMFME. In fact, it is essentially the well-known Sherman-Morrison-Woodbury formula, in which context we usually think of *n* as much smaller than *m*, so that  $I_m + AB$  is a low-rank update to  $I_m$ .

#### **Printed in the USA.**

*is a registered trademark.*

#### **Editorial Board**

product  $A_1 A_2 ... A_k$  to minimize the number of operations in the evaluation is a nontrivial problem, known as the matrix chain multiplication problem. Textbooks show that the problem

H. Kaper, *Editor-in-Chief, Georgetown University*  C.J. Budd, *University of Bath, UK* K. Burke, *University of California, Davis* C. Castillo-Chavez, *Arizona State University* H. De Sterck, *Monash University, Australia* A.S. El-Bakry, *ExxonMobil Production Co.* M.G. Gerritsen, *Stanford University* O. Ghattas, *The University of Texas at Austin* A. Hagberg, *Los Alamos National Laboratory*  J.M. Hyman, *Tulane University* L.C. McInnes, *Argonne National Laboratory* S. Minkoff, *University of Texas at Dallas* N. Nigam, *Simon Fraser University, Canada* A. Pinar, *Sandia National Laboratories* R.A. Renaut, *Arizona State University* G. Strang, *Massachusetts Institute of Technology*

#### **Representatives, SIAM Activity Groups**

**Linear Algebra**

Depending on the dimensions  $n_1$ ,  $n_2$ ,  $n_3$ , and  $n_4$ , evaluating  $J_g$  as  $(J_{f_3}J_{f_2})J_{f_1}$  or  $J_{f_3}(J_{f_2}J_{f_1})$  may be more efficient. More subtly, the expressions  $\left\{ \left\| J_g z \right\|_2 / \left\| z \right\|_2 : z \in \mathbb{R}^n \right\}$  $\left\{ \left\| J_{g} z \right\|_{2} / \left\| z \right\|_{2} : z \in \mathbb{R}^{n_{1}} \right\}$ and  $\left\{ \|w^T J_g\|_{2} / \|w^T\|_{2} : w \in \mathbb{R}^n \right\}$  $\left\{\left\|w^T J_g\right\|_2 / \left\|w^T\right\|_2 : w \in \mathbb{R}^{n_4}\right\}$  both give the 2-norm of  $J_{a}$ . If  $n_1 \neq n_1$  then one of these expressions will be easier to evaluate analytically, as it involves fewer

R. Renaut, *Arizona State University* **Discrete Mathematics** D. Hochbaum, *University of California, Berkeley* **Mathematical Aspects of Materials Science** Q. Du, *Columbia University* **Supercomputing** L. Grigori, *Inria Paris, France*  **Control and Systems Theory** F. Dufour, *Inria Bordeaux Sud-Ouest, France*

precisely when  $I_n + BA$  is.

A closer look at the matrix inversion formula leads to the realization that the conditions for the existence of the inverses of  $I_m + AB$  and  $I_n + BA$  must be the same. How can this be, given that  $AB \neq BA$  in general and that the two matrices can be of different sizes? In fact, *AB* and *BA* have quite a lot in common. They have the same trace, and the same determinant when  $m = n$ . Indeed, they have the same nonzero eigenvalues. More precisely, the sets of eigenvalues of *AB* and *BA* are the same except when  $m \neq n$ , in which case the larger matrix has additional zero eigenvalues. Therefore,  $I + AB$  is nonsingular

**Dynamical Systems** F. Diacu, *Yale-NUS College, Singapore* **Orthogonal Polynomials and Special Functions** P. Clarkson, *University of Kent, UK* **Geometric Design** J. Peters, *University of Florida* **Geosciences** T. Mayo, *University of Central Florida* **Life Sciences** T. Kepler, *Boston University* **Imaging Science** E. Miller, *Tufts University* **Algebraic Geometry** J. Draisma, *Universität Bern, Switzerland* **Computational Science and Engineering** P. Constantine, *Colorado School of Mines* **Applied Mathematics Education** P. Seshaiyer, *George Mason University* **Nonlinear Waves and Coherent Structures** K. Oliveras, *Seattle University* **Mathematics of Planet Earth** H. Kaper, *Georgetown University* **Uncertainty Quantification** E. Spiller, *Marquette University* **Optimization** A. Wächter, *Northwestern University*

#### *SIAM News* **Staff**

J.M. Crowley, *editorial director, jcrowley@siam.org* K. Swamy Cohen, *managing editor, karthika@siam.org* L. Sorg, *associate editor, sorg@siam.org*

Visit our website to view the results: sinews.siam.org



# **The World's Most Fundamental Matrix Equation**



*Cartoon created by mathematician John de Pillis.*

The WMFME is a mathematical—but not computational—equivalence. Generations of students have learned that the product  $xy^Tz$ , where *x*, *y*, and *z* are *n*-vectors, should be written and evaluated as  $x(y^Tz)$  (O(n) flops) rather than  $(xy^T)z$  $(O(n^2)$  flops). More generally, deciding where to put the parentheses in a matrix

(which does not ask for the matrix product to actually be formed) can be solved by dynamic programming in  $O(k^3)$  operations, but an  $O(k \log k)$  algorithm was devised by T.C. Hu and M.T. Shing [3].

The WMFME is also relevant in evaluating the Jacobian of a composition of functions. Consider  $g(x) = f_3(f_2(f_1(x))),$ where  $f_k$  maps  $\mathbb{R}^{n_k}$  to  $\mathbb{R}^{n_{k+1}}$ . The chain rule allows us to express the Jacobian of *g* in terms of the Jacobians of the constituent functions:

## $J_q(x) = J_{f_s}\left(f_2(f_1(x))\right)J_{f_s}\left(f_1(x)\right)J_{f_s}(x).$

unknowns. This is a form of duality, and

## **Siam news**

can be exploited to find explicit expressions for condition numbers [1].

Algorithmic differentiation (also called automatic differentiation, or AD), is a well-established subject of renewed interest because of its use in backpropagation in neural networks and deep learning. The difference between the forward and reverse modes of AD is essentially the order in which Jacobians are accumulated, rather similarly to the previous paragraph's discussion. I originally learned this interpretation from Mike Giles; it can

also be found in the book [2] by Andreas Griewank and Andrea Walther. Gil Strang includes this timely topic in his forthcoming book [5] as well.

A rather differ-

ent implication of the WMFME is the equation  $A(BA)^{1/2} = (AB)^{1/2}A$ , for any *A* and *B* such that the square roots exist. One can obtain the equation by iterating the symmetric form of the WMFME to attain  $A(BA)^k = (AB)^k A$ for all positive integers *k*, concluding that  $A p(BA) = p(AB)A$  for any polynomial *p*, and using the definition of matrix function via an interpolating polynomial.

Finally, we note that if *A* and *B* are symmetric positive definite, then *ABA* is symmetric positive definite, as it is congruent to *B*. Certain matrix trace considerations in quantum physics lead to the question of whether an arbitrary product formed from multiple copies of *A* and *B* (such as  $A^3BA$  or  $BAB^2AB$ ) has positive eigenvalues (the product is in general not symmetric). The answer is no, but examples with a negative eigenvalue are hard to find [4].

#### **References**

[1] Baboulin, M., & Gratton, S. (2009). Using dual techniques to derive componentwise and mixed condition numbers for a linear function of a linear least squares solution. *BIT Num. Math., 49*(1), 3-19.

[2] Griewank, A., & Walther, A. (2008). *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*. Philadelphia, PA: Society for Industrial and Applied Mathematics.

[3] Hu, T.C., & Shing, M.T. (1984). Computation of matrix chain products. Part II. *SIAM J. Comput., 13*(2), 228-251.

[4] Johnson, C., & Hillar, C. (2002). Eigenvalues of words in two positive definite letters. *SIAM J. Matrix Anal. Appl., 23*, 916-928.

[5] Strang, G. (2018). *Linear Algebra and Learning from Data*. Wellesley, MA: Wellesley-Cambridge Press. To appear, http://math.mit.edu/~gs/learningfromdata/.

*Nicholas Higham is the Richardson Professor of Applied Mathematics at The University of Manchester. He is the current president of SIAM.*

> Thank you for voting in the 2017 **SIAM General Elections. The** polls are now closed.

#### FROM THE SIAM PRESIDENT *By Nicholas Higham*

of periodicity that is a unit vector directed along the  $x_i$  direction,  $j=1,2$ . Thus, the average value of  $E(x)$  is the identity matrix. Applying an average electric field in a direction v generates a physical vector-valued electric field  $E(x) \cdot v$ ; if the field does not vanish for any x and  $v \neq 0$ , the determinant of  $E(x)$  cannot vanish and thus must maintain its sign throughout the material. Giovanni Alessandrini and Vincenzo Nesi [2] proved this result, which then led to improved bounds on the effective conductivity of composites. This naturally inspired the question of whether a similar result holds true for the determinant of the  $3 \times 3$ matrix-valued electric field  $E(x)$  for threedimensional composites.

Graeme Milton first thought about interlocking rings while on a bus in Rome, and Marc Briane and Vincenzo Nesi [8] developed the idea into a rigorous counterexample. A clue to the significance of highlyconducting interlocking rings is that when they are at different electrical potentials, the potential does not monotonically decrease (or increase) along the line joining their centers. Houman Owhadi pointed out that Alano Ancona [3] used a similar interlocking geometry to prove the loss of injectivity of the vector-valued potential associated with the matrix electric field  $E(x)$ . Thanks to David Bergman's work [4] on the Hall effect, perturbation theory proves that if one has a zero Hall coefficient outside a small test region in the unit cell and a nonzero constant Hall coefficient in the test region, the effective Hall coefficient is determined by the integral of a principal cofactor of the matrix  $E(x)$  over the test region. The appropriate cofactor is determined by the direction of the magnetic field, assumed aligned with one of the coordinate axes. For conduction in a plane with the magnetic field perpendicular to that plane, Alessandrini and Nesi's result [2] about the positivity of the determinant of  $E(x)$ implies that if the local Hall coefficient is

nonnegative everywhere, then the effective Hall coefficient is also nonnegative; no sign reversal can occur [5]. In the quest to find a three-dimensional counterexample, one would ideally want a geometry with cubic symmetry so that its response is isotropic. It is easy to visualize a plane filled by interlocking rings, which looks a bit like chain mail (medieval armor). When we contacted chain mail artist Dylon Whyte for permission to reproduce a beautiful picture he had created of this geometry, he asked—to our amazement—if we had considered the three-dimensional geometry of interlocking rings. That turned out to be exactly what was needed (see Figure 1, on page 1).

> [3] Ancona, A. (2002). Some results and examples about the behavior of harmonic functions and Green's functions with respect to second order elliptic operators. *Nagoya Math. J., 165*, 123-158.

The geometry that we proved would reverse the sign of the Hall coefficient [6] with three phases—highly-conducting interlocking rings, a background conducting region of much lower conductivity, and small spheres of high Hall-coefficient material—in the gaps between the rings where a cofactor of  $E(x)$  changes sign (see Figure 1b, on page 1). It was too complex to easily construct, even with state-of-theart manufacturing. But upon numerically analyzing the conducting ring structure, with void outside the rings and the rings themselves having a nonzero Hall coefficient, we found that we could achieve a sign reversal of the Hall coefficient—even in this simplified microstructure—in the presence of conducting bridges between the rings, on their inside sides [9]. Although this geometry still involved the cubic array of interlocking rings, the physical intuition for the Hall coefficient reversal was quite different, and based on the Hall voltage sign on the inside of the rings. Ramesh G. Mani and Klaus von Klitzing [13] noted that connecting leads to the inside surface of holes gives a reversed Hall voltage. However, we emphasize that their observation had nothing to do with homogenization and effective moduli. The Hall coefficient reversal using this single-phase interlocking ring structure, numerically predicted in [9], was then experimentally confirmed by Christian Kern [11] (see Figures

1c and 1d, on page 1). It is quite incredible to see the actual microstructures produced by three-dimensional laser printing.

The first half of 2017 saw considerable<br>news about the imminent impact of quantum computing (QC) on science, math, and data analysis [9]. Diverse viewpoints predict wildly-varying timescales—from years to decades—for initial impact, and debate what types of problems will first be affected. At the 2017 SIAM Annual Meeting, held in Pittsburgh, Pa., this July, we organized a minisymposium entitled "Identifying Computational Methods for Early Benefit from Quantum Computing," which addressed how QC will become useful to practicing computational scientists. We aimed to identify computational methods that are likely to benefit from QC in the next five years, and share the experiences of early QC application developers.

> This is not the end of the story on Halleffect materials. Another model predicted the parallel Hall effect [7], where the induced electric field is parallel to the magnetic field. A simplified microstructure exhibiting this behavior was designed and experimentally tested in [10] and [12], which noted that a split cylindrical shell of such a material might be useful for measuring the magnetic field's curl. Other interesting developments arise on the mathematical side as well. The vanishing of electric fields at certain points has turned out to be important to hybrid inverse problems, and conductivities  $\sigma(x)$ —involving geometries similar to interlocking rings, for which the stability of the reconstructions will inevitably degrade exist for any finite number of prescribed boundary conditions [1].

A QA-based processor is a special-purpose device that natively solves the *quadratic unconstrained binary optimization*  (QUBO) problem. The goal of a QUBO is to find the  $x_i \in \{0, 1\}$  that minimize

> $x^{\mathsf{T}}Qx$ (1)

for upper-triangular matrix *Q* with  $Q_i \in \mathbb{R}$ . The QUBO form is equivalent to the *unconstrained binary quadratic programming* (UBQP) problem and the *Ising model*.

> **Acknowledgments:** Muamer Kadic was supported by the Labex ACTION program (contact ANR-11-LABX-0001-01), and Graeme Milton was supported by the NSF through grant DMS-0411035.

#### **References**

[1] Alberti, G.S., Bal, G., & Di Cristo, M. (2017). Critical Points for Elliptic Equations with Prescribed Boundary Conditions. *Arch. Ration. Mech. Anal., 226*(1), 117-141.

[2] Alessandrini, G., & Nesi, V. (2001). Univalent σ-harmonic mappings. Arch. *Ration. Mech. Anal., 158*(2), 155-171.

[4] Bergman, D.J. (2010). Self-duality and the low field Hall effect in 2D and 3D metal-insulator composites. In G. Deutscher, R. Zallen, & J. Adler (Eds.), *Percolation Structures and Processes* (pp. 297-321). Jerusalem: Israel Physical Society.

[5] Briane, M., Manceau, D., & Milton, G.W. (2008). Homogenization of the twodimensional Hall effect. *J. Math. Ana. App., 339*(2), 1468-1484.



Figure 1. From left to right: Phenyl dendrimer molecular structure to the electronic structure graph and the resulting 8-concurrent graph partition*ing using a D-Wave system. Image credit: Susan Mniszewski, Los Alamos National Laboratory.*

[6] Briane, M., & Milton, G.W. (2009). Homogenization of the Three-dimensional Hall Effect and Change of Sign of the Hall Coefficient. *Arch. Ration. Mech. Anal., 193*(3), 715-736.

[7] Briane, M., & Milton, G.W. (2010). An Antisymmetric Effective Hall Matrix. *SIAM J. Appl. Math., 70*(6), 1810-1820.

[8] Briane, M., Milton, G.W., & Nesi, V. (2004). Change of sign of the corrector's determinant for homogenization in threedimensional conductivity. *Arch. Ration. Mech. Anal., 173*(1), 133-150.

[9] Kadic, M., Schittny, R., Bückmann, T., Kern, C., & Wegener, M. (2015). Hall-Effect Sign Inversion in a Realizable 3D Metamaterial. *Phys. Rev. X, 5*, 021030.

[10] Kern, C., Kadic, M., & Wegener, M. (2015). Parallel Hall effect from threedimensional single-component metamaterials. *Appl. Phys. Lett., 107*, 132103.

[11] Kern, C., Kadic, M., & Wegener, M. (2017). Experimental Evidence for Sign Reversal of the Hall Coefficient in Three-Dimensional Metamaterials. *Phys. Rev. Lett., 118*, 016601.

[12] Kern, C., Schuster, V., Kadic, M., & Wegener, M. (2017). Experiments on the Parallel Hall Effect in Three-Dimensional Metamaterials. *Phys. Rev. Applied, 7*, 044001. [13] Mani, R.G., & von Klitzing, K. (1993). Realization of dual, tunable, ordinary- and quantized-Hall resistances in doubly connected GaAs/AIGaAs heterostructures. *Z. Phys. B, 92*(3), 335-339.

*Marc Briane is a mathematician at the Institut de Recherche Mathématique de Rennes, France. Muamer Kadic is a physicist at the Institut FEMTO-ST, CNRS at the Université de Bourgogne Franche-Comté, Besançon, France. Christian Kern and Martin Wegener are physicists at the Institute of Applied Physics and Institute of Nanotechnology at Karlsruhe Institute of Technology, Germany. Graeme Milton is a distinguished professor of mathematics at the University of Utah. Dylon Whyte is a chainmail artist in Ontario, Canada.*

#### **Hall Effect**

*Continued from page 1*

# **How Will Early Quantum Computing Benefit Computational Methods?**

#### *By Phil Goddard, Susan Mniszewski, Florian Neukart, Scott Pakin, and Steve Reinhardt*

The conceptual appeal of QC systems is the use of their computational power, which grows exponentially with the number of quantum bits (or *qubits*), to reduce the time spent executing combinatorial algorithms, which on classical computers grows exponentially with the number of variables. The most advanced commercially available quantum computers are currently delivered by D-Wave Systems; the number of qubits in these systems has doubled every other year for the past six years, a trend that is expected to continue. We believe that D-Wave quantum computers will deliver high-quality solutions quickly and in a sustainable way.

#### **Quantum Annealing**

Scott Pakin of Los Alamos National Laboratory (LANL) described the current state of QC systems, where contemporary quantum computers implement one of two computational models: the *gate* or *circuit* model [4], or the *quantum annealing* (QA) model [5]. Here we focus on QA-based quantum computers, as they are the most commercially advanced.

One can think of a quantum annealer as a hardware implementation of simulated annealing that uses quantum effects superpositioning, entanglement, and quantum tunneling—to reduce the likelihood of getting stuck in a local minimum. In both quantum and simulated annealers, finding the  $x_i$  that truly minimize (1) is not guaranteed. Instead, the goal is normally to find good solutions quickly. A D-Wave quantum computer can propose a solution to (1) in only 5us even for  $N > 2,000$  (where the search space is greater than  $2^{2000}$ , as supported by a D-Wave 2000Q™ system.

Mapping computational problems into QUBO form, which requires creativity and ingenuity but can lead to encouraging results when accomplished, is a key challenge that all subsequently-described applications face.

#### **Applications**

**Graph Partitioning.** Combinatorial optimization as graph-theoretic problems is ubiquitous throughout mathematics, computer science, physics, chemistry, bioscience, machine learning, and complex systems. Many of these problems are NP-hard and therefore rely on heuristic solutions. The availability of quantum computers provides new opportunities to explore relevant quantum graph algorithms, particularly novel QA heuristics and hybrid methods that may out-perform classical approaches or efficiently solve new problem types.

Sue Mniszewski of LANL presented her team's work on graph partitioning algorithms using QA on the D-Wave 2X™ system [6], motivated by recent studies on graph-based electronic structure theory. Graph partitioning is a natural fit to the QUBO form solved by the D-Wave 2X system. One can naturally map unconstrained community clustering—based on the modularity metric—onto the QUBO, despite its status as a "very hard" problem for a classical computer. When con-

*See* **Quantum Computing** *on page 5*

noise and solution can be expressed in terms of Gaussian distributions, summarizing the posterior distribution by its mode amounts to computing its maximizer, the maximum a posteriori estimate  $x_{\text{MAP}}$ . Assuming for simplicity that *b* is corrupted by scaled white noise  $\Sigma = \sigma^2 I$ ,

ſ  $\overline{\phantom{a}}$  $\left\lceil \right\rceil$  $\bigg\}$ 2

where  $L$  is an invertible matrix related to  $\Gamma$ . Equivalently, since  $x_{\text{MAP}}$  is the minimizer of the functional



where  $\alpha = \sigma^2$ , we can think of it in numerical linear algebra as the solution of a penalized least squares and—in the context of inverse problems—a Tikhonov regularized solution.

$$
x_{\text{MAP}} = \operatorname{argmin} \left\{ \|Ax - b\|^2 \right\}
$$

$$
+ \alpha \|L(x - \overline{x})\|^2 \right\}
$$

Do we gain anything new in the deterministic setting by recasting the solution of our problem in probabilistic terms? One advantage of describing the solution

of the problems in terms of its posterior probability density is that in addition to summarizing it with a single point estimate, e.g., the mode, we can query the probability that realizations of the random variable are close to it. What is most exciting about the solution being a random variable is that there is great freedom in the assignment of the prior, which can be as specific or as loose as we believe the solution to be before considering the data. In particular, we can define prior distributions through stochastic simulations based on qualitative a priori beliefs that may be difficult to express analytically. I often think that in everyday life, we use a prior to state our opinion about events before gathering related data. Some priors are confirmed by data and others are in conflict with them. While the interpretation of the prior as a penalty term is currently very common regardless of the presence or absence of an underlying Bayesian framework, this was not the case in earlier days; a little over a decade ago, a referee commented that numerical linear algebra and Bayesian inference have absolutely nothing to do with each other! After warming up with traditional smoothness priors reminiscent of Tikhonov regularization functionals, it may be tempting to advance to more complicated priors, where we retain the Gaussian formalism but assume that entries of the covariance matrix are unknown — hence modeled as random variables. For consistency, we express our



**Figure 2.** *Three realizations from three different priors used for the reconstructions in Figure 1. From left to right: white noise prior, second order smoothness prior, and conditionally Gaussian inverse gamma hyperprior. Image credit: Daniela Calvetti* 

beliefs about these new random variables before accounting for the data in the form of a probability density, referred to as hyperprior. Conditionally Gaussian priors are particularly well suited when looking for sparse solutions, with appropriate choices of hyperpriors. State-of-the-art numerical methods allow us to efficiently compute an estimate of the solution by an innerouter iteration scheme. For some choices of hyperpriors, the results are remarkably similar to those obtained with sparsity-promoting regularization schemes, at a fraction of the computational cost.

Recently, I have applied these ideas to the reconstruction of brain activity from measurements of the induced magnetic field at the sensor of a magneto-encephalography device. In that context, where the number of unknowns is much larger than the number of measurements, utilization of qualitative a priori beliefs can have a major

impact on the quality of the computed solution. Preconditioners for Krylov subspace iterative linear system solvers related to a priori information about the organization of neurons, first shown in Santiago Ramón y Cajal's pioneering drawings, and belief in the sparsity of brain activity have produced highly accurate reconstructions at a very low computational cost. Powerful, stateof-the-art numerical analysis algorithms make it possible to compute the solution very efficiently. There is no question now that uncertainty is a crucial component of numerical computations; the challenge is using its quantification to design better numerical algorithms.

*Daniela Calvetti is the James Wood Williamson Professor in the Department of Mathematics, Applied Mathematics and Statistics at Case Western Reserve University.*

**Numerical Analysis**

*Continued from page 1*

# **Mitigating Bias in Science and Engineering**

*By Robin O. Andreasen*

We generally associate flowers with positive qualities, such as beauty and happiness, and insects with negative sensations, such as poison and fear. We do this despite the fact that flowers are sometimes poisonous and insects can sometimes be beautiful. These perceptions make up the basis of the implicit association test (IAT), developed by psychologists Anthony G. Greenwald, Debbie E. McGhee, and Jordan L.K. Schwartz. The test measures strength of association between a category or concept, such as race or gender, and evaluative terms (good, bad) or stereotypes (leader, caretaker). It can also expose people's hidden attitudes about members of certain social groups. For instance, I might explicitly believe that men and women are equally good at science, but unknowingly implicitly associate science with males and the liberal arts with females. You can discover your own implicit attitudes by taking an IAT (there are many!) on Harvard University's *Project Implicit* website.<sup>1</sup>

Implicit associations are natural. They are part of concept formation, and concepts are useful. They allow us to simplify and organize the mass quantities of information that we accumulate when navigating the world. They can also be statistically accurate. For example, it is true that women are underrepresented in the scientific workforce and overrepresented in the humanities. Implicit associations become problematic, however, when they are misapplied or biased by socialization. Socialization can lead us to wrongly associate the role of mathematics professor with a male and English teacher with a female. Accurate associations can also be misapplied. While it is true that roughly 85 percent of the directors of the National Science Foundation (NSF) have been male, assuming that the current director is male would be a mistake.

The role of implicit attitudes and their impact on women and other underrepresented groups in science, technology, engineering, and mathematics (STEM) was the subject of a minisymposium and

<sup>1</sup> https://implicit.harvard.edu/implicit/

panel discussion entitled "Implicit Bias, Stereotyping and Prejudice in STEM" at the 2017 SIAM Annual Meeting, held in Pittsburgh, Pa., this July. The panel was organized by Charles R. Doering (University of Michigan), and speakers included Nicholas P. Jewell (University of California, Berkeley), Denise Sekaquaptewa (University of Michigan) and Ron Buckmire (NSF). Jewell discussed the pervasiveness of implicit bias in academic evaluative contexts, such as hiring, promotion, and peer review. Sekaquaptewa examined the effects of bias and stereotype on the experiences of underrepresented groups in STEM, while Buckmire outlined the NSF's efforts to educate reviewers about the potential for—and impact of bias in the proposal review process. See accompanying sidebar for reports from Jewell and Sekaquaptewa.

It is well known that race and gender disparities exist in the STEM workforce. Women have earned roughly 50 percent of all STEM bachelor's degrees, 45 percent of all STEM master's degrees, and 40 percent of all STEM Ph.D.s awarded since the early 2000s. Yet they filled only 28 percent of all STEM occupations in 2015 [1]. That same year, black and Hispanic scientists, mathematicians, and engineers collectively constituted only 11 percent of that workforce [1]. Further disparities exist as well. Women and other underrepresented groups often receive lower pay, win fewer awards, and advance through the ranks more slowly than their male or white counterparts, even when they possess equal qualifications.

The existence and persistence of groupbased disparities in STEM are often explained in terms of a combination of interacting structural and social factors, including implicit bias. Our brains are not perfect. Everyone has implicit biases, even about members of their own group. The problem is that these types of biases often impose small disadvantages on women and other underrepresented groups, and small advantages to men and other dominant groups. These types of (dis)advantages can accumulate over time, resulting in largescale inequalities. Rates of pay serve as an

*See* **Mitigating Bias** *on page 6*

## **Stereotyping and Pay Inequities in STEM Fields**

Implicit bias influences all areas of academic life, including appointments, promotions, peer review, and leadership, thus affecting individuals and the institutional structures underlying these activities.

Gender pay equity has attracted national attention, particularly in recent years with the failure to enact major pay equity legislation. Despite its progressive reputation, academia has a poor record in this regard.<sup>1</sup> There have been substantial quantitative and methodological efforts to quantify bias in the area of pay equity. Statistical methods allow local academic leaders to consider pay data and assess whether a gender "gap" exists

<sup>1</sup> http://www.nytimes.com/interactive/ 2009/03/01/business/20090301\_Wage Gap.html

[1]; these methods reveal the general need for across-the-board adjustments when pay inequities are discovered. In addition, there is considerable evidence of what sociologist Robert Hironimus-Wendt coined "gated communities" in academia — the highest-paid academic disciplines tend to contain the highest percentage of male members, who also control community entry. Comparable worth evidenced through comparable pay is an ideal worth embracing.

*— Nick Jewell, University of California, Berkeley*

#### **References**

[1] Billard, L. (2017). Study of Salary Differentials by Gender and Discipline. *Statistics and Public Policy, 4*(1), 1-14.

## **Experiences of Women and Minorities**

An increasingly large research literature in the social sciences focuses on stereotyping and implicit bias regarding women and underrepresented racial/ethnic minorities (URMs) in STEM.

Research has also shown significant impact on targets of stereotyping. Studies on *stereotype threat* indicate that members of groups stereotyped as poor performers in math-intensive domains (including white women and URMs) actually perform more poorly on math tests when they become aware of these negative stereotypes. Knowing that others may be stereotyping them causes cognitive distraction; giving a poor math performance would, in turn, seem to confirm those stereotypes. This performancerelated concern consumes cognitive resources that could have been devoted to solving test problems [1]. When the relevance of the stereotype is reduced in the testing situation (via experimental manipulations in the lab), the scores of female, male, white, and URM students are not significantly different.

Social scientists have asserted that many STEM environments contain elements that "trigger" stereotyping and implicit bias. STEM settings that comprise very few women or URMs, or subtle cues—such as masculine décor in the setting, can activate stereotypes among everyone involved. This promotes implicit favorability towards men and white people in evaluation, and triggers the damaging stereotype threat experience among members of negatively-stereotyped groups. Thus, we must acknowledge the features of our STEM environments and consider making changes to reduce stereotypic elements and create a more inclusive environment for all.

— *Denise Sekaquaptewa, University of Michigan*

#### **References**

[1] Steele, C.M. (2010). *Whistling Vivaldi: And Other Clues to how Stereotypes Affect Us*. New York, NY: Norton. See also: http://reducingstereotypethreat.org.

straints are imposed (e.g., equal partitioning), QUBO reformulation is necessary. Mniszewski demonstrated concurrent partitioning based on the graph coloring problem, community clustering via modularity, and iterative multilevel partitioning with refinement (similar to METIS and KaHIP) on benchmark graphs and electronic structure graphs. Even graphs with approximately self-similar structure, which are traditionally difficult to partition, benefit from quantum graph partitioning (see Figure 1, on page 3). Graph partitioning results from quantum and hybrid classicalquantum approaches show that the D-Wave 2X system is comparable to current stateof-the-art methods, and sometimes better.

**Traffic Flow Optimization.** Florian Neukart from Volkswagen (VW) described the mapping of certain parts of the realworld problem of maximizing traffic flow into a form suitable for QA [7]. The objective is to reduce the time required for a set of cars to travel between their individual sources and destinations by minimizing total congestion over all road segments. To combat the limited size and connectivity of current-generation D-Wave systems, the VW team developed a hybrid quantum and classical workflow—based on the T-Drive trajectory dataset of the cars' GPS coordinates—that mimics traffic flow optimization in near-real time, integrating calls to the D-Wave system.

The team maximized simulated traffic flow between the Beijing city center and airport by redirecting a subset of 418 selected taxis to alternate routes, thus minimizing the number of *congested* (i.e., having more than a given number of vehicles at a given time) road segments. This required simultaneous optimization over all vehicles. The program considered three alternative routes, described by lists

of street segments, for each trip between the city center and airport, and assigned cars to routes that minimized the number of congested road segments. The left half of Figure 2 displays the traffic density on the Beijing road graph before optimization, and the right displays the density after optimization via D-Wave's qbsolv tool [2].

The VW team focused on finding good quality solutions within short periods of calculation. They ultimately showed that time-critical optimization tasks, such as continuous redistribution of position data for cars in dense road networks, are suitable candidates for quantum applications.

**Finance.** Phil Goddard of 1QB Information Technologies (1QBit) works with applications in computational finance, where many high-value problems can be cast as combinatorial optimization problems and are hence solvable with QA. Specific applications include multiperiod mean-variance portfolio optimization, (quantum) hierarchical risk parity feature selection for credit scoring, and tax loss harvesting [1]. While adhering to realistic investment constraints, the problem variables can be discretized and reduced through suitable transformations to the QUBO form solved by a D-Wave system. The size of the solvable optimization problem (measured in number of problem variables) depends on several factors, including the technique used to discretize the problem and the way it is embedded onto the Chimera graph topology in which the D-Wave system's qubits are laid out. Conceptually, the benefits of using QC will increase with problem size.

#### **Programming**

Steve Reinhardt of D-Wave Systems described the range of software tools available to solve problems on existing commercial quantum computers. Only in the last year or two have interfaces emerged that are higher level than the system-dependent quantum machine instruction exposed by D-Wave's low-level system interface [3]. Several groups of tool developers deliver interfaces that allow a problem to be stated as a polynomial and then converted to a QUBO. Two groups deliver *solvers* that solve a problem larger than that natively supported by the hardware by repeatedly decomposing the problem into chunks that can be executed on the system. These tools have become essential for application and higher-level tool development. QC Ware Platform [10] and edif2qmasm [8] are tools that enable subject-matter experts to express problems in high-level forms and map those problems to a QUBO for D-Wave execution.

#### **Summary**

When comparing techniques for the different applications, we see that effectively mapping a problem to QUBO form is essential to obtaining good results. Some problems map directly to QUBOs while others map with intermediate steps that may add ancillary variables. Either approach matches well with a D-Wave quantum computer, ideally resulting in a problem that is sufficiently hard, as D-Wave systems are more likely to deliver a performance advantage over classical systems in the case of hard problems. Additionally, programs solving real-world problems invariably execute in a hybrid classical-quantum mode. All of the aforementioned applications also take advantage of a decomposing solver to fit the problem—in chunks—onto the QC system.

#### **References**

[1] 1QB Information Technologies. *1Qbit: Our Thinking*. Retrieved from https://1qbit.com/our-thinking/.

[2] Booth, M., Reinhardt, S.P., & Roy, A. (2017). *Partitioning Optimization Problems for Hybrid Classical/Quantum Execution* (D-Wave Technical Report Series, 14-1006A-A). Retrieved from https://github.com/dwavesystems/qbsolv/ blob/master/qbsolv\_techReport.pdf.

[3] *Developer Guide for C.* (2017). Burnaby, British Columbia, Canada: D-Wave Systems, Inc.

[4] Feynman, R.P. (1986). Quantum mechanical computers. *Found. Phys., 16*(6), 507-531.

[5] Kadowaki, T., & Nishimori, H. (1998). Quantum annealing in the transverse Ising model. *Phys. Rev. E, 58*, 5355- 5363.

[6] Mniszewski, S.M., Ushijima-Mwesigwa, H., & Negre, C.F.A. (2017). *Graph partitioning using the D-Wave for electronic structure problems.* In *Identifying Computational Methods for Early Benefit from Quantum Computing* (minisymposium). 2017 SIAM Annual Meeting. Pittsburgh, PA, July 10-14, 2017.

[7] Neukart, F., Von Dollen, D., Compostella, G., Seidel, C., Yarkoni, S., & Parney, B. (2017). Traffic flow optimization using a quantum annealer. Preprint, *arXiv:1708.01625*.

[8] Pakin, S. (2017). *edif2qmasm: Run Hardware Descriptions on a Quantum Annealer*. Retrieved from https://github. com/lanl/edif2qmasm.

[9] Palmer, J. (2017). Here, There, and Everywhere: Quantum technology is beginning to come into its own. *The Economist, Technology Quarterly*. Retrieved from http://www.economist.com/news/ essays/21717782-quantum-technologybeginning-come-its-own.

[10] QC Ware Platform software. (2017). *QC Ware*. Retrieved from https://platform. qcware.com/.

*Phil Goddard is Head of Research at 1QBit, and president and principal consultant at Goddard Consulting. He specializes in applying cutting-edge techniques to high-value optimization and machine learning problems. Susan Mniszewski is a computer scientist at Los Alamos National Laboratory (LANL). Her research interests include solving optimization problems using quantum computing. Florian Neukart works as a principal scientist in the fields of artificial intelligence and quantum computing at Volkswagen Group of America, where he is conducting research on self-driving vehicles, quantum machine learning, self-optimizing robots, and artificial intelligence. Scott Pakin is a computer scientist who currently serves as the technical/scientific point of contact for LANL's D-Wave quantum annealer. He has researched numerous areas of high-performance computing. Steve Reinhardt has built hardware/ software systems that deliver new levels of performance via conceptually simple interfaces. He now leads D-Wave's efforts with customers to map early applications to D-Wave systems.*

# IT'S TIME TO **ONLINE RENEWAL** IS QUICK, EASY, AND EFFICIENT. GO TO **MY.SIAM.ORG MEMBERSHIP**

### THAT SIAM OFFERS, INCLUDING:

**RENEW TODAY FOR ACCESS TO ALL** 

- MEMBER DISCOUNTS ON CONFERENCES, BOOKS, **AND JOURNALS**
- 21 ACTIVITY GROUPS FOR SPECIALIZED **INTERESTS**
- SUBSCRIPTIONS TO SIAM NEWS AND SIAM REVIEW
- MORE THAN 175 STUDENT CHAPTERS WORLDWIDE
- PERSONAL GROWTH, CAREER ADVANCEMENT, **AND PEER NETWORKING**
- PROFESSIONAL AWARDS, PRIZES, **AND RECOGNITION**

### **LOGIN AT MY.SIAM.ORG AND RENEW TODAY!**



**Figure 2.** *Heatmaps of traffic congestion in unoptimized (left) and optimized (right) flows. Image credit: Florian Neukart, Volkswagen Group of America.*

#### **Quantum Computing**

*Continued from page 3*

example. If women consistently receive lower raises—even by a small amount than equally-qualified men, a gender pay gap will eventually emerge. Psychologist Virginia Valian calls this mechanism "accumulation of advantage." She argues that taken together, these factors can make significant headway in explaining the glass ceiling and other group-based career inequalities.

The good news is that something can be done. Although it may not be possible to eliminate implicit biases altogether, they can be reduced and modified. Awareness of implicit bias and its role in evaluation is an important first step. One should be mindful of common cognitive shortcuts that sometimes occur in the evaluation process. Examples include preferring people with qualifications and characteristics similar to one's own, undervaluing a person's work or research because it is unfamiliar, and making snap judgments by focusing on a few negatives rather than overall qualifications. Also important is recognition of the contexts in which implicit bias is likely to influence evaluation. Research shows that people are more likely to resort to implicit bias under specific circumstances, including when they lack information, experience time pressure, or are distracted or under stress. Taking measures to ensure that these factors are not at work during the evaluation process is essential. There are also a number of best practices that can be used to work around implicit attitudes. For instance, when serving on a hiring committee or awards panel, make sure that a variety of candidates are represented. If the pool lacks diversity, take active steps to deepen it and encourage individuals from underrepresented groups to apply. In any type of evaluation process—including hiring, peer review, appraisals, and promotion it is important for evaluators to establish

clear criteria and ways to weigh their relative importance prior to evaluation. Using those set criteria, take adequate time to review each candidate and consider his/ her qualifications as a whole. When group decision-making is involved, as when serving on a committee, complete your own assessment before hearing the views of others; committee chairs must be aware of power dynamics and allow everyone to share their views. Keep careful notes during the evaluation process and refer back to the preset criteria. A number of organizations, such as SIAM, the NSF, the Association for Women in Science, and the Mathematical Association of America are advocating for the aforementioned measures. Although completely eliminating one's biases might not be possible, appropriate steps can diminish and alter them, thus ultimately increasing diversity in STEM. Having a more diverse workforce taps into a broader talent pool. Perhaps more importantly, diversity in the work-

place and educational settings can promote broader and more creative thinking,

therefore enhancing the science itself.

#### **References**

[1] National Science Foundation & National Center for Science and Engineering Statistics. (2017). *Women, Minorities, and Persons with Disabilities in Science and Engineering: 2017* (Special Report NSF 17-310). Arlington, VA. Retrieved from www.nsf.gov/statistics/wmpd/.

#### **Further Reading**

MacNell, L., Driscoll, A., & Hunt, A.N. (2015). What's in a name: Exposing gender bias in student ratings of teaching. *J. Coll. Barg. Acad., 0*(53), 1-13.

*Robin O. Andreasen is an associate professor in the Department of Linguistics and Cognitive Science and research director of UD-ADVANCE at the University of Delaware.*

## **Mitigating Bias**

*Continued from page 4*

# **The Mathematics of Seeing Clearly: Deblurring Images for National Security**

#### *By Annette Hilton and Amanda Freuler*

A blurred image is often only a minor nuisance to photographers and everyday social media enthusiasts. But as Derek Jung learned as a graduate student intern in the National Science Foundation's (NSF) Mathematical Sciences Graduate Internship  $(MSGI)$  Program,<sup>1</sup> a blurry image becomes much more serious in the context of national security. Research designed to deblur images is vitally important to national security efforts, which attempt to identify unknown sensitive materials captured in photographs. Jung, a mathematics doctoral student at the University of Illinois at Urbana-Champaign, was tasked with finding a solution to deblur images.

> To find out more about these experiences and further opportunities in STEM, visit the ORISE website.2 ORISE supports the DOE and other federal agencies' missions to strengthen the nation's science education and research initiatives. ORISE is managed for the DOE by Oak Ridge Associated Universities. Applications are now open for the NSF's 2018 MSGI Program.<sup>3</sup>

The MSGI Program provides research opportunities and hands-on experience in the application of mathematics in nonacademic settings for Ph.D. students via internships at federal national laboratories, industries, and other facilities.

"I do mathematics because it helps me grow personally and build relationships," Jung said, reflecting on his decision to pursue the subject. "I'm allowed to think for hours about a problem, take regular walks around campus, and I'm apparently doing my job! Solving a problem leads to pride and self-confidence, while toiling for months is accompanied by support from my peers and family."



University of South Carolina doctoral student Erik Palmer returned to his hometown of *Berkeley, Calif., to perform research at Lawrence Berkeley National Laboratory. His work was made possible by the National Science Foundation Mathematical Sciences Graduate Internship Program. Photo used with permission.*

<sup>1</sup> https://orise.orau.gov/nsf-msgi/

While appointed to the Nevada National Security Site's Signal Processing and Applied Mathematics team north of Las Vegas, Jung integrated his mathematics background with an industry environment for the first time. To develop a solution for deblurring images, he first sought to understand how they become blurred. With the help of mentors Aaron Luttman and Kevin Joyce, Jung investigated model theories about the functioning of blurred images and attempted to prove their functionality with math. He based his research on measure theory, functional analysis, and harmonic analysis — all forms of advanced calculus that seek to describe spaces.

Focusing on key gaps in existing research, Jung made significant contributions that will soon be ready for publication. He continued to pursue new ideas to clarify blurry images after his return to the University of Illinois. When presenting his research to colleagues, Jung received a fresh perspective and suggestion, which he used to devise a solution to the last remaining gaps in the problem. His successful research contributes

to efforts to find and identify sensitive materials, thus advancing national security. "Before this summer

internship, I never had experience in applying mathematics to the real world,"

Jung said. "My background was pure mathematics, and I thought it would be difficult to find an opportunity to apply my skills in an industry setting. The experience was spectacular and unique; it was unbelievable how the NSF's MSGI Program set me up with a project and location that enabled me to contribute and feel comfortable."

> Luttman, Joyce, and Jung plan to submit their research to the *Journal of Mathematical Analysis and Applications*. Jung expects to receive his doctorate in 2019 and hopes to begin a postdoctoral position. He would

eventually like to teach at a university or conduct research at a federal laboratory.

Jung was among 40 doctoral students to benefit from the NSF's MSGI Program, all of whom were awarded spots for 10 weeks at federal laboratories, industry-based locations, and other approved facilities. Funded by the NSF, the The MSGI Program is administered through the U.S. Department of Energy's (DOE) Oak Ridge Institute for Science and Education (ORISE).

Erik Palmer of the University of South Carolina was inspired to pursue opportunities within the national laboratory system during a local SIAM student chapter talk. While stationed at Lawrence Berkeley National Laboratory, Palmer contributed to efforts to improve understanding of multiphase flows — the movement of materials with different states or phases. Multiphase flow research is used in a variety of applications, including advancing clean and efficient energy, delivering more precise medical therapies, and optimizing waste treatments.

At Lawrence Livermore National Laboratory, Benie Justine N'Gozan of the University of Texas, Arlington spent her

time developing new statistical learning algorithms to interpret complex machine learning models. Her research helps improve machine learning models—used widely in areas such as business and healthcare—that predict future events.

Steven Reeves of the University of California, Santa Cruz spent his time at Lawrence Berkeley adapting an existing cosmology simulation code to incorporate the influence of magnetic fields. The code, which is run on some of the world's largest supercomputers, is used to simulate the formation of structures throughout the universe.

*Annette Hilton holds a bachelor's degree in geology and is currently employed as an intern in the Scientific Assessment and Workforce Development unit of Oak Ridge Associated Universities (ORAU). Amanda Freuler received her bachelor's degree in mass communication from Middle Tennessee State University. She currently serves as ORAU's Communications and Marketing intern.*

<sup>3</sup> https://www.zintellect.com/Posting/ Details/3602



*Derek Jung, a doctoral student at the University of Illinois at Urbana-Champaign, takes a break from research to visit Nellis Air Force Base in Nevada during the National Science Foundation Mathematical Sciences Graduate Internship Program. Photo used with permission.*

CAREERS IN MATHEMATICAL SCIENCES

<sup>2</sup> https://orise.orau.gov/index.html

# **The Clever Mathematics Behind Wall Street Intrigue**

**The Money Formula: Dodgy Finance, Pseudo Science, and How Mathematicians Took Over the Market.** *By Paul Wilmott and David Orrell. Wiley, Cornwall, UK, June 2017. 264 pages. \$34.95.*

 $A$ <sup>s</sup> with almost everything else, mathe-<br>matics can be corrupted by big money. *The Money Formula: Dodgy Finance, Pseudo Science, and How Mathematicians Took Over the Market* lays bare the mathematical abuses behind the trillion-dollar swindles in London and on Wall Street. These are the false assumptions and claims used to bait both investors and the public, the "innovations" (mathematical models and algorithms) that hide risk and shift it to consumers while pretending to do the opposite. Meanwhile, greed, corruption, and regulatory capture—among other things—seem to prevent beneficial reforms from occurring. The lack of enforced ethical standards in economics and finance is no accident, and the possibility of even bigger financial crashes and scandals looms in the future.

Authors Paul Wilmott and David Orrell are both respectable applied mathematicians, writers, and critics. Wilmott is the consummate insider (or "quant") while Orrell is the outsider, having already tackled academic economics in his insightful book *Economyths*. Their chatty dialogue explains the key role of the Black-Scholes formula in setting realistic prices for various kinds of financial options but also emphasizes its limitations, so often ignored in practice. The authors are astonished by the number of quants who actually believe in the *efficient market hypothesis*, and note how it excuses all manner of selfish behavior; the extraordinary pay and bonuses don't hurt.

Wilmott exposes a litany of "mathematical tricks for betting on the markets," noting that traditional quant concepts like *modern portfolio theory* and *value at risk* tend to

"fail just when you need them most…when apparent stability breaks down." However, he notes that hedge funds are good at looking "for small pockets of predictability… while they last." They mostly exploit financial derivatives, which are

often "used to make highly leveraged bets — so models are critical for risk assessment." Wilmott's description of the now-infamous *collateralized* 

*debt obligations* and *credit default swaps* reveals that these derivatives functioned

as a kind of pyramid scheme to shift risk from insiders at the top of the pyramid to dupes at the base, with toxic mortgages camouflaged by corrupt credit rating agencies. Yet the mystique of the clever mathematics has served, quite literally, as "the perfect get-outof-jail card."

Meanwhile, Orrell wonders at the feasibility of modeling markets as a type of physical system (à la Issac Newton). The empirical and mathematical answer is that markets exhibit "complex dynamics that resist numerical predic-

tion," with power law distributions replacing





The summer school aims to introduce graduate student



**ASSOCIATION FOR WOMEN IN MATHEMATICS** 

## **Membership**

Has your department found it difficult to hire women? Do you have a female family member, student, or friend thinking about a career in mathematics? Do you hope they will find the support and environment they need to thrive?

Then it's time to join the Association for Women in Mathematics (AWM) (The membership year is October 1 through September 30).

Individual members of SIAM qualify for reciprocal membership rates in the AWM. AWM welcomes both men and women as members. Show your support by going to **WWW.awm-math.org** and joining AWM today!

## **Corporate Sponsorship**

AWM is the largest, most effective organization providing support and encouragement for female students in the mathematical sciences at the college and graduate school level. These women provide a prime talent pool for STEM careers.

Organizations and companies can help AWM achieve its goals by becoming a Corporate Sponsor of the AWM. Sponsorship includes benefits, such as free ads in our Newsletter and on social media, designed to bring sponsors in contact with our membership.

See www.awm-math.org for details about becoming a corporate sponsor and for a list of potential Executive Sponsorship Opportunities.

# **Support AWM!**

to the mathematical and computational aspects of inverse problems, particularly modern developments that emphasize the quantification of uncertainty in the inverse solution within the framework of Bayesian inference. The target audience is PhD and appropriate MS students in mathematics and related fields

such as computer science, statistics, engineering, and science.

Application Deadline: February 1, 2018 More information posted at http://www.siam.org/students/g2s3/

Gaussians — not at all surprising in view of the variety of irrational actions identified by behavioral economists like Daniel Kahneman and Amos Tversky. Even savvy investors need to heed John Maynard Keynes' admonition that "markets can remain irrational longer than you can stay solvent." Wilmott

and Orrell cite mathematical biology as a better example of applied mathematics. Good biological models are not based on Newton-type scientific laws; instead, statistics and observations inform simple math-

> ematical formulae that offer key qualitative insights into particular situations. In finance and economics, such models could be tailored to

the chaotic patterns of real-world economic behavior (booms, busts, unpredictability, etc.) and some such attempts have been

made, along the lines of *The Origin of Wealth* by Eric Beinhocker.

In the future, we might also get insights and guidance from comprehensive explorations and simulation of big data using higherdimensional nonlinear networks and systems, despite their black box nature. For example, hurricane tracking is done manually by eyeballing a selection of Monte Carlo simulations of complex forces and building off past experience. Why not employ similar methods for economic and financial forecasting to continually update vast-

ly more realistic models of risk?

Wilmott and Orrell fail to mention one of our biggest challenges — the need to identify and utilize better tools, not just interest rates, to guide the economy. For example, Modern Monetary Theory provides a sound basis for restoring the tools of fiscal policy in general, and the government as *employer of last resort* in particular. In *With Liberty and Dividends for All: How to Save Our Middle Class When Jobs Don't Pay Enough*, Peter Barnes demonstrates universal ownership of wealth-generating assets for the same purpose. In addition, the Federal Reserve could be pouring money directly into infrastructure public banks to develop renewable energy, affordable housing, and public transit, instead of pumping it into Wall Street to support speculation.

In essence, financial economics could be facilitating the economy we need, rather than an economy of greed. While the authors do hint at the possibility of monetary reform, they mostly offer worthy (but familiar) prescriptions, such as breakup of big banks, stronger regulation, a financial transaction tax, simplicity, and transparency. The need for a political revolution to overcome big money's power to resist even the most commonplace reforms is the unaddressed problem. Strangely, Wilmott and Orrell do not cite other insider critiques, such as Yves Smith's blog—"NakedCapitalism. com"—or *ECONned: How Unenlightened Self Interest Undermined Democracy and Corrupted Capitalism*, her book focused on the 2008 financial crash. Ultimately though, *The Money Formula* does offer quantitative types a much better understanding of what we're up against, and provides an opening for some "beyond Wall Street" sequels.

*Richard H. Burkhart received his Ph.D. in mathematics at Dartmouth College in 1976. He then taught at the University of North Carolina at Wilmington before moving back to his home territory, Seattle, where he worked for Boeing in scientific and engineering computing and algorithm development for 21 years. He took early retirement to become a full-time activist and independent researcher, especially in the areas of democracy and economics.*



WILEY

*The Money Formula: Dodgy Finance, Pseudo Science, and How Mathematicians* 

*Took Over the Market. By Paul Wilmott and David Orrell. Courtesy of Wiley.*

BOOK REVIEW *By Richard H. Burkhart*

# **A Water-based Solution of Polynomial Equations**

I would like to describe a "hydrostatic" calculator of roots—at least of positive real ones—of a polynomial of any degree. As a pure thought experiment, let us cut the shapes shown in Figure 1 out of a sheet of weightless styrofoam. The *n*th shape displaces the volume  $x^n$  when submerged to depth *x*, provided the thickness of the sheet  $=1$ . Now our "calculator" (see Figure 2) consists of a weightless rod with the "origin" 0 marked on it. The styrofoam monomials can be affixed at any position on the rod. In addition, the trivial monomial  $x^0$  = 1 is represented by a unit weight that can be slid to any position on the rod.

with positive  $a, b, c,$  and  $d$ . We let these coefficients and the signs determine the locations of the monomials on the rod, as shown in Figure 2. Since it is not buoyant but weighty, the constant term fol-

As an illustration, let us solve

 $ax^3-bx^2+cx-d=0,$  (1)



**Figure 2.** *Solving (1) by dunking the "scale.* 

lows the opposite rule: the minus sign in front of *d* places it to the right of 0.

With the "calculator" thus prepared, we hold the rod horizontally and slowly dunk

Data analysis requires a variety of tools, and one of the foundational tools for unsupervised analysis and data reduction is principal component analysis (PCA). Researchers use PCA to analyze data matrices where the rows correspond to objects and the columns correspond to features, so that the  $i, j$  entry is the measure of feature *j* for object *i*. After some preprocessing, PCA then reduces to apply the

To understand why this method works, note that the polynomial

 $ax^3-bx^2+cx-d$  is the torque relative to 0 of the forces acting upon the rod (see Figure 3). Therefore, the vanishing of the torque for a particular depth *x* amounts to  $x$  being a root of (1).

it *until the torque we exert with the hand to keep the rod horizontal becomes zero*, i.e., until our scale balances. The depth *x* that provides this balance is a root of (1). MATHEMATICAL **CURIOSITIES** *By Mark Levi*

Of course, all of the above applies to polynomials of any degree, although this method only produces positive real roots.

*The figures in this article were provided by the author.*

*Mark Levi (levi@math.psu.edu) is a professor of mathematics at the Pennsylvania State University.*



During the SIAM Invited Address<sup>1</sup> at the Joint Mathematics Meetings, to be held in San Diego, Calif., from January 10-13, 2018, I will demonstrate the wide-ranging utility of the CP tensor decomposition with



## **Tensor Decomposition: A Mathematical Tool for Data Analysis**

**During the SIAM Invited Address at the Joint Mathematics Meetings, Tamara Kolda will** *discuss the use of tensor decomposition, an extension of principal component analysis, to examine data.* 

singular value decomposition to the matrix. We can use the resulting matrix factors for data interpretation, unsupervised learning, dimensionality reduction, completion of missing entries, and more.

The problem occurs when deciding how to handle data that is not twoway. Imagine the previous scenario (object and features), except that now we take repeated measurements in time; this becomes a three-way data

array. We could average the features over time or just stack them all together, but these solutions tend to be unsatisfactory because understanding the relationships influenced by the time dimension becomes impossible. Using tensor decompositions, an extension of PCA to higher-order data, is the alternative. In fact, we need not stop at three-way data, but can handle four-way, five-way, and much higher as well. There are a variety of tensor decompositions, but I focus on canonical polyadic (CP) tensor decomposition, introduced by Frank

Lauren Hitchcock in 1927 but nearly lost to history until its rediscovery in 1970 under the name CANDECOMP by J. Douglas Carroll and Jih-Jie Chang and the name PARAFAC by Richard A. Harshman.

examples in neuroscience



Björn Sandstede will talk about nonlinear patterns and waves at the 2018 SIAM Annual *Meeting.* **Left.** *A planar spiral-wave profile.* **Right.** *The differences of spectra on unbounded (solid curves) versus bounded domains (black circles). Image courtesy of Stephanie Dodson.*

and chemical detection. Of course, multiway data usually means more data, which leads to not only more insights but also more problems. One such problem is the possession of too much data to process efficiently. The use of randomized methods offers a solution to this dilemma. I will present a novel randomized method (based on matrix sketching) for fitting the CP decomposition to dense

data that is more scalable and robust than standard techniques. I will further consider the modeling assumptions for fitting tensor decompositions to data and explain alternative strategies for various statistical scenarios, resulting in a generalized CP tensor decomposition that we can fit using a different randomized method (based on

stochastic gradient descent).

— *Tamara G. Kolda, Sandia National Laboratories*

1 https://tinyurl.com/ybtgw7w8



*Tamara G. Kolda, Sandia National Laboratories.*

## **Nonlinear Patterns and Waves: From Spectra to Stability and Dynamics**

Patterns and waves are all around us. Stripes and hexagonal patterns appear on animal coats, as water waves on lakes, on sand dunes in deserts, or in cloud patterns in the sky. Besides being aesthetically pleasing, they often serve important beneficial or detrimental functions. For instance, coherent structures organize transport and mixing in geophysical fluid flows and help facilitate spatial differ-

entiation during the early development of organisms, but they can also lead to tachycardia via reentrant cardiac arrhythmias caused by spiral waves in cardiac tissue.

Perhaps surprisingly, patterns and waves occur in many different systems and on vastly different scales in both time and space, and their dynamic behavior is similar across these systems. Mathematical techniques can help identify the ori-

gins and common properties of patterns and waves across various applications. Understanding the ways in which such structures are created can help experimentalists identify the mechanisms that generate them in specific systems; in the case of tachycardia, mathematics may also aid the design of new, less invasive

treatments to remove reentrant waves from cardiac tissue.

Despite many advances, understanding patterns and waves still poses significant

mathematical challenges. To illustrate the difficulties, consider a case in which one has developed a partial differential equations (PDE) model and is interested in assessing the stability of a spiral-wave pattern under small perturbations of its shape. A common strategy in dynamicalsystems theory computes the Jacobian of the model evaluated at the underlying pattern, studies its spectrum, and draws

core in the spiral wave's center is challenging, even on the linear level.

conclusions about the nonlinear dynamics based on the spectral properties of this linear differential operator. Using this approach for spiral waves is complicated. For instance, these spectra do not change continuously on the linear level when going from unbounded to large but bounded domains. Furthermore, disentangling the effects of the spiral arms' modulations in the far field from the movement of the *Björn Sandstede, Brown* 

> At the 2018 SIAM Annual Meeting, to be held July 9-13 in Portland, Ore., I will show how geometric dynamical systems ideas combined with PDE approaches can shed light on the stability and dynamics of spiral waves and many other patterns

> and nonlinear waves. I will also discuss applications and open problems.

*–– Björn Sandstede, Brown University*



*University.*

# **FOUND: Title Sponsor** Math Modeling Challenge \$100,000 Scholarships

 $\begin{array}{c} + \\ x + \\ y + \\ z \end{array}$ 



 $\dot{\mathsf S}$ 

# **Curious?**

Follow the story at M3Challenge.siam.org

**Challenge Weekend:** March 2-5, 2018

During Challenge weekend, an open-ended problem is revealed to high school teams and they work together, under time constraints, using the math modeling process to represent, analyze, make predictions and otherwise provide insight into that real-world problem's questions.

# M3Challenge.sia

**Title Sponsor** Announcement: Coming in Dec 2017 **Math Modeling Challenge**  High schools in the U.S., its territories, and DoDEA schools are eligible to participate in M3 Challenge 2018.

The National Association of Secondary School **Principals has placed this program on the NASSP<br>National Advisory List of Student<br>NASSP Contests and Activities since 2010.** NASSP<br>2016-2017

Presented by sıam.

| Society for Industrial and<br>| Applied Mathematics

Sponsored by



#### *By Guo-Wei Wei*

Technological advances in the past<br>
few decades have fueled the exponential growth of "omic" data in biology. Understanding the rules of life from existing omic data sets, which offer unprecedented opportunities for mathematicians, remains an important mission of the field. Biomolecular structurefunction relationship is a major rule of life, and recognizing this relationship is the holy grail of biophysics and a central issue in experimental biology.

Geometric modeling is vital to the comprehension of biomolecular structurefunction relationships. It also bridges the gap between biological data and theoretical models, such as quantum mechanics, molecular mechanics, statistical mechanics, thermodynamics, and multiscale models. However, geometry-based models are frequently inundated with too much structural detail and thus often computationally intractable. Topology provides the ultimate abstraction of geometric complexity by concerning only the connectivity of different components in a space, and characterizing independent entities, rings, and higher-dimensional faces of the space in terms of topological invariants or Betti numbers. To study topological invariants in a discrete data set—like atoms in a biomolecule—algebraic topology utilizes simplicial complexes under various settings, such as the Vietoris-Rips complex, Čech complex, or alpha complex. Specifically, a 0-simplex is a vertex, a 1-simplex an edge, a 2-simplex a triangle, and a 3-simplex a tetrahedron, as illustrated in Figure 1. Algebraic groups built on these simplicial complexes are used in simplicial homology to systematically compute Betti numbers for a given data set [7].

Nevertheless, traditional topology and homology are truly free of metrics or coordinates and thus keep too little geometric information to be practically useful for biomolecules. Persistent homology, a new branch of algebraic topology, embeds multiscale geometric information into topological invariants to achieve an interplay between geometry and topology [14]. It creates a variety of topological spaces of a given object by varying a filtration parameter, such as the radius of balls or the level set of a real-valued function. As a result, persistent homology can capture topological features continuously over a range of spatial scales, and the resulting analysis is often visualized by barcodes [6] or persistence diagrams [5]. As such, the changes of topological invariants over scales are recorded by the "birth," "death," and "persistence" of barcodes over filtration. Persistent homology has been applied to a variety of domains, including image/ signal analysis, chaotic dynamics, sensor networks, complex networks, shape recognition, and computational biology [13].

For nano- and biomolecules, persistent homology enables a quantitative topological analysis—which reveals biomolecular "topology-function relationships"—via



## Are you a professional writer?

Do you like writing about cutting-edge applied mathematical and computational science research? Do you have a background in applied mathematical sciences and experience in scientific writing?

### **SIAM News is looking for writers like you!**

Successful SIAM News writers combine a strong mathematical background with the ability to explain technical concepts to our multidisciplinary audience, all the while piquing reader interest in the broad applications of mathematics.

topological fingerprints (TFs) [9, 11]. Contrary to popular belief, short-lived topological events are not noise, but rather part of TFs; they play a valuable role in the quantitative topological analysis of protein folding stability [9] and fullerene curvature energy [8]. Differential geometry has been utilized to derive partial differential equation-based persistence for biomolecules [8]. Multidimensional persistence induced by a multiresolution analysis [12] is particularly useful for resolving illposed inverse problems in cryo-electron microscopy structure determination [10].

TFs provide biomolecules with a systematic and unique representation that cannot be literally cast into traditional physical interpretation. Fortunately, this representation is ideally suited for machine learning (particularly deep learning), which captures nonlinear and high-order interactions among features in sufficiently large and intrinsically complex data sets. One of the first integrations of machine learning and TFs offered an encouraging classification of tens of thousands of proteins involving hundreds of tasks [4]. However, persistent homology neglects chemical and biological information during topological simplification and is thus not as competitive as geometry or physics-based representation in quantitative predictions. Elementspecific persistent homology, or multicomponent persistent homology built on colored biomolecular networks, has been introduced to retain chemical and biological information during topological abstraction [2]. This approach enciphers biological properties—such as hydrogen bonds, van

der Waals interactions, hydrophilicity, and hydrophobicity—into topological invariants, rendering a potentially revolutionary representation for biomolecules [1, 3].

Rational drug design is an imperative life science problem that ultimately tests our understanding of biological systems. Designing efficient drugs to cure disease is one of the most challenging tasks in the biological sciences. Multicomponent persistent homology plays a crucial role in hot-spot prediction, drug-binding pose analysis, binding affinity prediction, structure optimization, toxicity analysis, and pharmacokinetic simulation. For example, the integration of machine learning with multiscale weighted colored graphs and multicomponent persistent homology provided the best free energy ranking for Set 1 (Stage 2) in D3R Grand Challenge  $2$ ,<sup>1</sup> a worldwide competition in computer-aided drug design.

http://bit.ly/2h4Vm6q

#### **References**

[1] Cang, Z.X., & Wei, G.W. (2017). Analysis and prediction of protein folding energy changes upon mutation by element specific persistent homology. *Bioinform.*, doi: 10.1093/bioinformatics/btx460.

[2] Cang, Z.X., & Wei, G.W. (2017). Integration of element specific persistent homology and machine learning for protein-ligand binding affinity prediction. *Inter. J. Numer. Meth. Biomed. Eng.*, doi:10.1002/cnm.2914.

[3] Cang, Z.X., & Wei, G.W. (2017). TopologyNet: Topology based deep convolutional and multi-task neural networks for biomolecular property predictions. *Plos Comp. Bio., 13*(7), e1005690.

[4] Cang, Z.X., Mu, L., Wu, K., Opron, K., Xia, K., & Wei, G.W. (2015). A topological approach to protein classification. *Mol. Based Math. Bio., 3*, 140-162.

[5] Edelsbrunner, H., & Harer, J. (2008). Persistent homology — a survey. *Cont. Math., 453*, 257-282.

[6] Ghrist, R. (2008). Barcodes: The persistent topology of data. *Bull. Am. Math. Soc., 45*, 61-75.

[7] Kaczynski, T., Mischaikow, K., & Mrozek, M. (2004). *Computational Homology*. In *Applied Mathematical Sciences* (Vol. 157). New York, NY: Springer-Verlag.

[8] Wang, B., & Wei, G.W. (2016). Object-oriented persistent homology. *J. Comp. Phys. 305*, 276-299.

[9] Xia, K.L., & Wei, G.W. (2014). Persistent homology analysis of protein structure, flexibility and folding. *Inter. J. Num. Meth. Biomed. Eng., 30*, 814-844.

[10] Xia, K.L., & Wei, G.W. (2015). Persistent topology for cryo-EM data analysis. *Inter. J. Num. Meth. Biomed. Eng.,* 

Interested writers may email a resume and three science writing samples to sinews@siam.org for consideration.

# sinews.siam.org

**SIAM**. Society for Industrial and Applied Mathematics

*31*, e02719.

[11] Xia, K.L., Feng, X., Tong, Y.Y., & Wei, G.W. (2015). Persistent homology for the quantitative prediction of fullerene stability. *J. Comp. Chem., 36*, 408-422.

[12] Xia, K.L., Zhao, Z.X., & Wei, G.W. (2015). Multiresolution topological simplification. *J. Comp. Bio., 22*, 1-5.

[13] Yao, Y., Sun, J., Huang, X.H., Bowman, G.R., Singh, G., Lesnick, M.,… Carlsson, G. (2009). Topological methods for exploring low-density states in biomolecular folding pathways. *J. Chem. Phys., 130*, 144115.

[14] Zomorodian, A., & Carlsson, G. (2005). Computing persistent homology. *Dis. Comp. Geo., 33*, 249-274.

*Guo-Wei Wei is a professor of mathematics at Michigan State University.*

# **Persistent Homology Analysis of Biomolecular Data**



**Figure 1.** *An illustration of topological invariants (left), basic simplexes (middle), and proteinpersistence barcodes (right).* **Left.** *From top to bottom: a point, a circle, an empty sphere, and a torus. Betti-0, Betti-1, and Betti-2 numbers are, respectively, 1, 0, and 0 for a point; 0, 1, and 0 for a circle; 0, 0, and 1 for a sphere; and 1, 2, and 1 for a torus. Two auxiliary rings are added to the torus to explain Betti-1=2.* **Middle.** *Four typical simplexes.* **Right.** *Topological fingerprint (bottom) for a protein (top). Image credit: Zixuan Cang.*

2018

#### **Georgia Institute of Technology** *School of Mathematics*

The School of Mathematics at Georgia Tech is accepting applications for **tenure-track faculty in statistics**. Applications by highly-qualified candidates, and especially those from groups underrepresented in the mathematical sciences, are particularly encouraged. See **www.math.gatech.edu/resources/employment** for more details

and application instructions.

#### **Georgia Institute of Technology** *School of Mathematics*

The School of Mathematics at Georgia Tech is accepting applications for **non-tenure track post-doc faculty in pure and applied mathematics and statistics**. Applications by highlyqualified candidates, and especially those from groups underrepresented in the mathematical sciences, are particularly encouraged. See **http:// math.gatech.edu/employment-opportunities** for more details and application instructions.

#### **Georgia Institute of Technology**

*School of Mathematics*

The School of Mathematics, in cooperation with the Transdisciplinary Research Institute for Advancing Data Science (TRIAD) at Georgia Institute of Technology, is accepting applications for a **postdoctoral position within TRIAD on interdisciplinary and foundational research of data sciences applications** by highly-qualified candidates. Applications especially from groups underrepresented in the mathematical sciences are particularly encouraged. See **https:// www.isye.gatech.edu/about/employmentopportunities/postdoctoral-position-georgiatech** for more details and application instructions.

**Northwestern University** *Department of Engineering Sciences and* 

*Applied Mathematics* **Overview:** The Department of Engineering Sciences and Applied Mathematics is soliciting applications for a **postdoctoral fellowship in quantitative biological modeling** that will be available starting September 1, 2018. This position is part of a National Science Foundation Research Training Grant (NSF-RTG). **Duties:** The postdoctoral fellow will conduct research on the quantitative modeling of biological systems and teach three quarter courses per year in the department. The position will typically be for three years. Additionally, the postdoctoral fellow will participate in RTG-related training and career development activities.

S IAM has initiated a new Science Policy<br>
S Fellowships Program to engage earlycareer professionals in science policy and advocacy. The fellowship recipients will learn about the workings of science policy as it pertains to our discipline by participating in SIAM's Committee on Science Policy (CSP) meetings and conducting relevant activities to further SIAM's science policy efforts.

The winners of the fellowships, which will begin January 1, 2018, are as follows:

> **Environment:** The postdoctoral fellow will be part of an interdisciplinary environment focusing on current problems in experimental and computational biology. The fellow will gain experience from training in mathematical modeling, numerical methods, and modern data analysis/statistical tools relevant to biological problems. Research internships outside of Northwestern will broaden the fellow's perspectives. The fellow's research will be mentored by faculty from both applied mathematics and a biological discipline. Ongoing collaborations exist with faculty in neurobiology, molecular biosciences, environmental engineering, and preventive medicine, and additional areas of interest are welcome. An overall goal of the program is to broaden computational biological modeling in the department and at Northwestern.

> **Requirements:** Applicants must be U.S. citizens or permanent residents. Interested candidates should submit a curriculum vitae, three reference letters (one addressing teaching qualifications) and brief research and teaching state-

The 2017 Germund Dahlquist Prize was<br>awarded to Per-Gunnar Martinsson at the 2017 International Conference on Scientific Computation and Differential Equations, held September 11-15, 2017 at the University of

> ments online at the following URL: **https:// openposition.mccormick.northwestern.edu/ apply/index/NjY=**. If desired, one or two representative publi-

cations may also be submitted. For full consideration, applications should be received by January 5, 2018.

Northwestern University is an Equal Opportunity, Affirmative Action Employer of all protected classes including veterans and individu-

als with disabilities. Women and minorities are encouraged to apply.

**Direct inquiries about this position to:**  Hermann Riecke, Engineering Sciences and Applied Mathematics, Northwestern University, 2145 Sheridan Road Evanston, IL 60208-3125. **Phone:** (847)-491-3345. **Email:** h-riecke@ northwestern.edu. **http://www.mccormick. northwestern.edu/applied-math/**.

#### **The Chinese University of Hong Kong, Shenzhen**

*School of Science and Engineering*

The Chinese University of Hong Kong, Shenzhen [CUHK(SZ)] is seeking a professor/associate professor/assistant professor/lecturer in the School of Science and Engineering. CUHK(SZ) is a research university located in the Longgang District of Shenzhen and established in 2014 through a Mainland-Hong Kong collaboration, with generous support from the Shenzhen Municipal Government. CUHK(SZ) confers academic degrees and inherits the fine academic traditions of the Chinese University of Hong Kong. The university is developing academic programs in phases and currently offering courses in the Schools of Science and Engineering, Management and Economics, and Humanities and Social Science. English is the main language for course instructions.

## **SIAM Science Policy Fellowships**

• Natalie Sheils, *University of Minnesota* • Sheri Martinelli, *Pennsylvania State University*

• Robert Edman, Adventium Labs • Rosalie Belanger-Rioux, Massachusetts Institute of Technology

• Emily Evans, *Brigham Young University*

• Jason Pries, *Oak Ridge National Laboratory*

• Sucheta Soundarajan, *Syracuse University*

Fellowships will pay for travel to the biannual SIAM CSP meetings. Each spring, the CSP meets with representatives of agencies (such as the National Science Foundation and the Department of Energy) relevant to our discipline and visits congressional offices to promote the importance of research funding, graduate training, and undergraduate education in applied mathematics and computational science.

During the fall meeting, the CSP meets with agency representatives and formulates priorities for the following year.

Fellows will also participate in training and webinars to explore various facets of science policy and advocacy, learn how to effectively communicate science, and engage with policy makers on topics of interest to the SIAM community.

— *James Crowley, executive director of SIAM*



THEIR REFERRAL, YOU'LL GET A SIAM T-SHIRT FOR YOUR EFFORTS!\*

excludes students

**SIAM**. SOCIETY for INDUSTRIAL and APPLIED MATHEMATICS

Bath, U.K. The Germund Dahlquist Prize is awarded for original contributions to fields

associated with Swedish mathematician Germund Dahlquist, especially the numerical solution of differential equations and numerical methods for scientific computing.

"The pioneering work of Germund Dahlquist has been an inspiration to me for a long time," Martinsson said. "He played a key role in establishing numerical analysis as an area of particular research excellence in Sweden, and I was

opportunity to start my studies in applied mathematics in that environment."

The prize honors Martinsson for fundaand scientific computing that

mental contributions to numerical analysis

are having a significant impact in data science applications. The prize committee cites two of Martinsson's contributions

in particular: (1) the development of linear time algorithms for dense matrix opera-

tions related to multidimensional elliptic partial differential equations and integral equations, and (2) deep and innovative contributions to the development of probabilistic algorithms for the rapid solution of certain classes of large-scale linear algebra problems.

"The speed of any computational task depends in part on how fast the hardware is and in part on how effective our algorithms are," Martinsson

said. "Getting faster algorithms for solving common linear algebraic tasks means

very fortunate to have the *of Oxford.*

that we can now perform much more accurate computational simulations of physical phenomena since we can include more details and work with more realistic models. The computational tasks on which we have been focusing are also core building blocks in machine learning and data mining, so this has led to better search algorithms, smarter smartphones, faster algorithms for genomics, etc."

Martinsson is currently Professor of Numerical Analysis at the University of Oxford. He received his Ph.D. in computational and applied mathematics in 2002 from the Institute for Computational Engineering and Sciences at the University of Texas at Austin.

"I am very enthusiastic about the new methods that my collaborators and I have developed over the last several years," Martinsson said. "Besides providing new tools for computational scientists, I hope that these results have opened up possibilities for new exciting research at the interfaces between mathematics, numerics, and applications. If this award helps to draw attention to randomized methods and fast direct solvers, then that would be very exciting."



## **Visiting Assistant** Professorships

The Department of Mathematics in the College of Arts and Sciences at The Ohio State University is accepting applications for Hans J. Zassenhaus (ZAP), Arnold Ross (RAP) Visiting Assistant Professorships and one Visiting Assistant Professorship in Scientific Computation (VAP-SC).

Pending approval, these positions would be available effective Autumn Semester 2018. These term positions are renewable annually for up to a total of three years. The emphasis of ZAPs and the VAP-SC is teaching and research, while RAPs focus primarily on teaching. While teaching loads are subject to change, the teaching load for a ZAP or a VAP-SC is 2-1 (two courses in the autumn and one in the spring semester). A RAP will be expected to teach one course and two recitations (or equivalent assignment) each semester.

Qualifications: All candidates are required to have a Ph.D. in mathematics and to present evidence of excellence in teaching and research.

> **Applicant Instructions:**<br>All candidates should apply online at http://www.mathjobs.org.

A complete application consists of a cover letter, curriculum vitae, research and teaching statements, and three letters of reference. Inquiries may be directed to Denise Clark at **clark.879@osu.edu.** Applications will be considered on a continuing basis, but the annual review process begins October 16, 2017.

The Ohio State University is an equal opportunity employer. All qualified applicants will receive consideration for employment without regard to race, color, religion, sex, sexual orientation or gender identity, national o

SIAM PRIZE SPOTLIGHT

# **2017 Germund Dahlquist Prize**



*Send copy for classified advertisements and announcements to: marketing@siam.org; For details visit www.siam.org/advertising.*

*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*.

## Professional Opportunities and Announcements

**Post Specifications: The School of Science and Engineering** (**http://sse.cuhk.edu.cn/en**) invites applications for faculty positions in focused areas of **statistical science**, **data science**, **mathematics**, **financial engineering** and **quantitative finance**, and **bioinformatics**, though excellent applicants in all related areas will be considered.

Junior applicants should have **(i)** a Ph.D. degree (by the time of reporting to duty) in related fields and **(ii)** high potential in teaching and research. Candidates for associate and full professor posts are expected to have demonstrated academic leadership and strong commitment to the highest standards of excellence. Appointments will normally be made on a contract basis for up to three years initially, leading to longer-term appointment or tenure later subject to review. Exceptional appointments with tenure will be considered for candidates of proven abilities. **Salary and Fringe Benefits:** Salary will be comparable to international standards and commensurate with experience and accomplishments. Employee benefits will be provided according to the relevant labor laws of the People's Republic of China as well as CUHK(SZ) regulations. Subsidies from various government-sponsored talent programs will also be made available to eligible candidates (see **http://www.cuhk.edu. cn/UploadFiles/talentsProgramoutline.pdf**). An application package, including a CV and personal statements in teaching and research, as well as contact information of three references who will write recommendation letters on behalf of the candidate, should be sent via email to **Talents4SSE@cuhk.edu.cn**. All applicants need to specify the rank(s) of the position being applied to in their application cover letters. Upon submission of applications, applicants should request three recommendation letters to be directly sent to **Talents4SSE@cuhk.edu.cn**.

# **Direct Current Transmission and the Future of Electricity**

#### *By James Case*

In the not-too-distant-future, the U.S. will<br>ipoin the growing community of nations In the not-too-distant-future, the U.S. will that save money and energy by transporting electricity through direct current (DC) rather than alternating current (AC) transmission lines. The 700-mile-long Plains & Eastern Clean Line will supply the 9 million customers of the Tennessee Valley Authority with 3,500 megawatts (MW) of electric power from the wind farms of the Oklahoma panhandle. Operating at 600 kilovolts instead of the usual 400, the highvoltage direct current (HVDC) line will also supply Pope County, Ark., with an additional 500 MW.

HVDC transmission line losses are quoted at less than three percent per 1,000 km, some 30-40 percent lower than AC lines operating at similar voltages. The lineloss advantage is even greater for ultrahigh-voltage direct current (UHVDC) lines. Neither advantage is high enough to justify the use of HVDC or UHVDC lines over traditional distances, but both are well worth exploiting for the longer distances that wind and solar power will soon need to travel to link the sunniest and windiest parts of the planet with existing population centers. Long-distance DC lines are also cheaper to build than AC lines because DC cables can carry significantly more power than AC cables of equal cross section — largely due to something known as the "skin effect." Among other things, this permits reduction of the supporting pylons' footprint.

"Skin effect" refers to the fact that the distribution of AC in a cylindrical conductor is far from uniform, as indicated in Figure 1. In reality, the current density decreases exponentially from the surface toward the central axis. The "skin depth" *d* is defined as the depth at which the current density is just 1/*e* (about 37 percent) of the value at the surface. This varies from one installation to another, depending on the frequency of the current and the electromagnetic properties of the conductor itself.

Like most other HVDC and UHVDC lines, the Plains & Eastern Clean Line will accept low-voltage AC from nearby wind farms at the Pioneer Sky Energy Center outside Guymon, Okla., step it up to the required voltage via conventional transformers, convert it to DC, and ship it (in this case) eastward. At the Delta Landing Energy Center in Millington, Tenn.—not far from Memphis—the process will be reversed. Arriving high-voltage DC will be "inverted" into AC, stepped down to conventional voltages, and injected into the local power grid for use by existing cus-

tomers. In addition, the Traveler Junction Energy Center in central Arkansas will siphon off and invert roughly an eighth of the power, delivering it for use in nearby Oklahoma. GE Energy Connections has been chosen to build the converter stations for the Plains & Eastern Clean Line.

To transform AC to DC and back, the energy centers will use banks of *thyristors*, similar to the ones long used as logic gates in electronic circuitry before finding application in the power transmission industry. Thyristors differ from transistors in that they comprise four (rather than two) alternating blocks of N- and P-type semiconducting material. They have an anode A at one end, a cathode C at the other, and a gate connected by wire to the P block nearest the cathode (see Figure 2).

Thyristors can be at rest in either an "open" (conducting) or "closed" (nonconducting) state, and can toggle back and forth between the two states using signals received via the gate wire. Once placed in a particular state, they tend to remain "locked" in that state until switched to the other by a signal. Because thyristors are individually small, entire buildings of them are required to rectify and invert industrialstrength currents. They are also expensive; the converter stations along the Plains & Eastern Clean Line will cost approximately one billion dollars, roughly 40 percent of the entire project's budget.

Although thyristor installations can both rectify and invert electrical currents, most HVDC and UHVDC power lines are optimized—as is the Plains & Eastern Clean Line—for transmission in one direction only. The HVDC line beneath the English Channel, intended to send excess U.K. production to France and vice versa, is an exception. Despite the short distance separating the two nations, DC transmission is economical because AC line losses are exaggerated by underwater transmission. For similar reasons, several other shorthaul underwater DC transmission lines such as the Sardinia-Italian mainland line, which also provides power to the island of Corsica—operate in parts of Europe. DC transmission can also connect incompatible grids, such as one operating at 50 hertz (as is common in much of Europe) with another operating at 60 hertz.

 $A$  lgebraic vision is an emerging view-<br>point of geometric problems in computer vision that aims to examine polynomial models through the lens of algebra. Modeled as problems in applied algebraic geometry, the fundamental questions take

> The U.S. will hardly be the first country to reap the benefits of DC transmission over long distances. China began its exploitation of UHVDC technology in 2010 with the completion of an 800-kilovolt line with 6,400-megawatt capacity—from the Xiangjiaba Dam in remote Yunnan province to Shanghai. The Jinping-Sunan line, completed in 2013, carries 7,200 MW of power from hydroelectric plants along the Yalong River in Sichuan province to coastal Jiangsu province. Presently under construction is a 12,000 MW line from coal and wind-rich regions in the far northwest to Anhui province, 2,000 miles away in the east. While 75 percent of China's coal is located in the far north and west of the country and 80 percent of its hydroelectric power is in the southwest, most of the country's vast population is in the east, thousands of miles from these abundant sources of energy. So successful is China's venture into UHVDC technology that the State Grid Corporation of China, the country's monopolistic electricity utility, has begun building

elsewhere. In 2015, it won a contract to build a 1,500-mile line in Brazil, from the Belo Monte hydropower plant on an Andean tributary of the Amazon to Rio de Janeiro.

India is also climbing aboard the UHVDC bandwagon. When finished and operating at full capacity, its 1,000-mile North East-Agra line will transmit 6,000 MW from Assam to Uttar Pradesh, one of the country's most populous regions. A second line of the same capacity will carry power 875 miles from power plants near coal fields in the northwest, past an intermediate inversion station near New Delhi, to end users in the east. Siemens, General Electric, and the Swedish-Swiss multinational Asea Brown Boveri—rather than State Grid—are building the Indian lines.

50Hertz, the firm that operates the electric power grid in northeast Germany, is currently planning to exploit the pointto-point nature of DC transmission lines. Almost half of the firm's generated power comes from renewable sources, particularly wind. It would like to send much of that power to southern Germany and on into Austria. But any extra power it puts into its own grid ends up energizing the Polish and Czech grids on its way to Bavaria, irritating all those involved.

The proposed solution is a new UHVDC line, known as the SuedOstLink, extending from the shores of the North Sea to an inversion station in Bavaria. Within 10 years, UHVDC lines could stretch from the far north of Sweden to Bavaria, Austria, and much of central Europe. Their creation could even lead to a true UHVDC grid in Europe, in which DC transmission lines connect with one another as well as AC suppliers and servers.

In Asia, an even more ambitious plan is afoot. State Grid intends to have 23 point-to-point UHVDC links in operation by 2030, and is looking for additional opportunities. In March 2016, the company signed a memorandum of understanding with the Russian firm Rosseti, the Japanese firm SoftBank, and the Korea Electronic Power Corporation for the development of a system to move electric power from windswept Siberia to populous Seoul.

Such projects—which are transnational as well as transcontinental—are not without risk. A country that outsources a significant proportion of its electricity generation to another nation invests great trust in the latter's political stability and good faith. A lack thereof appears primarily responsible for the failure of an enterprise called Desertec, intended to connect the Sahara's all-but-limitless potential for solar power generation with European markets. If and when built, such installations will qualify as "supergrids," where HVDC and UHVDC trunk lines connect AC grids *and one another* across natural barriers and national boundaries alike. The command and control of such networks, to account for the day-to-day and even hour-to-hour fluctuations of supply and demand, will be both complex and critical. While the physical know-how to construct such networks already exists, the managerial know-how to keep them operating efficiently over long periods of time has yet to be developed.

*James Case writes from Baltimore, Maryland.*



**Figure 2.** *Schematic diagram of a thyristor. Image credit: James Case.*



**Figure 1.** *Illustration of the skin effect in the cross-section of an alternating current (AC) transmission line. Image credit: James Case.*

## **Algebraic Vision**

on a new life that makes them amenable to algebraic methods in both geometry and optimization. These formulations have resulted in a greater understanding of the structural properties of problems in vision, thus enabling the design of algorithms that exploit structure. Moreover, they have brought the role of real algebraic geometry in such applied problems to the forefront. Problems in vision have also led to exciting and novel advanc-

es in mathematics because of questions that might not have been asked or answered without this external stimulus. A diverse group of researchers—including experts from vision, computational algebraic geometry, classical algebraic geometry, combinatorics, numerics, linear algebra, and optimization—have come together to collaborate on algebraic vision problems.

A key problem in computer vision is the estimation of the three-dimensional shape of a world scene from images and the parameters of the cameras that captured them. This problem, studied under the name *structure from motion* or *multiview* 

*geometry*, has its origins in photogrammetry and perspective drawings. The modeling language for these problems is projective geometry, which naturally leads to polynomial models for multiview geometry. While the needed polynomials are clear in some instances, they may be harder to identify in others. Up to this point, algebraic vision's focus has been in multiview geometry and its immediate relatives.

In my talk at the 2018 SIAM Annual Meeting, to be held July 9-13 in Portland, Ore., I will convey the main philosophy of algebraic vision and illustrate the impact of algebraic methods on some of the foundational problems in vision.

*— Rekha R. Thomas, University of Washington*

![](_page_11_Picture_15.jpeg)

*Washington.*

![](_page_11_Figure_33.jpeg)

*Rekha R. Thomas will discuss algebraic vision and its application to geometry and optimization at the 2018 SIAM Annual Meeting.*