

## A Computationally Efficient Solution of Large-Scale Image Reconstruction Problems

By Paul Davis

During an up-close and personal encounter with medical technology, few patients likely ponder the underlying science. SIAM members might be exceptions, especially those who heard Misha Kilmer of Tufts University speak about image reconstruction at the 2017 SIAM Conference on Computational Science and Engineering (CSE17), held this February in Atlanta, Ga.

Much of Kilmer's work is motivated by diffuse optical tomography (DOT), an imaging protocol that passes near-infrared light through tissue in search of tumors.

Image reconstruction identifies a set of tissue properties that best accounts for the patterns seen in a given image. The medical question is whether those properties signal dangerous tissue anomalies.

The theme of Kilmer's invited presentation at CSE17 was choosing "ingredients for a computationally efficient solution of image reconstruction problems." In effect, she invited the audience to improve critical components of the image reconstruction process in order to deliver better answers more efficiently.

Kilmer identified five categories of "ingredients" drawn from medical imaging,

hydrology, deblurring, and other reconstruction problems that warrant the expert attention of the CSE community:

(i) Representation of images to enhance reconstruction of the particular features that are important in a given setting

(ii) Efficient approximations to the forward model, e.g., efficient computational simulation of the image produced by a hypothetical tissue sample with specific material properties

(iii) Regularization to reduce sensitivity to measurement and computational errors

(iv) Optimization tools to quickly and reliably find the material properties that best explain a given image

(v) Quantification of the uncertainty inherent in noisy inverse problems.

Kilmer focused on the first two: the selection of a "natural image space" within which to describe images, and more efficient evaluation of the computational model for the physical processes that produce them. A well-chosen image space can guide the reconstruction process towards physically reasonable material properties while offering some built-in stability to random error.

Model evaluation consumes the lion's share of the computational time in most image reconstructions. For example, the computation that simulates a DOT image for a given set of tissue properties is the solution of a discretized, time-dependent partial differential equation (PDE). The tissue properties—spatially-varying coefficients of photon diffusion and absorption—appear both as coefficients in the PDE and as the unknowns sought by the image reconstruction. Since the model could be asked to produce an image for every tissue property distribution considered, efficient evaluation of the forward model could pay huge dividends in reducing the time needed for an image reconstruction.

Kilmer and her colleagues have advanced two ideas for modeling the image space: dictionary learning and low-order parameterization. The dictionary approach extracts a catalog of vectorized prototype subimages—of fixed size—from a training image. Given an image requiring reconstruction, machine-learning techniques and a low-rank approximate factorization combine to produce a regularized, approximate rep-

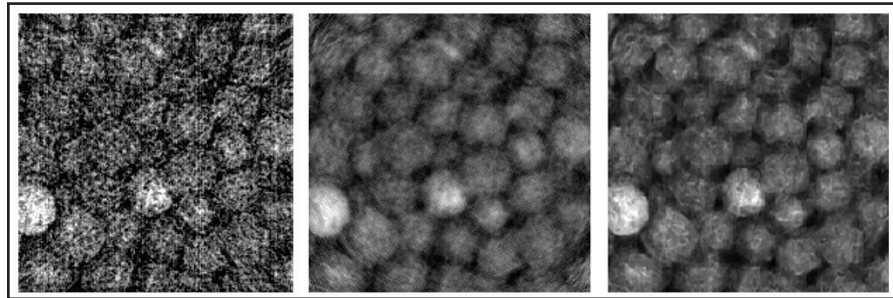


Figure 1. A comparison of reconstructions of an image of peppercorns using three different techniques. Left. Filtered Back Projection. Middle. Classic Tikhonov regularization. Right. A tensor-based form of dictionary reconstruction. Image courtesy of [2]. Image credit: Samuli Siltanen.

See Image Reconstruction on page 3

## Phytoplankton Exhibit Rapid Shape-shifting in Response to Turbulence

By Anupam Sengupta, Francesco Carrara, and Roman Stocker

Phytoplankton are photosynthetic microorganisms that form the base of most aquatic food webs, impact global biogeochemical cycles, and produce half of the world's oxygen. Many species of phytoplankton are motile and migrate through the water column via gravitaxis, directional movement in response to gravity. They move upward toward light during the day and downward toward higher inorganic nutrient concentrations at night [7]. Despite the minute size of individual organisms, phytoplankton's immense numbers make these migrations some of the largest and most important on Earth. Understanding how physicochemical cues from the environment—such as light, nutrients, and turbulence—affect migration greatly impacts our ability to predict the diel vertical migration of phytoplankton. This type of migration contributes significantly to the biological pump, the process driving carbon sequestration from the atmosphere to the deep ocean through sinking particulate organic matter [1].

Ramon Margalef, one of the founding fathers of modern marine biology, was among the first to recognize the fundamental role of turbulence in phytoplankton ecology [6]. Strong turbulence can be detrimental to phytoplankton, as it has the potential to cause flagellar or body wall damage, increased physiological stress, and reduced growth [10]. To cope with environmental stressors such as turbulence and yield adaptive strategies, phytoplankton exploit the intrinsic plasticity of their functional traits [9]. For instance, over the course of several hours in regions of strong turbulence, the dinoflagellate *Ceratocorys horrida* reduces the length of its spines to enhance sinking [11], presumably down to calmer ocean layers, while *Alexandrium catenella* forms chains to alter swimming behavior as an

active response to hydrodynamic shear [4]. However, while scientists have long recognized that turbulence is a primary determinant of plankton fitness and succession, it is unclear whether phytoplankton can actively respond to turbulence over behavioral timescales. Given that turbulent disturbances can be highly localized and intermittent [5], it is possible that phytoplankton evolved avoidance mechanisms by modulating migration based on turbulent cues.

Over the past decade, the interaction of phytoplankton motility with fluid flow has drawn major attention from both the biology and physics communities. This has led to a deeper understanding of how fluid mechanical cues in the ocean impact the vertical migration of phytoplankton. For example, fluid flow can cause gravitactic cells to form thin layers [3] and microscale patchiness [2]. Recent work indicates that members of two major groups of phytoplankton, raphidophytes and dinoflagellates, display an active, behavioral response to repeated overturning events—imposed through the flipping of an experimental chamber and representative of turbulent cues associated with the smallest turbulent eddies in the ocean [8]. The typical range of values for ocean turbulence lies between  $10^{-9}$  and  $10^{-5}$  W/kg [5], which corresponds to a Kolmogorov timescale  $\tau_K = (\nu \epsilon)^{1/2}$  in

the range 0.1-30 s, where  $\epsilon$  is the energy dissipation rate and  $\nu$  the kinematic viscosity of seawater. Small-scale eddies are experimentally generated by overturnings

See Phytoplankton on page 4

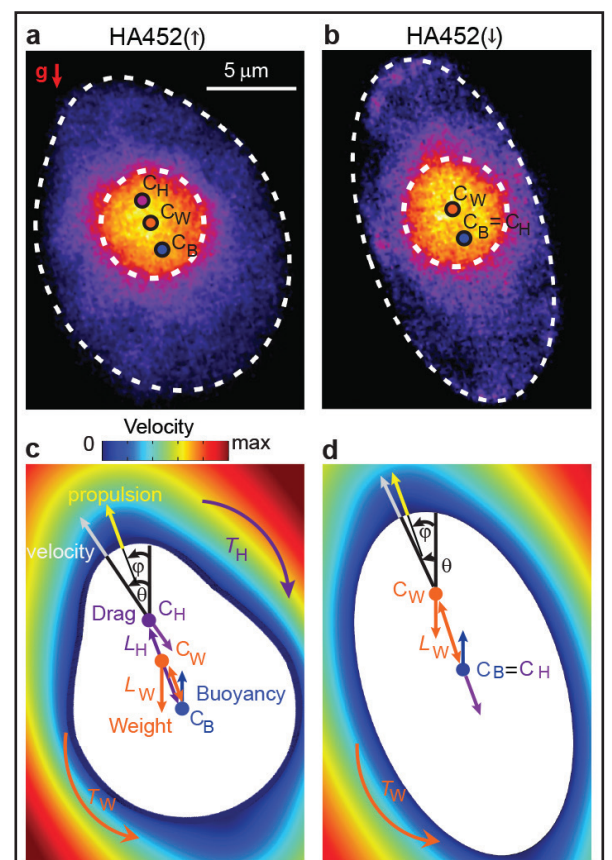


Figure 1. A change in morphology underpins the emergence of a downward swimming subpopulation in *Heterosigma akashiwo* strain HA452. **1a** and **1b**. False-color epifluorescence micrographs of upward swimming—HA452(t)—and downward swimming—HA452(l)—subpopulations. White dashed lines denote the contour of the cell body and nucleus (bright orange).  $C_W$ ,  $C_B$ , and  $C_H$  are the centers of mass, buoyancy, and hydrodynamic stress, respectively. **1c** and **1d**. Free body diagrams showing the forces acting on the cell overlaid on the numerically-computed flow field around the cell (not to scale). **1c**. HA452 cells swimming upwards after exposure to turbulent cues for 30 minutes are top-heavy ( $C_W$  above  $C_B$ ) and fore-aft asymmetric ( $C_H$  above  $C_B$ ); thus,  $T_W$  and  $T_H$  act in opposition. **1d**. HA452 cells swimming downwards after exposure to turbulent cues for 30 minutes are fore-aft symmetric ( $C_H$  coincides with  $C_B$  and thus  $T_H$  vanishes) and top-heavy ( $C_W$  above  $C_B$ ), so that  $T_W$  causes cells to orient downwards. Adapted from [8].

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## 5 Extended Functionality and Interfaces of the PRIMME Eigensolver

Eigenvalue equations model physical systems at subatomic, molecular, and human scales. Andreas Stathopoulos, Eloy Romero, and Lingfei Wu describe the PReconditioned Iterative MultiMethod Eigensolver (PRIMME) software package, useful for solving large, sparse Hermitian standard eigenvalue problems.

## 6 What Characteristics Make Mathematicians Suited for Industry?

With an increase in mathematical science Ph.D.s and dwindling numbers of academic positions, it's becoming more and more important for graduate students to look elsewhere for jobs. Drawing on his own industrial experience and conversations with mathematics Ph.D.s working in industry, Bill Satzer outlines attributes desirable for non-academic careers in the field.



## 8 Paying Tribute to Alan Turing's Life and Work

Ernest Davis reviews *The Turing Guide*, a collection of 42 essays covering various aspects of Turing's personal life and career. Mathematicians, computer scientists, philosophers, engineers, biologists, historians, and relatives offer insight on Turing's work and its impact in the 60 years since his death.

## 10 SIAM Student Chapters Put Funds to Good Use

SIAM awarded over \$64,000 to more than 120 student chapters for events and activities in the 2016-2017 academic year. From poster sessions on relevant topics to keynote lectures by leading researchers in the field, read about a sampling of events held over the past year.



## 11 Professional Opportunities and Announcements

# The Evolution of Mathematical Word Processing

The book *Track Changes: A Literary History of Word Processing* by Matthew G. Kirschenbaum, published last year by Harvard University Press, presents a history of word processing up to around 1984. Kirschenbaum explores early software and hardware that authors used in their daily workflow, focusing mainly on nontechnical writing. Many of the initial developments have had a big influence on how we use computers in our writing today. In fact, some of the early software is still in use, notably by George R.R. Martin, author of the *Song of Ice and Fire* fantasy novels that were adapted into the HBO series *Game of Thrones*; Martin does all of his writing in Wordstar<sup>1</sup> 4.0 (1987) on a DOS machine.

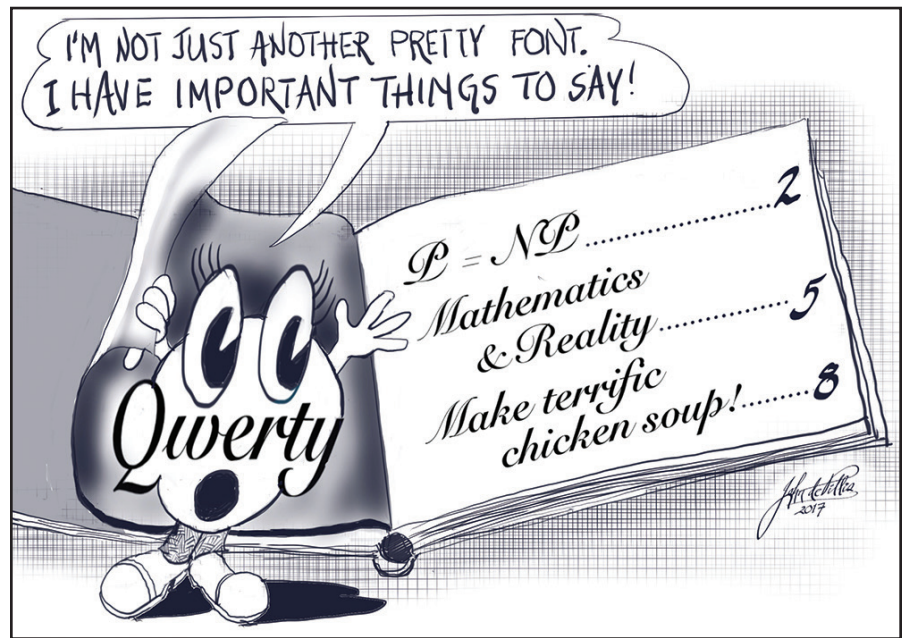
Reading *Track Changes* led me to reflect on my own early experiences with word processors and TeX to produce mathematical papers, and wonder in what ways computers have simplified mathematical writing over the last three decades.

In the early to mid-1980s, some institutions had minicomputers providing access to the Unix typesetting system troff, while others had the newer—and still evolving—TeX. Both typically outputted to laser printers, which at the time were huge and very expensive. Those of us without such facilities but with access to microcomputers (Apple II, Commodore PET, etc.), either wrote our own word processors (too basic to do more than write letters in my case) or cajoled standard word processors to produce mathematics. As a graduate student, I customized a program called Vizawrite for the Commodore 64 to output codes enabling access to Greek and other special characters built into the ROM of an Epson dot matrix printer (see my previous article<sup>2</sup> for details). This was all great fun, and the output was good enough for submission to journals.

Nowadays, everyone has easy access to TeX and LaTeX, and to inexpensive laser printers providing output at 300dpi. Moreover, advances in computer hardware mean that the time it takes to TeX a document is now almost negligible. When I was writing the first edition of *Accuracy and Stability of Numerical Algorithms* (published by SIAM in 1996), it took seven and a half minutes to typeset the book in LaTeX. By the time the (longer) second edition came out in 2002, that figure was down to five seconds (and has barely decreased since, not least because TeX does not take advantage of multicore processors).

<sup>1</sup> <https://arstechnica.co.uk/information-technology/2017/03/wordstar-a-writers-word-processor/>

<sup>2</sup> <https://sinews.siam.org/Details-Page/mathematical-word-processing-historical-snippets>



Cartoon created by mathematician John de Pillis.

But do computers really make it much easier to write papers now versus 30 years ago? In the 1980s, we had spell checkers, outliners, and even software for checking grammar. While spell checkers are now ubiquitous, grammar checkers are almost unheard of. Indeed, if my experience is anything to go by, some students treat their advisors as their grammar checkers!

Outlining is a way of gathering your thoughts by creating lists containing sections of text that you reorganize, extend, and gradually turn into a complete document. Again, tools for outlining in text editors and word processors have barely advanced over the last three decades, save for the wonderful Org mode in Emacs.

The great memory capacity of today's machines means that unlimited "undo" is a standard software feature, and disks are so fast that documents can be auto-saved every few minutes without any impact on the user. Combined with version control and a sensible backup strategy, there is no reason to ever lose anything you have typed. This insurance is very different from the days when people kept files temporarily on RAM disks before saving them to much slower mechanical hard disks — losing everything if the RAM disk unexpectedly crashed.

My favorite story from Kirschenbaum's book concerns the Bravo word processor written at Xerox PARC in the 1970s. Bravo had modes (like the classic Vi editor available on all Unix systems).<sup>3</sup> Kirschenbaum notes, "If a user typed the four-character sequence E, D, I, T into Bravo while it was in the wrong 'mode,' rather than echoing the word 'edit' on the screen, the system would do the following: first, it selected the Entire

<sup>3</sup> If you accidentally enter Vi, type ":q!" to get out.

document; second it Deleted it; third, it would Insert whatever the next character to be entered happened to be — in this case, T."

In the 1980s, authors could barely have contemplated real-time collaborative writing. Overleaf,<sup>4</sup> originally called writeLaTeX, provides this for LaTeX through browsers. I have not tried it—I can't see myself ever doing serious writing in a browser—but the company is partnering with several journal publishers, providing templates and "one-click submission" to journals. If you think it would be useful for SIAM to offer such a facility, please let me know.

Another potentially-useful capability that is not widely available is the ability to automatically produce a précis of a piece of text. Microsoft Word used to have an autosummarize function that "identifies the key points in a document," but this function was discontinued in Word 2010. With recent advances in machine learning, perhaps we will see such a function reappear. Could it produce a reasonable first draft of an abstract, given the paper? Could it even, in many cases, improve upon a published abstract?

Two modern ideas can offer real writing help. The first is "distraction-free writing," in which all the things that vie for our attention when we look at our screens are hidden, leaving just a full-screen window containing the text being typed. While various recent editors have been designed to be distraction-free, good general-purpose editors can also be made so with appropriate customization (for example, see my blog post).<sup>5</sup> If you've never tried this kind of minimal, zen-like writing, you should; there is something quite liberating about a screen containing just text and no extraneous features.

Finally, while TeX is the ultimate markup language for mathematicians, it can be overkill, especially at the outlining stage. The Markdown language, invented by John

See *Word Processing* on page 4

<sup>4</sup> <https://www.overleaf.com/>

<sup>5</sup> <https://nickhigham.wordpress.com/2016/01/14/distraction-free-editing-with-emacs/>

## Errata and Clarifications

In the article "Nonsmooth Dynamical Systems in Neuroscience" by Wilten Nicola and Sue Ann Campbell, which appeared in the June issue of *SIAM News*, equations (1) and (2) were mistakenly written as

$$\dot{x} = -2\eta x - y + F(t) \quad (1)$$

$$\dot{y} = x. \quad (2)$$

They should appear as

$$\dot{y} = -2\eta y - x + F(t) \quad (1)$$

$$\dot{x} = y. \quad (2)$$

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# Obituaries

By Jon Bashor

James “Jim” Corones, professor emeritus of mathematics at Iowa State University, passed away on April 28, 2017. He was 71.

Colleagues remember Jim for his leadership, ability to forge collaborations, and wide-ranging interests. But his enduring legacy is the Department of Energy’s (DOE) Computational Science Graduate Fellowship (CSGF) program, which he developed and led while at Ames Laboratory. The program became the centerpiece of the Krell Institute,<sup>1</sup> which Jim founded in 1997.

“In many conversations, Jim lamented the fact that DOE labs didn’t get due credit for their role in advancing computational science,” said Robert Voigt, who has been involved with the CSGF program since its onset and now provides technical advice. “He was passionate about improving awareness of the DOE’s role and contributions, and saw the fellowship as one way to raise that awareness.”

The CSGF program was created to train Ph.D. students in the then-emerging field of computational science, explicitly viewed as a closely-coupled combination of mathematics, computer science, and a scientific or engineering application. The fellowship is unique in requiring each fellow to obtain a substantive level of knowledge in all three components.

“There’s no question that the program helped give us all a foundation for the field of computational science, which didn’t really exist in the early 1990s,” said David Brown, director of the Computational Research Division at Lawrence Berkeley National Laboratory and, like Voigt, a long-time member of the CSGF steering and selection committees. “It’s widely viewed as one of the most successful fellowship programs in the world, and has served as a model for many other programs.”

Students specializing in a science or engineering application are required to take high-level computer science and math courses, while math or computer science students must take high-level science/engineering courses. All are required to spend one summer working at a DOE national lab on a

project that differs from their thesis research. To date, nearly 350 students have completed the program and are working at universities, national labs, and industry-based locations.

“Jim was incredibly smart and creative, and he devoted years of his life to the amazing CSGF program,” said Margaret Wright of the Courant Institute at New York University, who served on both the steering and student selection committees for many years. “He made it a success and protected it. People kept trying to change it, but he was the front line in defending it. Jim was firm as well as diplomatic, and was always successful in maintaining the principles of the program.”

Kevin Kreider, a postdoctoral researcher who worked on inverse scattering under Jim at Ames Lab from 1987-1989, remembers his energy and good sense of humor. “I always think of him as a visionary,” said Kreider, current chair of the Department of Mathematics at Akron University. “At the time, software packages were just being developed for solving problems involving partial differential equations, and Jim always talked about pushing that computing frontier. He was always looking to the future.”

Barbara Helland, associate director of the Advanced Scientific Computing Research program in the DOE’s Office of Science, began working for Jim as a computer scientist, administering his group’s computers at Ames Lab. Due to Jim’s leadership, the group was always a few steps ahead of the rest of the pack in deploying the newest systems, whether it be a VAX, a LISP machine, or the lab’s first distributed computing system.

“He pushed me out of the nest and freed me up to come to Washington,” said Helland, who followed Jim to the Krell Institute and worked for him for over 20

years. “He taught me a lot of what I needed to do this job — how to pull people together, build coalitions, and start discussions to move in new directions.”

Helland also noted Jim’s knack for anticipating new scientific thrust areas; he selected CSGF students to “seed the pipeline” in fields such as bioinformatics and machine learning before they were mainstream.

Roscoe Giles, a professor in Boston University’s Department of Electrical and Computer Engineering and member of the CSGF steering committee, said that



James “Jim” Corones, 1945-2017. Image courtesy of the Krell Institute.

the annual CSGF fellow selection meetings showcased Jim’s talent for getting people to work together and agree on the final outcome. This process was punctuated by fierce discussions, as dozens and dozens of applications were whittled down to just 20, with each committee member reviewing every application and then serving as an advocate for two or three in the final round. “Without Jim’s passion, our discussions would not have been nearly so rich and thoughtful,” said Giles.

“We had genuine disagreement, but we remained collegial,” added Wright, who adopted some of Jim’s committee management techniques in selecting SIAM Fellows. “We’d always end up happy with the fellows we chose.”

Jim Hack, director of the National Center for Computational Sciences at Oak Ridge National Laboratory, remembers Jim’s passion for many things, from ancient Greek coins to baseball — especially his beloved Boston Red Sox and the hated Yankees.

“I was always amazed at the breadth of things he could talk about,” said Hack, who served on the CSGF steering committee since its creation. “I always felt I learned something new when I chatted with him.”

Among Jim’s other interests were jazz, blues, and classical music; football, bas-

ketball, and golf; national and international politics and political history; science education and national science policy; religious and philosophical underpinnings of Western thought; gardening; fishing; poetry and literature; history of the 20th century, particularly of Eastern Europe and life behind the Iron Curtain; and visual arts such as painting, sculpture, and film, including classic science fiction and film noir. Voigt also recalls Jim’s passion for fine wines and food, which were celebrated in a special meal (at personal expense) at the end of the annual selection process.

“He was the quintessential great leader,” said Wright. “He was highly knowledgeable and dedicated to doing what was right.”

“We loved working for him and he challenged us to do our best,” added Helland. “And he inspired loyalty — you knew he’d be true to you.”

Jim, who earned his B.S. and Ph.D. in physics from Brown University and Boston University respectively, led the applied mathematics program at Ames Lab. His research was in the field of linear and nonlinear wave propagation, including extensive work in acoustic and electromagnetic inverse scattering.

Jim is survived by Lou Lamb Corones, his wife of 30 years; sons Michael John Corones of Brooklyn Heights, N.Y., and Matthew John Corones of Ames, Iowa; and Kathy Corones of Ames, the mother of his sons.

In lieu of flowers, donations may be made to the work of surgeon Peter Scardino at Memorial Sloan Kettering Cancer Center<sup>2</sup> or to the research of radiation oncologist Russell Hales and neurologist Scott Newsome, both of Johns Hopkins Medicine.<sup>3</sup> A scholarship will also be established in his name through the Krell Institute.

*Jon Bashor is the communications manager for the Computing Sciences organization at Lawrence Berkeley National Laboratory. He worked with Jim Corones on various projects, with Jim helping track down the definitive Latin translation of “It shouldn’t be this difficult,” which Bashor uses in his email signature: “Tam difficile non debet.”*

<sup>2</sup> www.mskcc.org

<sup>3</sup> www.hopkinsmedicine.org

## Image Reconstruction

Continued from page 1

resentation of that image in terms of a relatively sparse set of dictionary images. The optimization problem of finding the best match to the given image is thereby reduced in size and restricted to images that are inherently better-behaved.

Figure 1 (on page 1) compares a more sophisticated form of dictionary reconstruction with two contenders: Filtered Back Projection, which Kilmer called “for many years, the gold standard,” and classic Tikhonov regularization, each applied to an image of peppercorns. Tensor dictionary reconstruction, the best of the three methods shown in Figure 1, extends the dictionary idea by replacing the approximate matrix factorization that slims the dictionary with a tensor counterpart.

Low-order parametrization entirely abandons the idea of reconstructing tissue properties via point-by-point inversion of an image. In its simplest form, it turns instead to a shape-based approach that models variations in a sample’s absorption coefficient, for example, using characteristic (or indicator) functions that have value 1 within the suspect region, 0 outside. That formulation provides a low-order parametric representation of the coefficient’s level sets, which delineate the margins of a potential tumor in a computationally efficient manner.

Low-order parameterization is attractive, in part because DOT imaging of breast tissue seeks only to differentiate among three types of tissue: adipose, fibroglandular,

and tumor. Knowledge of the precise material properties at every point in the tissue is unnecessary when the fundamental goal is to locate tumor tissue.

Figure 2 illustrates how a few compactly supported radial basis functions can capture potentially challenging level sets, such as the square shown on the right. Kilmer calls such representations “pretty remarkable, given that they are *radial* basis functions.” Those basis functions also provide built-in regularization and a best-match optimization problem of low dimension. Trust region methods seem well suited to the optimization itself.

Evaluating the forward model—finding the image produced by a given distribution of material properties—is the computational bottleneck in nonlinear image reconstruction problems like DOT and hydraulic tomography. To break that dam, Kilmer and her colleagues have studied two classes of ideas: approximation of the forward model operator and reduced-order modeling.

If the forward model is a linear operator, then low-rank approximations to the matrix operators can be practical. If the forward model is a time-dependent PDE, then transfer functions—an idea borrowed from control theory—are the silver bullets: evaluating particular transfer functions at selected frequencies provides the various function values necessary for optimization. Coupling this approach with both low-order parametrization of the image space and trust region optimization can efficiently solve DOT problems.

Reduced-order modeling is motivated by the recognition that it is possible to estimate

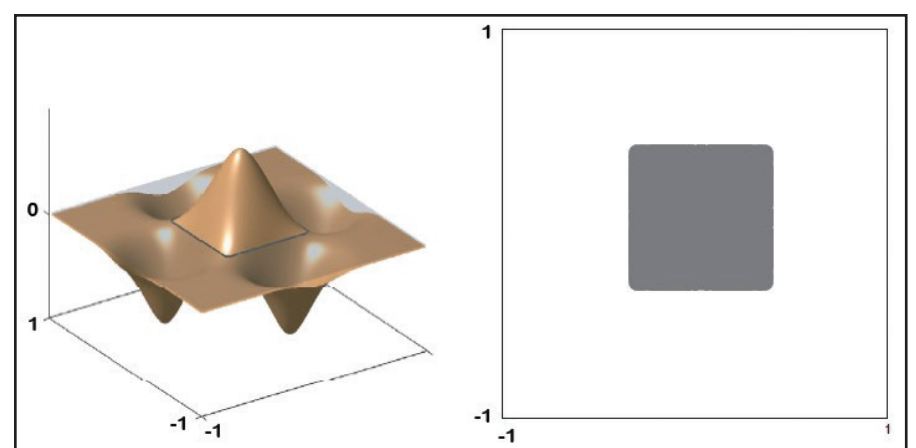


Figure 2. A parametric level set representation of the boundary of a nearly square level set (right) formed using radial basis functions (left). Image courtesy of [1].

the residual from a given image reconstruction using data from a much smaller collection of randomly selected detectors. Although the smaller problems are solved more quickly, the corresponding reductions in the residual may stall short of a good reconstruction. Swapping in a few well-chosen sources and detectors can restart the optimization productively. Kilmer describes this approach as “randomize, then optimize.”

As Kilmer made clear, image reconstruction, like many other important areas of CSE, has an immense river of mathematical ideas running through it. Her careful descriptions of the power of some of those ideas amply demonstrate the potential of CSE-wide community collaboration, which she espoused, “Complementary scientific computing techniques working together have the best chance of improving the speed and maintaining the accuracy of image reconstruction.”

*Kilmer’s CSE17 presentation is available from SIAM either as slides with synchronized audio, or as a PDF of slides only.<sup>1</sup>*

## References

- [1] Aghasi, A., Kilmer, M., & Miller, E.L. (2011). Parametric Level Set Methods for Inverse Problems. *SIAM Journal on Imaging Sciences*, 4(2), 618-650.
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*Paul Davis is professor emeritus of mathematical sciences at Worcester Polytechnic Institute.*

<sup>1</sup> <https://www.pathlms.com/siam/courses/4150/sections/5824>



## Phytoplankton

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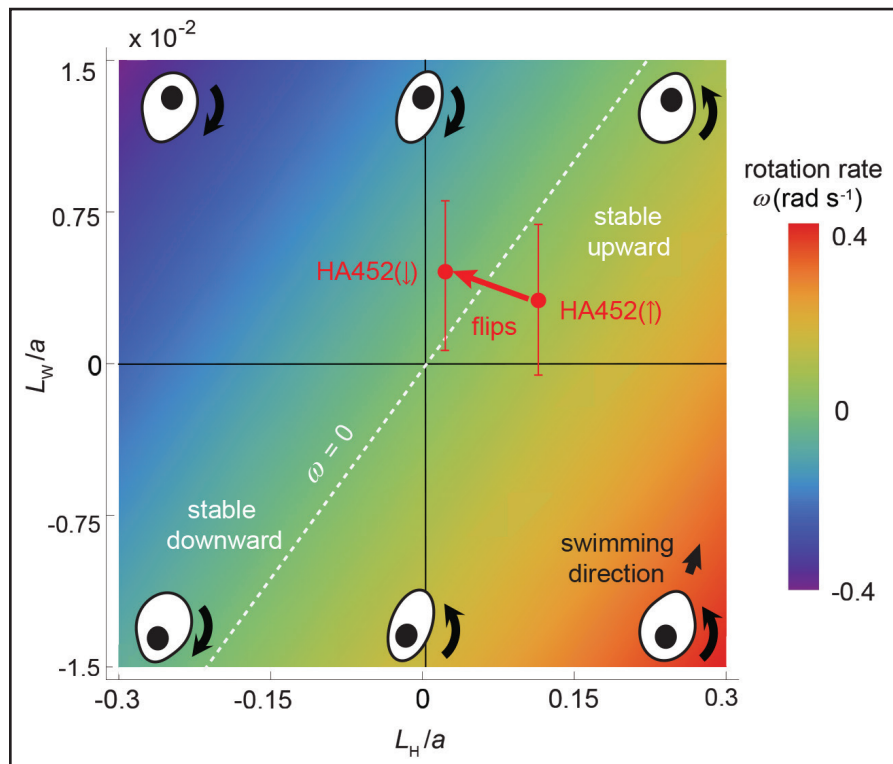
(flippings) of a millifluidic chamber in the vertical plane over a period of 18 s, which corresponds to a turbulent dissipation rate  $\epsilon = 3 \times 10^{-8}$  W/kg.

Within minutes of experiencing overturning, an upward-swimming population splits into two subpopulations: one that continues to swim upward and one that begins to swim downward. The split is triggered by changes in the cell orientation relative to gravity, as implied by the absence of splitting when flipping occurs in the horizontal plane. This result indicates that the cue for behavioral differentiation is not fluid velocity gradients, but rather changes in the cell orientation relative to gravity, a simple yet fundamental effect of small-scale turbulent eddies that has been previously neglected.

where  $P$  is the propulsion force, acting along the major axis of the cell ( $\phi$  relative to the vertical), and  $D$  is the drag force, acting at an orientation  $\theta$  relative to the vertical. Additionally, balancing the torques around the centre of buoyancy yields

$$D \sin(\theta - \phi)L_H - W \sin \phi L_W = R\eta\omega. \quad (2)$$

$L_H$  and  $L_W$  are the two cellular length scales that correspond to the offset length between  $C_B$  (the geometric center where the buoyancy force acts) and  $C_H$  (the center of hydrodynamic stress where the net hydrodynamic force acts) or  $C_W$  (the center of mass where the weight,  $W$ , acts) respectively (see Figure 1, on page 1). The position of these three points, relevant for cell



**Figure 2.** Regime diagram of cell stability. Colors denote the cell rotation rate  $\omega$  following an orientational perturbation:  $\omega > 0$  denotes negatively gravitactic cells (stable upward),  $\omega < 0$  denotes positively gravitactic cells (stable downward), and  $\omega = 0$  (white dashed line) denotes neutrally stable cells. Sample asymmetry configurations corresponding to different locations on the regime diagram are illustrated by the black and white schematics. Full circles denote experimental data [8]. The morphological adaptation of HA452 cells in response to overturning causes the population stability to switch (red arrow crossing the white dashed line). The original population splits into a subpopulation swimming downward HA452(↓) and a subpopulation swimming upward, HA452(↑). Adapted from [8].

Quantitative morphological analysis of the raphidophyte *Heterosigma akashiwo* (strain HA452), which forms harmful algal blooms, revealed that a change in cell shape accompanies this behavior; the cells that reversed their swimming direction did so by morphing from an asymmetric “pear shape” to a more symmetric “egg shape.” For an axisymmetric cell of volume  $V$  and density  $\rho_{\text{cell}}$  swimming in a fluid of density  $\rho_{\text{fluid}}$ , the equations for translational and rotational motions are decoupled. This allows one to write force-free conditions along the major- and minor-axis directions as follows:

$$P \sin \phi = D \sin \theta \quad (1)$$

$$P \cos \phi - D \cos \theta = (\rho_{\text{cell}} - \rho_{\text{fluid}}) V g,$$

stability, is obtained using the cell contour, the size and position of the nucleus (determined by epifluorescence microscopy), and the flow field around the cell (obtained via a fluid dynamics model) [8]. The relative position of these points within the cell regulates the strength of the hydrodynamic and gravity torques, determining the cell’s swimming stability and thus ultimately its swimming direction. At a given swimming speed, numerical solution of the system of equations (1) and (2) yields the rotation rate  $\omega(\theta)$  as a function of the swimming orientation to the vertical  $\theta$ . The swimming direction  $\theta$  is set by the competition between the gravitational torque  $T_W$  and the hydrodynamic torque  $T_H$  about  $C_B$ . Two physical features—summarized

## Word Processing

Continued from page 2

Gruber in 2004, provides a simple plain text markup syntax (for example, `*italic text*`, `**bold text**`) and is widely supported by applications, often in modified forms (for instance, at GitHub and Stack Exchange). Unfortunately it is not standardized, and various syntaxes for expressing mathematics are in use. Tools such as Pandoc<sup>6</sup> can convert files between many different formats, including from Markdown to LaTeX.

Anyone interested in writing a history of mathematical word processing (which is outside the scope of *Track Changes*), will find past issues of *SIAM News* to be a treasure trove of information. Especially in the 1980s, *SIAM News* regularly carried

articles reviewing and comparing word processing and typesetting systems, as well as adverts for such systems.

In conclusion, developments in computing over the last 30 years have not done as much as one might have thought to make writing mathematics easier. If I had to pick a favorite tool, it would be markup languages and the ability to convert between them. I write my *SIAM News* columns in Emacs Org mode, print drafts by exporting to LaTeX or html, and submit final copy to SIAM by exporting to Word via Pandoc. This workflow is great fun to use, and as Donald Knuth has said, “The enjoyment of one’s tools is an essential ingredient of successful work.”

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

by two morphological length scales—determine cell stability: the asymmetry in shape, quantified by  $L_H/a$ , and the mass distribution, quantified by  $L_W/a$ , where  $a$  is the semi-major axis (see Figure 1, on page 1). The characteristic reorientation timescale determines cell stability based on the fact that greater stability will cause faster reorientation toward the stable orientation after a cell’s perturbation. In the phase space of cell stability defined by the two cellular length scales  $L_H$  and  $L_W$ , the loss of fore-aft asymmetry corresponds with the crossing of the line that divides upward and downward stability regimes (see Figure 2).

These findings illustrate that phytoplankton are capable of precise control over movement behavior through fine-scale control of cellular morphology in rapid response to environmental cues. This discovery paves the way for a new class of mathematical models in which single phytoplankton cells sense turbulent cues and rapidly adapt their motility strategy. By establishing a mechanistic link between turbulence, cell physiology, and emergent behavior, the proposed framework contributes to our understanding of phytoplankton distributions in current and future oceans.

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<sup>1</sup> <https://sengupta.mit.edu>

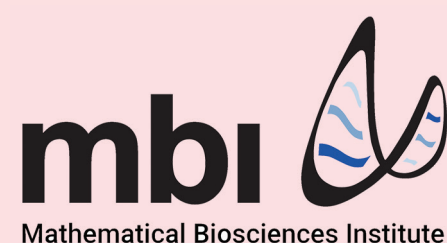
## MBI Online Colloquia

The Mathematical Biosciences Institute (MBI) is hosting a novel online colloquium in important and emerging areas of mathematical biology. These web-based colloquia give individuals and groups the opportunity to watch talks and ask questions of the speaker. Audience members can interact with leading researchers, either from their classroom or the comfort of their own office. These interactive colloquia are held monthly on Wednesdays at noon Eastern Standard Time. If you are unable to make a talk, you can view it on-demand at a later date. All talks from the 2016-2017 academic year are now available on the MBI website.

The MBI Colloquium has several goals. The colloquium presents an opportunity to create local math biology communities, with get-togethers organized around the monthly talks; enables large numbers of researchers to hear about recent advances in the field; and facilitates access to top-notch speakers for researchers and students at smaller schools.

This year’s talks, and details of how to connect to them, are available on the MBI website.<sup>1</sup> Jim Collins (Department of Biological Engineering, Massachusetts Institute of Technology) will give the first fall 2017 talk on Wednesday, September 20. Subsequent fall talks will feature John Tyson (Department of Biological Sciences, Virginia Tech), Kristin Swanson (Department of Neurosurgery, Mayo Clinic, Phoenix), and Lisa Fauci (Department of Mathematics, Tulane University).

<sup>1</sup> <https://mbi.osu.edu/go/sn/colloquium>



<sup>6</sup> <http://pandoc.org/>



# Extended Functionality and Interfaces of the PRIMME Eigensolver

By Andreas Stathopoulos, Eloy Romero, and Lingfei Wu

Nearly three centuries after Leonhard Euler's discovery of principal axes of quadratic forms, eigenvalues and eigenvectors are center stage in the study of matrices and linear operators. No other equation has arguably come so close to describing our physical world as succinctly as the eigenvalue equation. The spiritual powers seem to concur, as the Dirac equation (a relativistic form of the Schrödinger equation) is the only equation engraved on the floor of Westminster Abbey.

Eigenvalue equations model physical systems at subatomic, molecular, and human scales. As tools, eigenvalues and the related singular value decomposition (SVD) help us analyze stability and partition graphs, obtain low-rank approximations, and discover information in data sciences. Many of these applications give rise to large, sparse matrices that are often Hermitian, and for which we must compute a small part of the spectrum. Iterative methods are the computational tool for this calculation.

Hermitian eigenproblems have well-conditioned, real eigenvalues that enable the development of many efficient methods. As it happens, practitioners have responded by demanding the solution of more eigenvalues of even larger matrices. Today, it is not uncommon to see eigenproblems of sizes greater than one billion.

With larger matrix sizes and denser spectra, the Lanczos method, which is theoretically optimal over all polynomial methods in terms of the number of matrix-vector multiplications, becomes computationally less attractive than other restarted methods. ARPACK, a remarkable theoretical and software development of the 1990s, is a widely-used, restarted eigensolver with minimal tuning requirements. It is present in virtually all problem-solving environ-

preconditioning), more efficient algorithms, high performance computing (HPC) improvements, a C99 code base, and interfaces to a host of modern problem-solving environments.

PRIMME differs from other eigenvalue libraries in several crucial ways. First, it focuses only on Hermitian eigensolvers, where algorithmic expertise can translate to highly-optimized code. Second, it implements a parametrized inner-outer method, which—by appropriate settings—can turn into any family of methods, including the near-optimally restarted versions of generalized Davidson and Jacobi-Davidson. The parametrization also controls many algorithmic components, such as blocking, locking, projections, and the extraction method, all of which can be combined to provide a continuum between traditional methods. This is one of the most complete set of algorithmic features available in today's eigensolvers.

Although expert users may cherish PRIMME's power and extended control, we have focused much of our efforts on creating a simple yet expressive interface that requires no parameter setting to provide almost the entire span of benefits to non-expert users. Depending on problem size, the number of eigenvalues needed, and the tolerance required, all parameters receive default values based on theoretical arguments and/or our experience. If the user provides additional parameters, the rest of the defaults are set accordingly. In addition, runtime measurements allow the method to adapt to the given problem. The resulting default dynamic method runs consistently within five to ten percent of the time of optimal choice.

```
% Download https://www.cise.ufl.edu/research/sparse/mat/Bates/sls.mat
A=load('sls.mat'); A=A.Problem.A;

% Computing the 20 smallest singular values with default settings
opts.tol = 1e-6;
[U,S,V,resNorms,stats]=primme_svds(A,20,'S',opts);
stats.elapsedTime %1601s

% Using Jacobi preconditioner on A*A, P=diag(A'*A)
P=diag(sum(abs(A).^2));
precond.AHA = @(x)P\x;
[U,S,V,resNorms,stats]=primme_svds(A,20,'S',opts,precond);
stats.elapsedTime %139s

% If the preconditioner is good, Generalized Davidson may perform better
% than Jacobi-Davidson. Change the method of the underneath eigensolver to GD.
opts.primme.method = 'DEFAULT_MIN_MATVECS';
[U,S,V,resNorms,stats]=primme_svds(A,20,'S',opts,precond);
stats.elapsedTime %130s

% Large basis size and block methods may improve convergence and performance
opts.maxBasisSize = 80;
opts.maxBlockSize = 4;
[U,S,V,resNorms,stats]=primme_svds(A,20,'S',opts,precond);
stats.elapsedTime %88s

% LOBPCG may perform well if the gap between wanted and unwanted eigenvalues is large.
% This turns out not to be the case here.
opts.primme.method = 'LOBPCG_OrthoBasis';
[U,S,V,resNorms,stats]=primme_svds(A,20,'S',opts,precond);
stats.elapsedTime %209s
```

Figure 2. Various options for computing the 20 smallest singular values of sls. This is the second-largest matrix in number of nonzero elements of a least squares problem in the University of Florida Sparse Matrix Collection. Runtimes are reported on a machine with an Intel® Core™ CPU i7-6700K and 16GiB of physical memory. We could not run MATLAB's svds because more than 16GiB is required to compute the sparse QR factorization, which MATLAB uses for inverse iteration on  $R^{-1}$ .

## SOFTWARE AND PROGRAMMING

stantial interest in the package and a wider user base; both factors are important for the code's sustainability on new architectures.

PRIMME is also based on performance-aware software practices that make state-of-the-art theoretical advancements widely accessible. Of course, this is not the end of the road. Support for the generalized eigenvalue problem and algorithmic improvements for the SVD are under development, and we are experimenting with polynomial filtering options, with an eye to exascale. Improved kernels (such as block orthogonalization and blocked inner solvers) and a graphics processing unit-enabled version are also in the works. With PRIMME's multiplatform availability, we welcome new users and would love to hear about their use of PRIMME in exciting applications.

### Further Reading

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Andreas Stathopoulos is a professor of computer science at the College of William & Mary and currently serves as the section editor for *Software and High Performance Computing for the SIAM Journal on Scientific Computing*. His favorite research is on eigenvalue methods and software, and on high performance aspects of scientific computing. Eloy Romero is a research associate at the College of William & Mary. He works on the high performance solution of large-scale eigenvalue and singular value problems. His major software contributions can be found in SLEPc and PRIMME. Lingfei Wu is a postdoctoral researcher of cognitive computing at IBM T. J. Watson Research Center. His research interests span large-scale machine learning and data mining, big data analytics, high-performance mathematical software, and numerical linear algebra.

Randall J. LeVeque (rjl@uw.edu) of the University of Washington, Seattle, is the editor of the *Software and Programming column*.

```
# Python: Compute 100 largest singular triplets of A with default parameters
[U,S,V] = Primme_svds(A, 100, which='L')

# R: Compute the 6 smallest eigenpairs of A with default parameters
r = eigs_sym(A, 6, "A", tol=1e-6)
r$values

% MATLAB/Octave: Compute the 6 smallest eigenvalues using ILU(0) as a preconditioner
[L,U] = ilu(A, struct('type','nofill'));
opts.tol = 1e-10;
evals = primme_eigs(A, 6, 'SA', opts, [], L, U);
```

Figure 1. Three examples of PRIMME's use in Python, R, and MATLAB/Octave with only basic parameter settings.

ments (PSEs) for scientific computing. However, the problems' increasing difficulty requires eigensolvers with advanced features, such as preconditioning and inner-outer methods that must also perform well on current computer architectures. Methods that offer these key features are not strictly Krylov, and often require expert tuning to achieve their potential.

PRIMME, pronounced "prime," stands for PReconditioned Iterative MultiMethod Eigensolver<sup>1</sup> and was first released in 2005 as a C software package for finding a few selected eigenpairs of large Hermitian matrices. It was developed with the goal of bringing state-of-the-art preconditioned eigenvalue methods from "bleeding edge" to production with the best possible robustness and efficiency, while simultaneously offering a highly-usable interface that requires minimal or no tuning. Over the last few years, PRIMME's functionality has grown significantly, with the software now supporting the computation of singular value triplets (the first such package to support

PRIMME carries a 3-clause BSD license for integration into a variety of open source and commercial platforms. It has a minimal dependency on the widely-available BLAS and LAPACK libraries through wrappers that could be reassigned. The interface uses a simple C struct and function pointers, rather than the object-oriented approaches of other libraries that depend on particular ecosystems, such as PETSc or Trilinos. Together with the lightweight dependencies, this helps reduce the amount of effort required to port the full interface of PRIMME to other applications.

An increasing amount of scientific and engineering computations are currently performed on PSEs. Such PSEs use optimized numerical libraries and offer multithreading and even distributed parallelism, blurring the line with traditional HPC. Therefore, besides the C and Fortran interfaces of PRIMME, we have recently developed interfaces for both eigenvalue and singular value functionality in MATLAB/Octave, Python (compatible with SciPy), and R (see examples of usage in Figures 1 and 2). We are also aware of the availability of an independent Julia interface. These interfaces, which can be viewed as extensions of the eigs() and svds() routines in MATLAB, have generated sub-

<sup>1</sup> Download PRIMME from [www.github.com/primme/primme](http://www.github.com/primme/primme). Documentation available at [www.cs.wm.edu/~andreas/software](http://www.cs.wm.edu/~andreas/software).

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# What Characteristics Make Mathematicians Suited for Industry?

By Bill Satzer

While the number of Ph.D.s in the mathematical sciences continues to grow, the availability of academic positions—especially those leading to long-term employment—remains stagnant. According to the American Mathematical Society’s recent survey, 52 percent of new math-based Ph.D.s in the United States held academic positions in 2014–2015. Three-fourths of that 52 percent were hired in postdoctoral positions. Nonacademic U.S. hiring was at 35 percent, a five-year high. If history is a guide, many of those postdocs will not find permanent academic employment.

What happens to these unemployed Ph.D.s? Does their training and experience in graduate school prepare them for the world they must now face? I seek to identify the characteristics that make mathematics Ph.D.s attractive candidates for positions outside the academic world and prepare them for nonacademic careers. Sometimes this environment is simply called “industry,” but I find that term too limiting and even misleading. Jobs that employ mathematicians now cover a broad spectrum—from government to retail sales (e.g., Amazon and Target); management consulting (e.g., McKinsey & Co.); manufacturing (e.g., Dow Chemical Co., DuPont, Corning Inc., 3M); data analysis and software development (e.g., Google); medical technology; pharmacology; drug development; and so on. But for lack of a better word, I’ll continue to use the term “industry” to encompass all non-academic employers.

I identify three general categories of attributes desirable for industrial employment: technical capability, communication skills, and flexibility. Ph.D. students typically focus most on technical skills and general technical aptitude. These are significant, but only part of the picture. Communication and flexibility matter quite a bit, and may be as important as technical capability.

The following analysis is based on my experience in industry, as well as conversations, interviews, and discussions with mathematics Ph.D.s working in industry; the people who hire them; and the people who work with them. Though the suggestions pertain to Ph.D.s in the mathematical sciences, many also apply to related fields, such as physics.

## Technical Capability

A mathematics Ph.D.’s most important technical skill is a capacity for sustained

logical and analytical work. Writing a thesis tests one’s ability for extended, independent work, and the discipline and persistence necessary to carry it through. This is true regardless of a student’s specialization area, though specializations in more applied areas may make finding a nonacademic position easier.

At the same time, there are general areas where a solid technical background—equivalent to what one would learn in an advanced undergraduate course—is highly desirable. These include probability and statistics, data analysis, mathematical modeling, and the basics of numerical analysis (particularly numerical linear algebra). Experience with mathematical software like MATLAB, Mathematica, or Maple can be very useful, as is familiarity with writing code in languages such as C. However, some companies—particularly those doing heavy-duty data work—may actually require experience in coding with Python, C, or something similar.

Many potential employers continue to view mathematics Ph.D.s as impractical or too specialized, interested only in the abstract and skilled only in proving theorems. Thus, evidence of breadth is important—serious interest, curiosity, and experience in areas unrelated to one’s Ph.D. specialty.

The ability to learn and continue learning is another essential strength. Being able to jump into a situation, assess it, and quickly gauge what one needs to know is invaluable. Adaptability in an unfamiliar work environment is a prime asset.

Recognizing that not every problem demands a full-scale attack and rigorous solution is also important. Sometimes new Ph.D.s want to demonstrate their analytical skills by pursuing a fully robust solution and a proof, but this often suggests a lack of perspective and perhaps poor judgment. The effort required to solve a problem can be highly dependent on the situation. Often the best results emerge from back-of-the-envelope calculations. Learning to evaluate a problem and justify the corresponding level of effort is highly regarded.

It is important to note that rarely (and in my experience, never) is someone hired to fill a position as a mathematician. A mathematician’s value to a company is not as a mathematician, but as an individual with a versatile skill set who happens to be a mathematics Ph.D. Scientists, engineers, and mathematicians are hired for industrial jobs with the expectation that they have, or



Applied mathematics plays an important role in the manufacture of goods such as aluminum. Mathematicians design prototypes, optimize and verify designs, automate processes, and help manage supply chains. SIAM photo.

will develop, relatively broad capabilities in that industry to contribute technically to a company’s goals. Industrial managers assume that their employees are there to do the job and handle any technical issues that arise, regardless of the scientific or engineering discipline.

## Communication Skills

Unsurprisingly, Ph.D.s should be able to share information with colleagues—who come from a variety of backgrounds—in a nonacademic environment. Part of this is simply learning some of the technical language used by engineers, chemists, biologists, computer scientists, and others. I find that this helps in understanding and appreciating their perspectives. Sometimes

the real technical issues and problems do not begin to emerge until the language issue is addressed. More than once, I’ve found myself working on a problem that I presumed was well posed

in a technical area with which I had little experience, only to find that the problem described to me was not the right one at all. Resolving language and cultural differences between technical specialties in advance helps avoid the “correct solution-wrong problem” dilemma. The process of developing “shared knowledge” in a work environment begins with developing a shared vocabulary, shared goals, and perhaps a shared perspective.

Relevant communication skills include both speaking and writing, formal and informal. For example, knowing how to assemble a concise presentation on short notice is a valuable skill. And clear, well-organized, and articulate writing is still rare enough not to go unnoticed.

While the aforementioned approaches largely apply to communication with fellow engineers and scientists, most companies have a variety of other personnel—including sales, marketing, manufacturing, financial, legal, and management groups—with whom one must interact. While the worldviews of other engineers and scientists may differ from yours, the perspectives of individuals from such diverse areas can be mind-bogglingly at odds with your own. Nonetheless, to work with them you’ll have to understand something about them, their goals, and the effects of their actions. Additionally, while academic work can be mostly solitary, teamwork is far more common in industry. This requires considerable adaptability to accommodate differences in technical language, culture, work style, and personality.

New Ph.D.s with teaching experience can use that experience to their advantage. Teaching, either one-to-one or in small groups, is very common in industrial settings, as people naturally educate one another in everyday situations. Knowing how to present ideas and concepts clearly and concisely, as well as how to identify and approach areas of misunderstanding, is a notable skill. This offers solid evidence of the ability to communicate to a potential employer.

## Flexibility

It is increasingly common for people, especially technical professionals, to make one or two major career changes during the course of their working lives. Flexibility is a survival skill; it requires that Ph.D.s view themselves as broadly capable, engaged with the world, and open to challenge. To be successful in a nonacademic environment, new Ph.D.s must be willing to immerse themselves thoroughly in the projects with which they are involved.

In some cases, the most critical need for flexibility arises when recent Ph.D.s realize how they must reinvent themselves and realign their expectations for nonacademic positions. Unfortunately, I have often witnessed new mathematics Ph.D.s in industry-based positions who feel that they have failed as mathematicians and disappointed their advisors and mentors because they were not doing what they were trained to do. The adjustment can be traumatic, but Ph.D.s must resolve this before they start actively looking for jobs. Uncertainty in job interviews is not a good strategy. The necessary self-assessment and realignment of expectations is best done as early as possible in one’s graduate school career.

## Conclusion

New mathematics Ph.D.s have much to offer. To insure that they find personally fulfilling careers and put their talents to the best use, I’ve suggested a collection of skills and attributes that increase their desirability for positions in industry. These, I think, would be beneficial no matter the direction of their future careers.

*Bill Satzer received his Ph.D. in mathematics from the University of Minnesota working on a problem in celestial mechanics under advisor Dick McGehee. Almost all of his career has been in industry; he recently retired from the 3M Company.*

## CAREERS IN MATHEMATICAL SCIENCES



Mathematicians often use their skills to help streamline production and distribution systems in industry. SIAM photo.



# Update from the Division of Mathematical Sciences

By Michael Vogelius, Tie Luo, and Henry Warchall

With this article, the management team of the Division of Mathematical Sciences (DMS) at the National Science Foundation (NSF) would like to provide an update about recent program activities from the DMS and an outlook for the future. The DMS plays a critical role in providing about 64 percent of all U.S. federal support for basic research at the frontiers of discovery in the mathematical sciences. It also supports training through research involvement of the next generation of mathematical scientists, conferences and workshops, and a portfolio of national mathematical sciences research institutes.<sup>1</sup>

Here we call attention to four recent funding opportunities that we find particularly newsworthy. Two are calls for development of large-scale interdisciplinary research centers/institutes that involve collaboration between mathematical scientists and researchers from other scientific areas, and two are calls for activities to enhance and broaden graduate education in the mathematical sciences.

## 1. Transdisciplinary Research in Principles of Data Science

The Transdisciplinary Research in Principles of Data Science (TRIPODS) program<sup>2</sup> aims to bring together the statistics, mathematics, and theoretical computer science communities to develop the theoretical foundations of data science through integrated research and training activities. Phase I will support the development of small collaborative institutes. Phase II (to be described in an anticipated future solicitation, subject to availability of funds) will support a smaller number of larger institutes via a second competitive proposal process. All TRIPODS institutes will involve significant and integral participation by all three communities.

The TRIPODS program is a part of the NSF initiative “Harnessing Data for 21st Century Science and Engineering,” one of the “10 Big Ideas for Future NSF Investments.”<sup>3</sup> It is co-funded equally by the NSF Division of Computing and Communication Foundations and the DMS. These investments are augmented by funds from the “Growing Convergent Research at the NSF” initiative and the Office of Multidisciplinary Activities of the Mathematical and Physical Sciences Directorate. It is the hope of the DMS that the TRIPODS program will emphasize to academic institutions forming programs in data science that such efforts naturally involve computer scientists, mathematicians, and statisticians. The TRIPODS Phase I proposals are currently under review, and it is anticipated that up to 12 three-year awards of approximately \$500,000 per year will be made.

## 2. NSF-Simons Research Centers for Mathematics of Complex Biological Systems

The NSF-Simons Research Centers for Mathematics of Complex Biological Systems<sup>4</sup> (MathBioSys) is a new program that expects to fund centers of five-year duration from a one-time call for proposals. The program focuses on research to understand emergent properties in biological systems. It welcomes proposals to establish centers at which sustained collaborations are facilitated between mathematical scientists and biologists to develop

novel mathematical, computational, and statistical approaches. Such approaches will advance fundamental understanding of how and why emergent properties arise in molecular, cellular, and organismal systems. The program strongly encourages projects aimed at developing predictive frameworks for understanding phenotypes. Projects are expected to include plans for significant effort in cross-disciplinary training of cohorts of future scientists, such as postdoctoral research associates, graduate students, and/or undergraduates from mathematical sciences and related areas of the biological sciences. Each center is also envisaged to conduct convening activities, including short-term and/or long-term visitors’ programs, workshops, and/or outreach activities.

The MathBioSys program is part of the NSF “Understanding the Rules of Life: Predicting Phenotype” initiative, another of the “10 Big Ideas for Future NSF Investments.” The program is co-funded equally by the Simons Foundation and

the NSF, with 30% of the total investment furnished by the DMS and 20% furnished by the NSF Directorate for Biological Sciences. Letters of intent and proposals are due August 10 and September 29, 2017, respectively. It is anticipated that three centers devoted to collaboration between mathematicians, statisticians, and biologists will be funded. Each center will be funded for a five-year duration with an annual budget of \$2 million.

## 3. Mathematical Sciences Graduate Internships

By means of this activity, the DMS aims to provide opportunities to enrich the training of graduate doctoral students in the mathematical sciences through summer research internships in nonacademic settings. The DMS has partnered with the Oak Ridge Institute for Science and Education (ORISE), which is managed by Oak Ridge Associated Universities for the Department of Energy, to estab-

lish the Mathematical Sciences Graduate Internship program.<sup>5</sup>

The immediate goal of the program is to arrange and support internships for approximately 40 students annually, primarily at U.S. National Laboratories. The program is intended to introduce doctoral students in the mathematical sciences to important applications of mathematical or statistical theories outside of academia. The internships are aimed at students who are interested in learning about such applications, regardless of whether they plan to pursue an academic or nonacademic career. Interns will not only gain experience in the diverse uses of advanced mathematical tools at National Laboratories, but also become aware of the additional skills required for success in employment outside the traditional academic setting. The program is equally intended for students in pure and

See *Division of Math Sciences* on page 9

<sup>5</sup> [https://www.nsf.gov/publications/pubsumm.jsp?ods\\_key=nsf17042](https://www.nsf.gov/publications/pubsumm.jsp?ods_key=nsf17042)

## William Benter Prize in Applied Mathematics 2018

### Call for NOMINATIONS

The Liu Bie Ju Centre for Mathematical Sciences of City University of Hong Kong is inviting nominations of candidates for the William Benter Prize in Applied Mathematics, an international award.

#### The Prize

The Prize recognizes outstanding mathematical contributions that have had a direct and fundamental impact on scientific, business, financial, and engineering applications.

It will be awarded to a single person for a single contribution or for a body of related contributions of his/her research or for his/her lifetime achievement.

The Prize is presented every two years and the amount of the award is US\$100,000.

#### Nominations

Nomination is open to everyone. Nominations should not be disclosed to the nominees and self-nominations will not be accepted.

A nomination should include a covering letter with justifications, the CV of the nominee, and two supporting letters. Nominations should be submitted to:

##### Selection Committee

c/o Liu Bie Ju Centre for Mathematical Sciences  
City University of Hong Kong  
Tat Chee Avenue  
Kowloon  
Hong Kong

Or by email to: [lbj@cityu.edu.hk](mailto:lbj@cityu.edu.hk)

Deadline for nominations: 30 September 2017

#### Presentation of Prize

The recipient of the Prize will be announced at the **International Conference on Applied Mathematics 2018** to be held in summer 2018. The Prize Laureate is expected to attend the award ceremony and to present a lecture at the conference.

The Prize was set up in 2008 in honor of Mr William Benter for his dedication and generous support to the enhancement of the University’s strength in mathematics. The inaugural winner in 2010 was George C Papanicolaou (Robert Grimmett Professor of Mathematics at Stanford University), and the 2012 Prize went to James D Murray (Senior Scholar, Princeton University; Professor Emeritus of Mathematical Biology, University of Oxford; and Professor Emeritus of Applied Mathematics, University of Washington), the winner in 2014 was Vladimir Rokhlin (Professor of Mathematics and Arthur K. Watson Professor of Computer Science at Yale University). The winner in 2016 was Stanley Osher, Professor of Mathematics, Computer Science, Electrical Engineering, Chemical and Biomolecular Engineering at University of California (Los Angeles).

The Liu Bie Ju Centre for Mathematical Sciences was established in 1995 with the aim of supporting world-class research in applied mathematics and in computational mathematics. As a leading research centre in the Asia-Pacific region, its basic objective is to strive for excellence in applied mathematical sciences. For more information about the Prize and the Centre, please visit <http://www.cityu.edu.hk/lbj/>



<sup>1</sup> <https://www.nsf.gov/funding/programs.jsp?org=DMS>

<sup>2</sup> <https://www.nsf.gov/funding/programs.jsp?org=DMS>

<sup>3</sup> [https://www.nsf.gov/about/congress/reports/nsf\\_big\\_ideas.pdf](https://www.nsf.gov/about/congress/reports/nsf_big_ideas.pdf)

<sup>4</sup> [https://www.nsf.gov/funding/pgm\\_summ.jsp?pims\\_id=505392](https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=505392)



# Paying Tribute to Alan Turing's Life and Work

**The Turing Guide.** By Jack Copeland, Jonathan Bowen, Mark Sprevak, and Robin Wilson. Oxford University Press, New York, NY, March 2017. 545 pages. \$115.00.

June 23, 2012 was the 100th birthday of the renowned Alan Turing. 2012 was designated as “the Alan Turing Year,” and 21 different countries celebrated with numerous events, conferences, books, and journal special issues. *The Imitation Game*, a 2014 biopic loosely based on Turing’s decryption work during World War II, was enormously successful.

A little late to the party but still very welcome is *The Turing Guide*, a collection of 42 fascinating essays covering every aspect of Turing’s life and work. It traces the consequences of Turing’s ideas and labors in the 60 years since his death. The essays are deeply researched, well written, and cogently argued, and the book itself is beautifully produced and amply illustrated with photographs, line drawings, diagrams, and cartoons.

Jack Copeland, a logician and historian at the University of Canterbury in New Zealand, appears to be *The Turing Guide*’s chief moving spirit. He has authored or coauthored 13 of the essays in this volume, having previously written a full-length biography of Turing and five other books on aspects of his work. Other contributors include mathematicians, computer scientists, logicians, philosophers, psychologists,

engineers, biologists, historians, and museum professionals. Turing’s nephew, Sir John Dermott Turing, and novelist David Leavitt also offer insight. Seven of the contributors who knew Turing personally wrote about their interactions at Bletchley Park—the site for British codebreakers during World War II—and one contributor described his work with Turing on his theory of morphogenesis.

Turing’s revolutionary achievements and wide-ranging scientific interests, his work’s lasting and future significance, and his personal tragedy are recounted and analyzed in depth. Most of the book naturally deals with the four great milestones of his career:

(i) **Computation theory.** Turing’s amazing 1936 paper, “On Computable Numbers,” laid the foundations of computation theory, defined the Turing machine and confirmed the existence of a universal Turing machine, demonstrated the undecidability of the machines’ fundamental problems, and—almost in passing—answered David Hilbert’s “Entscheidungsproblem” by proving that provability is undecidable.

(ii) **Code breaking.** In World War II, Turing was the scientific leader of the team at Bletchley Park that broke the German’s naval Enigma code. This was of enormous value to the Allied powers, particularly in protecting trans-Atlantic shipping from U-boat attacks.

(iii) **Electronic computer.** After the war, Turing was deeply involved with the development of electronic computers in Great Britain. Turing’s 1945 report on the Automatic Computing Engine established a detailed design of a stored-program computer. In 1948, he joined Max Newman’s lab in Manchester and played

a leading role in the development of the Manchester computer.

(iv) **Artificial intelligence.** Turing was a pioneer and early visionary in artificial intelligence (AI). He developed the first chess-playing program by proposing a number of research methods—some have been fruitful, others may yet be fruitful—and positing the Turing test as a measure of successful realization of machine intelligence.

There is much else besides. In the early 1950s, Turing developed a powerful theory of biological morphogenesis. In fact, the paper describing that theory has more citations on Google Scholar than any of his papers on computation theory or AI. However, as Margaret Boden noted in her essay, this likely says more about the limitations of Google Scholar’s citation count as a measure of impact than about the actual relative importance of the work. Turing worked in a number of mathematical areas beyond logic and computation theory, including

the central limit theorem, the theory of normal numbers, the word problem in group theory, and the Riemann hypothesis. Working with Christopher Strachey, he created the first computer music; in 1951, the Manchester computer gave a small concert consisting of “God Save the King,” Glenn Miller’s “In the Mood,” and “Baa Baa Black Sheep.” Additionally, in an often-ignored section of his paper on “Computing

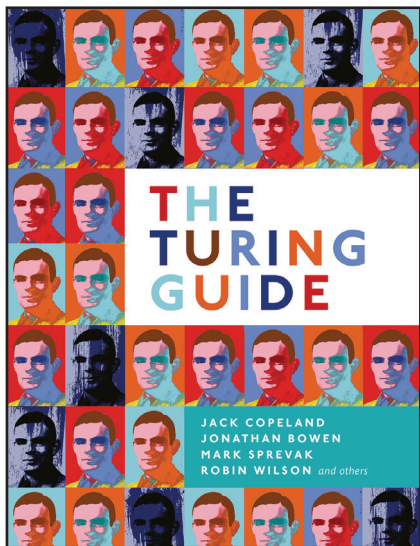
Machinery and Intelligence,” which introduced the Turing test, Turing also endorsed parapsychology; Leavitt’s chapter in the book discusses the scientific and cultural context of that unexpected intrusion.

The essays do at times go a bit overboard in their worshipful attitude. A book focused on a single individual inevitably and reasonably emphasizes the importance of its hero, but this can be taken too far. It seems quite unfair, in an extended historical discussion of computation theory and the Turing machine, to leave entirely unmentioned Emil Post’s independent discovery of essentially the identical model (it was actually slightly simpler), which published six months later. Furthermore, it is pretty much meaningless to claim, as Copeland does, that “If Isaac Newton had known about [the Turing machine], he probably would have wished he had thought of it first.” I am not sure what the proper consequent is for the counterfactual “If Newton had known about the Turing machine,” but it seems clear that, if Newton had known about it, he would have thought of it before Turing. Boden expresses absolute certainty that a large collection of handwritten mathematical notes, which were found after Turing’s death and have thus far been indecipherable, are a “treasure trove” of mathematical insights of potential relevance to theoretical biology; perhaps they are, but that is pure speculation.

Also, despite *The Turing Guide*’s joyous celebration of Turing’s growing fame, there seems to be a steady undercurrent of resentment that he isn’t even more famous. Of course, Turing was gravely undervalued for decades—the Bletchley work was kept so secret that Turing’s own mother, who

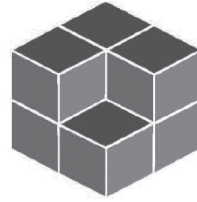
## BOOK REVIEW

By Ernest Davis



*The Turing Guide.* By Jack Copeland, Jonathan Bowen, Mark Sprevak, and Robin Wilson. Courtesy of Oxford University Press.

See Alan Turing on page 11



**Institute for Computational and Experimental Research in Mathematics**

## APPLY TO BECOME AN ICERM POSTDOC

*The Institute for Computational and Experimental Research in Mathematics (ICERM) at Brown University invites applications for its 2018-2019 postdoctoral positions.*

**Postdoctoral Institute Fellows:** ICERM supports two academic-year Postdoctoral Institute Fellows with salary and benefits.

**Postdoctoral Semester Fellows:** ICERM supports five four-month Postdoctoral Fellows each semester with salary and benefits.

**The 2018-2019 Semester Programs are:**

- Nonlinear Algebra (Fall)
- Computer Vision (Spring)

**Eligibility for all ICERM positions:**

Applicants must have completed their Ph.D. within three years of the start of the appointment. Documentation of completion of all requirements for a doctoral degree in mathematics or a related area by the start of the appointment is required.

**For full consideration:** Applicants must submit an AMS Standard Cover Sheet, curriculum vitae (including publication list), cover letter, research statement, and three letters of recommendation by January 1, 2018 to Mathjobs.org.

*Brown University is an Equal Opportunity/Affirmative Action Employer.*



More details can be found at:

<https://www.mathjobs.org/jobs/ICERM>

**To learn more** about ICERM programs, organizers, program participants, to submit a proposal, or to submit an application, please visit our website:

<http://icerm.brown.edu>

**Ways to participate:**

*Propose a:*

- semester program
- topical workshop
- summer undergrad program
- small group research project

*Apply for a:*

- semester program or workshop
- postdoctoral fellowship

*Become an:*

- academic or corporate sponsor

**About ICERM:** The Institute for Computational and Experimental Research in Mathematics is a National Science Foundation Mathematics Institute at Brown University in Providence, Rhode Island. Its mission is to broaden the relationship between mathematics and computation.

121 S. Main Street, 11th Floor  
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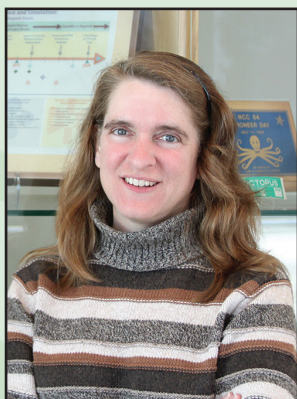
# Announcing Candidates for the Upcoming 2017 SIAM General Election

This fall, SIAM members will elect a President-Elect, Vice President at Large, and Secretary, as well as three members to serve on the SIAM Board of Trustees and four members to serve on the SIAM Council. We would like to introduce you to the following candidates standing for election. Be sure to make your voice heard on who will make important decisions for the organization — by voting! Look out for the email announcing elections in September to cast your vote!

## Vice President at Large



**Ilse Ipsen\***  
North Carolina State  
University



**Carol Woodward**  
Lawrence Livermore  
National Laboratory

## Board of Trustees

- **Russel Cafflich\***, University of California, Los Angeles
- **Charles Doering**, University of Michigan
- **Tamara G. Kolda\***, Sandia National Laboratories
- **Esmond Ng**, Lawrence Berkeley National Laboratory
- **Helena J. Nussenzweig Lopes**, Federal University of Rio de Janeiro
- **Henry Wolkowicz**, University of Waterloo

\* indicates incumbent

## President-Elect



**Tony Chan**  
Hong Kong University of  
Science and Technology



**Lisa Fauci**  
Tulane University

## Secretary



**Thomas Grandine**  
Boeing Company



**Chen Greif**  
University of British  
Columbia

## Council

- **Suncica Canic**, University of Houston
- **Hector Cenicerros**, University of California, Santa Barbara
- **Raymond Chan\***, The Chinese University of Hong Kong
- **Laura Grigori**, INRIA Paris
- **Geoffrey McFadden\***, National Institute of Standards and Technology
- **Lois Curfman McInnes**, Argonne National Laboratory
- **Michael Ng**, Hong Kong Baptist University
- **Padma Raghavan\***, Vanderbilt University

## Division of Math Sciences

Continued from page 7

applied areas. It is planned to continue this collaboration with in 2018.

### 4. Improving and Supporting the Transition to Graduate School in the Mathematical Sciences

The NSF Directorate for Education and Human Resources and the DMS invite proposals for projects designed to encourage and prepare U.S. students to pursue and succeed in graduate doctoral study in the mathematical sciences. Particular emphasis is placed on broadening participation of students from underrepresented populations, including racial/ethnic groups underrepresented in mathematics and statistics, individuals with disabilities, and women. The activity aims to support projects that are scalable—to serve large numbers of students without large increases in cost—and sustainable, that is, have continued impact without ongoing large influxes of grant funding. Projects are expected to involve mathematical sciences research as part of student training, and/or educational research that produces new knowledge to help the community understand for whom—and under what circumstances—proposed activities are effective in preparing a diverse population of students to be successful in graduate school.<sup>6</sup>

### About These New Initiatives

The DMS considers the first two aforementioned activities to be parts of the DMS research institutes portfolio, which currently constitutes approximately 12 percent of the annual DMS investment. These new opportunities represent the continued evolution of the DMS institute portfolio, which the division aims to keep current, dynamic, and responsive to emerging needs of the mathematical sciences community.<sup>7</sup> Both new programs were developed in close consultation with the communities involved, in particular through workshops that provided insight into current activity in these areas and perceived future needs. Both new programs are centered on an intellectual partnership between the mathematical sciences and another discipline, matched by significant financial investment from the other disciplinary partner. This arrangement reflects the worth of the interdisciplinary activity from a scientific viewpoint, in that it certifies the importance of these activities to both disciplines. It also greatly leverages DMS investments. The DMS is particularly pleased to be able to initiate a close partnership with the Simons Foundation in support of the new MathBioSys program.

The DMS considers the third and fourth activities to be parts of the DMS workforce program portfolio, which currently constitutes approximately 10 percent of the annual DMS investment. These new opportunities address two distinct community needs

in support of the development of the next generation of mathematical scientists. First, employment data<sup>8</sup> show that the majority of mathematical sciences Ph.D. recipients take employment other than conventional academic tenure-track positions; yet many U.S. graduate programs in the mathematical sciences do not provide students with needed information about potential non-academic career paths. The Mathematical Sciences Graduate Internship program is an early step towards raising doctoral students' awareness of potential, rewarding non-academic careers. Second, despite substantial efforts by the mathematical sciences community and investment by funding agencies, current data indicate that both the percentage of women and the percentage of students from underrepresented groups entering doctoral programs and receiving doctoral degrees in the mathematical sciences have remained relatively constant since 2004. These levels are well below the representation of these groups in the general population. The activity in Improving and Supporting the Transition to Graduate School in the Mathematical Sciences aims to catalyze cost-effective community projects based on proven techniques to address this underrepresentation.

### Outlook for the Future

As of this writing, the Congressional appropriation for the fiscal year 2017 budget has not been finalized. The expected fiscal year 2017 budget for the DMS is

\$233,512,000, which represents a small decrease of approximately \$400,000 from the 2016 level. The President's fiscal year 2018 budget request to Congress for the NSF<sup>9</sup> will result in a decrease in the DMS budget of approximately \$24,000,000, roughly a 10 percent reduction. The highest priorities for the DMS in this challenging budgetary climate are to maintain—to the extent possible—investments in its core activities, namely the disciplinary programs that fund unsolicited proposals for research by individual investigators and the research institutes portfolio.

Looking further into the future, the Mathematical Sciences Research Institutes program will hold an open competition<sup>10</sup> in fiscal year 2019. Proposals are invited for new institute projects from U.S. sites, as are renewal proposals from any of the currently-supported U.S.-based Mathematical Sciences Research Institutes. Awards from this competition are anticipated to begin in fiscal year 2020. The DMS is committed to maintaining investment in its research institutes portfolio at a level of 12-14 percent of the total DMS investment over the long term.

*Michael Vogelius is the division director of the Division of Mathematical Sciences (DMS) at the National Science Foundation. Tie Luo is the deputy division director of the DMS. Henry Warchall is the senior advisor at the DMS.*

<sup>6</sup> [https://www.nsf.gov/publications/pub\\_summ.jsp?ods\\_key=nsf17078](https://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf17078)

<sup>7</sup> <http://www.ams.org/notices/201511/moti-p1375.pdf>

<sup>8</sup> <http://www.ams.org/profession/data/annual-survey/annual-survey>

<sup>9</sup> <https://www.nsf.gov/about/budget/fy2018/index.jsp>

<sup>10</sup> [https://www.nsf.gov/funding/pgm\\_summ.jsp?pims\\_id=5302](https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=5302)



# SIAM Student Chapters Put Funds to Good Use

## Texas Tech Chapter Sponsors Graduate Minisymposium

The West Texas Applied Math Graduate Minisymposium took place this past April at Texas Tech University in Lubbock, Texas. Organized by Sara Calandrini and Giacomo Capodaglio, respectively the president and vice president of the Texas Tech University Chapter of SIAM, the event was open to all graduate students and postdoctoral associates in the field of applied mathematics. It was meant to foster the creation of a network for young researchers that could be useful for future collaborations and career development.

The minisymposium featured 11 talks by researchers from the University of New Mexico, Texas A&M University, the University of Texas at Arlington, the University of Texas at El Paso, in addition to Texas Tech. The talks covered various fields of applied mathematics, such as virus infection modeling, flow in porous media, reduced order modeling, and even mathematical tools for the detection of gravitational waves. Max Gunzburger (Florida

State University) served as the keynote lecturer, and his presence enhanced the event. Additionally, a poster presentation—with ten presenters—took place during the lunch break, giving attendees the opportunity to enjoy food while perusing posters and interacting with presenters.

A barbecue held the following day for all conference participants and Texas Tech's Department of Mathematics and Statistics celebrated the minisymposium's success. A plan to organize the minisymposium again next spring is in the works.

To read more about the symposium, please visit the webpage<sup>1</sup> or contact giacomo.capodaglio@ttu.edu. The event was sponsored by the Texas Tech University Chapter of SIAM and the Department of Mathematics and Statistics of Texas Tech.

— Giacomo Capodaglio, vice president of the Texas Tech University Chapter of SIAM

<sup>1</sup> <http://www.math.ttu.edu/Department/Calendar/Conferences/wtamgm/>



From left to right: Giacomo Capodaglio, vice president of the Texas Tech University Chapter of SIAM, keynote speaker Max Gunzburger (Florida State University), and Sara Calandrini, president of the Texas Tech University Chapter of SIAM. Photo credit: Sanjeeva Karunarathna.



From left to right: Kyle Henke, Juan Pablo Madrigal Cianci, and Geoffrey Schuette enjoy lunch and the accompanying poster presentation. Photo credit: Sanjeeva Karunarathna.

## Central Valley Regional SIAM Student Chapter Conference

Over 80 participants from universities in Northern and Central California attended the second annual Central Valley Regional SIAM Student Chapter Conference, held in April. Hosted by the University of California, Merced Chapter of SIAM, the event showcased student research in applied math.

The conference recognized students from UC Merced; the University of California, Davis; San Jose State University; and California State University, Fresno for institutional and geographic diversity and their work in expanding undergraduate participation.

Jessica Taylor—who received the SIAM Student Chapter Certificate of Recognition “for her outstanding efforts and accomplishments” on behalf of the UC Merced chapter—aims to increase promotion of undergraduate research at the university.

Taylor, the SIAM chapter president and a Ph.D. candidate in UC Merced's Applied Mathematics graduate group, spoke about motivating more undergraduates to get involved with the chapter and increasing collaboration between the chapter and other student organizations at the university.

Daniella Calvetti, the James Wood Williamson Professor of mathematics at Case Western Reserve University, delivered the keynote address. She spoke about her work on interactions and synergies of uncertainty quantification and numerical analysis.

With a focus on interdisciplinary research, the conference invited participants from various departments across the university. The event ended with a poster session spanning diverse areas, such as sea level rise and malaria immunity.

— Adapted from UC Merced University News

## GW Chapter Hosts Regional Conference

The George Washington University Chapter of SIAM: Conference on Applied Mathematics, held in late April at George Washington University (GW) in Washington, D.C., brought together speakers from universities and companies to present their work.

Researchers from Columbia University; John Hopkins University; the University of Maryland, College Park; George Mason University; and Fugue, Inc. delivered lectures. Attendees included undergraduate and graduate students, postdoctoral researchers, and experts from institutions in the Washington, D.C., metro area.

“We were excited to bring together students and faculty from the East Coast,” Chong Wang, president of the GW chapter, said. “The conference—with great diver-

sity—was very successful, and it was all possible due to the generosity of SIAM and the GW Department of Mathematics. Many students expanded their networks and definitely learned something new!”

“I liked that the event brought in people of diverse backgrounds,” one attendee remarked. “The topics were interesting, professional, and covered a nice range.”

The George Washington University Chapter of SIAM would like to thank SIAM and GW's Department of Mathematics for the financial support. We look forward to hosting students from across the region again in 2018.

— Chong Wang, Debdeep Bhattacharya, Eric Shehadi, and Yanxiang Zhao, for the George Washington University Chapter of SIAM



From left to right: SIAM student chapter faculty advisor Noemi Petra; Jessica Taylor, UC Merced student chapter president and recipient of the SIAM Student Chapter Certificate of Recognition; and keynote speaker Daniella Calvetti (Case Western Reserve University). Photo credit: Veronica Adrover, University Communications at UC Merced.



Attendees of the George Washington University Chapter of SIAM: Conference on Applied Mathematics. Photo credit: Chong Wang.



Keynote speaker Daniella Calvetti (second from right) sits among attendees of the second annual Central Valley Regional SIAM Student Chapter Conference. Photo credit: Veronica Adrover, University Communications at UC Merced.



# Benford's Law and Accelerated Growth

Benford's law, discovered by Simon Newcomb [2], is an empirical observation that in many sets of numbers arising from real-life data, the leading digit of a number is more likely to be 1 than 2, which in turn is more likely than 3, and so on. Figure 1 shows a count of leading digits from the 107 NASDAQ-100 prices,<sup>1</sup> sampled around noon on June 14, 2017. Although the monotonicity is clearly violated, there is a bias in favor of low leading digits.

The following example illustrates a mathematically rigorous deterministic (as opposed to probabilistic) counterpart of Benford's law. Consider a geometric sequence, for instance

$$1, 2, 4, 8, 16, 32, 64, 128, 256, \dots,$$

and extract from it the sequence of leading digits:

$$1, 2, 4, 8, 1, 3, 6, 1, 2, \dots$$

<sup>1</sup> <http://www.cnbc.com/nasdaq-100/>

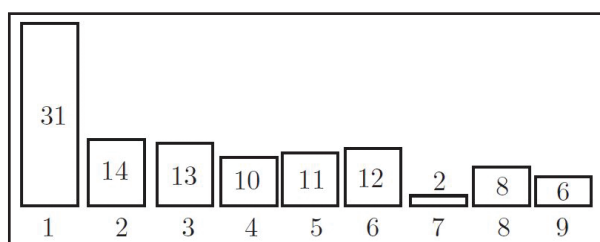


Figure 1. A snapshot of the distribution of leading digits in NASDAQ-100 stock prices.

It turns out that the frequency  $p_k$  of digit  $k$  is well defined and given by

$$p_k = \lg(k+1) - \lg k, \quad (1)$$

see [1]. In particular, the frequency decreases with  $k$ :

$$p_1 = \lg \frac{2}{1} > \lg \frac{3}{2} > \dots > \lg \frac{10}{9} = p_9. \quad (2)$$

In light of this example, if the price of a stock undergoes an exponential-like growth (in a loose analogy with the geometrical sequence), then the bias illustrated in Figure 1 may not be that surprising.

What is behind Benford's frequency bias (2) for the geometric series? A one-word answer is "acceleration." To see why, consider a continuous counterpart of 2<sup>n</sup>—say, the exponential function  $e^t$ , visualizing the point  $x = e^t \in \mathbb{R}$  as a particle moving with time along the  $x$ -axis.

Figure 2 shows the  $x$ -axis cut into segments  $[10^j, 10^{j+1})$  and stacked on top of each other, all of them scaled (linearly) to the same length. This cutting and scaling allows us to see the leading digit of  $e^t$  at a glance. Now the reason for Benford's law becomes

## MATHEMATICAL CURIOSITIES

By Mark Levi

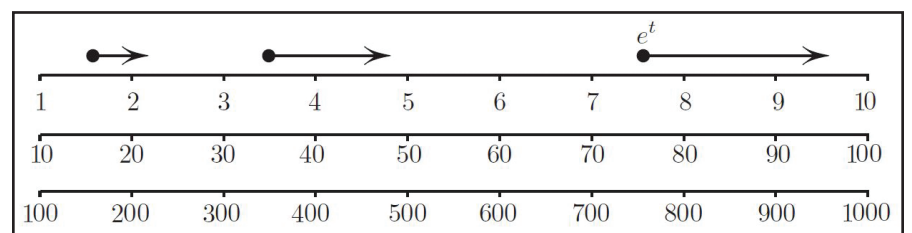


Figure 2. The intuition behind Benford's law.

clear: since  $e^t$  accelerates, it passes the higher-digit segments faster and is thus less likely to be found there.

Figure 2 makes it easy to compute the probability, i.e., the proportion of time, of observing the leading digit  $k$ . To that end, we find the time spent having the leading digit  $k$  while traversing the  $j$ th row in Figure 2:

$$\ln[(k+1)10^j] - \ln[k10^j] = \ln \frac{k+1}{k}.$$

We then divide it by the time of traversal  $\ln[10 \cdot 10^j] - \ln 10^j = \ln 10$ ; both times are independent of  $j$ , and thus the proportion of time spent with the leading digit  $k$  over time  $[0, T]$  approaches

$$\frac{\ln \frac{k+1}{k}}{\ln 10} = \lg \frac{k+1}{k},$$

## Alan Turing

Continued from page 8

died in 1976, never knew what her son had done—and the book makes a cogent case that, in general, British accomplishments in computer development have remained underappreciated compared to American achievements. However, one would think that Turing is largely getting his due at this point. Nonetheless, Boden seems bothered that Francis Crick and James Watson's discovery of the structure of DNA overshadowed Turing's theory of morphogenesis. Copeland appears irked by the observation that Albert Einstein is more famous than Turing, and notes that Einstein had a long head start. Most preposterous is a claim by

as  $T \rightarrow \infty$ , the same as the discrete result (1).

The figures in this article were provided by the author.

## References

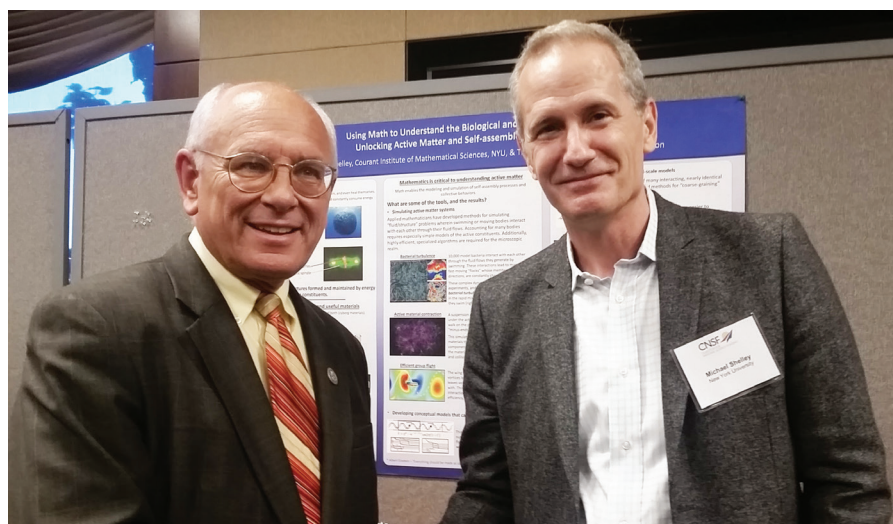
[1] Arnold, V.I. (1983). *Geometrical Methods in the Theory of Ordinary Differential Equations*. New York, NY: Springer-Verlag.

[2] Newcomb, S. (1881). Note on the frequency of use of the different digits in natural numbers. *American Journal of Mathematics*, 4(1), 39-40.

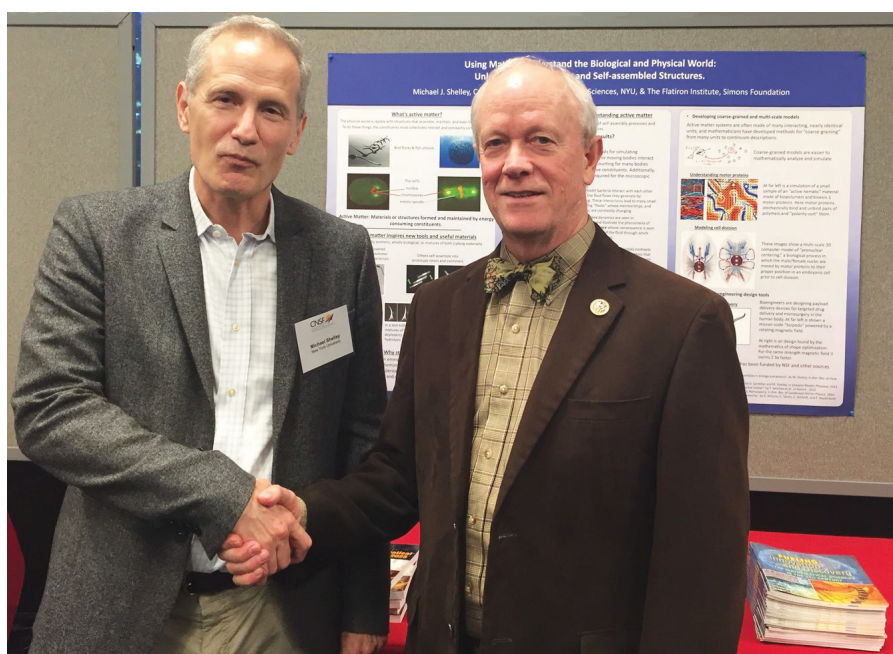
Mark Levi ([levi@math.psu.edu](mailto:levi@math.psu.edu)) is a professor of mathematics at the Pennsylvania State University.

## SIAM at the CNSF Exhibition

The 23rd Annual Coalition for National Science Funding (CNSF) Capitol Hill Exhibition, which took place on May 16th in Washington, D.C., was a success. Mike Shelley effectively represented the SIAM community, and spoke with Representatives Paul Tonko (D-NY) and Jerry McNerney (D-CA). He also conversed with France Córdoba, director of the National Science Foundation (NSF); Joan Ferrini-Mundy, acting chief operating officer of the NSF; Jim Ulvestad, acting assistant director of the Mathematical and Physical Sciences at the NSF; Debbie Lockhart, deputy assistant director of the NSF; and NSF senior advisor Henry Warchall.



Mike Shelley (right) meets with Representative Paul Tonko (D-NY) at the 23rd Annual Coalition for National Science Funding (CNSF) Capitol Hill Exhibition, which took place in Washington, D.C., this May. Photo credit: Eliana Perlmutter.



Mike Shelley (left) shakes hands with Representative Jerry McNerney (D-CA) at the recent 23rd CNSF Capitol Hill Exhibition, which was held this May in Washington, D.C. Photo credit: Miriam Quintal.

## Professional Opportunities and Announcements

Send copy for classified advertisements and announcements to [marketing@siam.org](mailto:marketing@siam.org). For rates, deadlines, and ad specifications visit [www.siam.org/advertising](http://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](http://www.siam.org)) or proceed directly to [www.siam.org/careers](http://www.siam.org/careers).

### The California Institute of Technology Department of Computing and Mathematical Sciences

The Department of Computing and Mathematical Sciences (CMS) at the California Institute of Technology invites applications for the position of lecturer in computing and mathematical sciences. This is a (non-tenure-track) career teaching position, with full-time teaching responsibilities. The start date for the position is ideally **September 1, 2017**, and the initial term of appointment can be up to three years.

The lecturer will teach introductory computer science courses, including data structures, algorithms, and software engineering, and will work closely with the CMS faculty on instructional matters. The ability to teach intermediate-level undergraduate courses in areas such as software engineering, computing systems, and/or compilers is desired. The lecturer will also assist in other aspects of the undergraduate program, including curriculum development, academic advising, and monitoring research projects. The lecturer must have a track record of excellence in teaching computer science to undergraduates. In addition, the lecturer will have opportunities to participate in research projects in the department. An advanced degree in computer science or a related field is desired but not required.

Applications will be accepted on an ongoing basis until the position is filled.

Please view the application instructions and apply online at <https://applications.caltech.edu/job/cmslect>.

The California Institute of Technology is an Equal Opportunity/Affirmative Action Employer. Women, minorities, veterans, and disabled persons are encouraged to apply.

### The Institute for Pure and Applied Mathematics

#### One-year Postdoctoral Position

The Institute for Pure and Applied Mathematics (IPMA) invites applications for a one-year postdoctoral position (renewable) with a monthly stipend of BRL 8.900,00 (after taxes). The position is intended for young researchers working on applied mathematics. Applications focusing on mathematical methods for solving problems of interest to some productive sector in Brazil are particularly welcome. Candidates with doctorates in areas other than mathematics areas are encouraged to apply.

The IPMA is committed to the principles of diversity and equal opportunity; in particular, women are encouraged to apply.

Details about the application procedure and necessary documentation can be found at [https://impa.br/en\\_US/page-noticias/novo-pos-doutorado-de-excelencia-no-imp/](https://impa.br/en_US/page-noticias/novo-pos-doutorado-de-excelencia-no-imp/). Applications should be made online, until October 15th, 2017.

The decision will be announced on November 2017. The selected candidate should start his/her activities at the IPMA at any time between January 1st and June 1st, 2018. Further inquiries should be addressed to [pdopen@impa.br](mailto:pdopen@impa.br).



# Data-enabled, Physics-constrained Predictive Modeling of Complex Systems

By Karthik Duraisamy

Even with recent advances in computing power and algorithms, a multitude of first-principles-based computations of physical problems remains out of reach, even on the most powerful supercomputers. This situation is unlikely to change for many decades for a number of important problems, such as those that involve bridging the gap between atomistic and continuum scales in materials science and combustion, climate and weather prediction, and structure formation and evolution in the universe. As a result, the scientific community continues to rely on physical intuition and empiricism to derive approximate models for prediction and control.

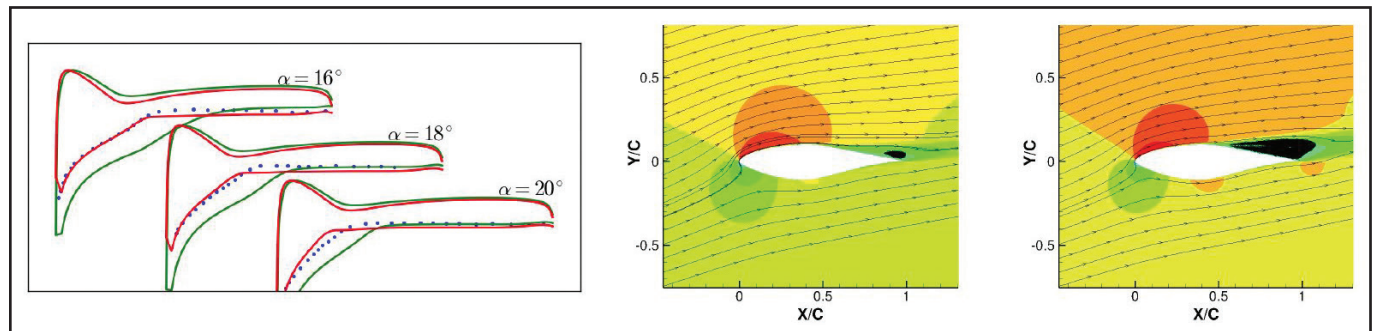
With the proliferation of high-resolution datasets and advances in computing and algorithms over the past decade, data science has risen as a discipline in its own right. Machine learning-driven models have attained spectacular success in fields such as language translation [3], speech and face recognition, bioinformatics, and advertising. The natural question to ask then is: Can we bypass the traditional ways of intuition/hypothesis-driven model creation and instead use data to generate predictions of physical problems? In other words, can one extract cause-and-effect relationships and create reliable predictive models based on a large number of observations of physical phenomena? The instinctive response from the physical modeler is typically along the lines of “curve-fitting is not physics,” and the like. The data scientist or statistician, on the other hand, exudes more optimism based on faith in approximation theory,

reinforced by successes in some application domains. Though application has been restricted to simple problems, inference and machine learning have indeed been used to extract operator matrices [6], discover dynamical systems [1, 10], and derive the solution of differential equations [7]. To develop improved predictive models of complex real-world problems, however, one may need to pursue a more balanced view. Data cannot be an alternative for physical modeling, but when com-

physics; we may not have enough data in all regimes of interest; and the data may be noisy and of variable quality. As a result of these challenges, if one were to apply machine learning directly to datasets (as in a speech recognition/translation example), the validity of the resulting models may be limited around the specific circumstances that generated the data. In other words, the predictive model might not be generalizable. Therefore, a pragmatic solution is to combine physics-based models with

Combining physical models with data-driven techniques yields the potential to derive predictive and generalizable models in a number of disciplines. While one can argue that model creation has always been data-enabled, renewed opportunities exist, courtesy of access to a high quality and quantity of data, better tools/techniques, and more powerful computers.

Against this backdrop, the scientific computing community is beginning to recognize the promise of data-enabled model-



**Figure 1.** Example of data-augmented, physics-based modeling applied to turbulent flow prediction. Predictive improvement is achieved based on inferring force data over another airfoil and constructing machine-learned model augmentations. **Left.** Pressure over airfoil surface. Green: baseline physics model. Red: machine learning-augmented physics model. Blue: experimental measurements. **Middle.** Baseline flow prediction (pressure contours and streamlines). **Right.** Flow prediction using machine learning-augmented physics model. Image adapted from [8].

combined with—and informed by—a detailed knowledge of the physical problem and problem-specific constraints, it is likely to yield successful solutions.

Consider a true process  $\mathbf{u}$  governed by a set of equations that are either unknown or too expensive to discretize. Assuming we want to derive *data-driven* models for a surrogate variable  $\bar{\mathbf{u}}$ , a few challenges arise: there may exist several latent variables  $\bar{\mathbf{v}}$  (which may encode the relationship between  $\mathbf{u}$  and  $\bar{\mathbf{u}}$ ) that might not be identifiable without a knowledge of the

data-based methods and pursue a hybrid approach. The rationale is as follows: by blending data with existing physical knowledge and enforcing known physical constraints [4] (mass and energy conservation, for instance), one can improve model robustness and consistency with physical laws and address gaps in data. This would constitute a *data-augmented physics-based* modeling paradigm.

In traditional modeling approaches, it is typical to write down a set of physics-based governing equations  $\mathcal{M}(\bar{\mathbf{u}}, \bar{\mathbf{v}}) = 0$ , where  $\mathcal{M}$  is a model operator. Using this model as a starting point, data-augmented models may seek a model form  $\mathcal{M}^\gamma(\bar{\mathbf{u}}, \bar{\mathbf{v}}, \beta(\bar{\mathbf{u}}, \bar{\mathbf{v}}), \alpha) = 0$ , where  $\alpha$  may be a set of parameters,  $\beta$  may be a functional form, and  $\mathcal{M}^\gamma$  may be an augmented set of operators, likely derived based on available data and selection of priors.

In some applications, the use of machine learning can be direct and powerful. For instance, researchers have used manifold learning to extract a constitutive relationship in solid mechanics directly from data [2]. They have successfully employed machine learning to learn density functionals [9] in electronic structure calculations. In many problems, however, the information extracted from the data can be defined only in the context of the model. This aspect can restrict the use of machine learning on the data, even if the starting point is a physics-based model. As an example, a constitutive relationship  $\beta(\bar{\mathbf{u}}_{data}, \bar{\mathbf{v}}_{data})$  extracted directly from the data may become inconsistent with the rest of the model in a predictive modeling setting because the latent variable in the model  $\bar{\mathbf{v}}_{model}$  might be an operational variable, whereas its counterpart in the data  $\bar{\mathbf{v}}_{data}$  might be a physical variable. Consequently, machine learning must be preceded by statistical inference in many problems. Statistical inference thus uses data to derive problem-specific information that consistently connects model augmentations to model variables. If the goal is predictive rather than reconstructive modeling, the outputs of several such inverse problems (on different datasets representative of the physical phenomena) must be transformed into general functional forms  $\beta(\bar{\mathbf{u}}, \bar{\mathbf{v}})$  using machine learning [5]. Figure 1 shows an example where lift data from one airfoil is used to infer and reconstruct functional forms of turbulence model discrepancies on other airfoils at flow conditions different from those in which the model was trained.

ing of complex physics. Initial successes have been noted, albeit on academic problems. For these techniques to have a significant impact in application domains, scientific rigor in data preparation, selection of priors, feature engineering, model training, and model deployment must be combined with domain expertise.

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Karthik Duraisamy is an associate professor of aerospace engineering and director of the Center for Data-driven Computational Physics at the University of Michigan, Ann Arbor.

## 2017 Kovalevsky and Reid Prizes

Liliana Borcea is the recipient of the 2017 AWM-SIAM Sonia Kovalevsky Lecture. The Lecture, intended to highlight significant contributions of women to applied or computational mathematics, is awarded annually at the SIAM Annual Meeting. Borcea is being recognized for distinguished scientific contributions to the mathematical and numerical analysis of wave propagation in random media, array imaging in complex environments, and inverse problems in high-contrast electrical impedance tomography, as well as model reduction techniques for parabolic and hyperbolic partial differential equations. “I am honored to be in the company of the outstanding women mathematicians that have won this award,” Borcea said.



Liliana Borcea, University of Michigan.

Borcea is the Peter Field Collegiate Professor of Mathematics at the University of Michigan. She received her M.S. and Ph.D. in scientific computing and computational mathematics from Stanford University, and is an elected member of the SIAM Council. “My work and research interests are motivated by my view of applied mathematics as a science that reaches across disciplines to computer science, physics, statistics, and experimental science,” Borcea said. “SIAM is a unique forum for applied mathematicians to exchange ideas and pursue interdisciplinary research.”

The AWM-SIAM Sonia Kovalevsky Lecturer receives a certificate signed by the presidents of AWM and SIAM.

### SIAM PRIZE SPOTLIGHT

Jean-Michel Coron has been awarded SIAM’s 2017 W.T. and Idalia Reid Prize in Mathematics. The prize recognizes outstanding work in, or other contributions to, the broadly defined areas of differential equations and control theory. Coron is being honored for fundamental contributions with lasting impact to both the analysis and control of nonlinear ordinary and partial differential equations, and in particular the Coron return method for feedback stabilization of nonlinear systems using time-varying controls, as well as applications of control theory to practical problems.



Jean-Michel Coron, Université Pierre et Marie Curie.

Coron is a full professor at Université Pierre et Marie Curie and a member of the French Academy of Sciences. He received his Thèse d’Etat (Ph.D.) in mathematical sciences from Université Pierre et Marie Curie. “The W. T. and Idalia Reid Prize is one of the most prestigious prizes in control theory, as confirmed by the outstanding level of previous laureates,” Coron said. “I am strongly honored to receive this award. It is for me a very important recognition of my works in control theory.”

The W.T. and Idalia Reid Prize recipient receives a cash prize of \$10,000 and an engraved medal, awarded at the SIAM Annual Meeting.