sinews.siam.org

Volume 50/ Issue 3 April 2017

Special Issue on the Mathematics of Planet Earth

In honor of Earth Day on April 22, we present articles on food security, sustainability, resource estimation and management, sea ice modeling, and more in this **special issue**!



Image courtesy of Steffen et al

In an article on page 5, Hans Kaper and Mary Lou Zeeman illustrate how mathematical and computational skills can help model food systems.

Assessing Risks to **Global Food Security** How Mathematicians Can Help

By James Case

The inaugural SIAM Conference on Mathematics of Planet Earth, held last September in Philadelphia, Pa., featured a public lecture by Molly Jahn of the University of Wisconsin, Madison (UW-Madison). Jahn, whose talk was entitled "Risks and Resilience in Global Food Systems: An Invitation for Mathematicians," holds appointments in the Department of Agronomy, the Global Health Institute, and the Center for Sustainability and the Global Environment. She has served as dean of the university's College of Agriculture and Life Sciences, director of the Wisconsin Agricultural Experiment Station, and Deputy and Acting Under Secretary of Research, Education, and Economics at the U.S. Department of Agriculture.

Jahn began her lecture by conceding that the current agricultural establishment (farmers, agribusinesses, and the agricultural research community) has been "stunningly successful" in improving agricultural productivity and efficiency. How else could we possibly be feeding a global population that has grown from under 2 billion to over 7 billion in the last century? She hastened to add, however, that the existing food delivery system is by no means ideal. It leaves some 800 million people undernourished, while 1.5 billion are overweight or obese. Meanwhile, estimates indicate that 1.4 billion tons of food are wasted each year. Though this is a small fraction of the total quantity produced, it is still significant more than enough to feed the 1.4 billion people subsisting on \$1.25 per day, or the 1.5 billion people who reside on degrading land. According to the Commission on Sustainable Agriculture and Climate Change (CSACC), more than 30 million acres of agricultural land are degraded each year due to overgrazing and other poor agricultural practices, climate change, groundwater depletion, urban sprawl, and additional human activities.

Cropland degradation, however, is not the only way in which current practices are overtaxing the planet. According to Jahn, the historic focus of research and intensive inputs

See Global Food Security on page 4



Filling the Sea Ice Data Gap with Harmonic Functions A Mathematical Model for the Sea Ice Concentration Field in Regions Unobserved by Satellites

By Courtenay Strong and Kenneth M. Golden

ea ice is frozen seawater that forms on \mathbf{O} the ocean surface in the Arctic basin and around the continent of Antarctica. Sea ice packs cover millions of square kilometers of our planet's surface and provide a habitat crucial to a diverse array of microorganisms, small crustaceans, marine birds, and mammals. Observed declines in sea ice amounting to approximately half a million square kilometers per decade are impacting global climate and ecosystems, and positive sea ice-albedo feedback is accelerating melting [2]. Sea ice has a very high albedo, meaning that it reflects most of the incoming sunlight. Declining ice coverage due to melting results in more solar energy entering the climate system, which leads to more warming and hence more melting. In fact, the September minimum of Arctic sea ice

extent dropped to about 3.4 million square kilometers in 2012, which is less than half of the 1979-2000 average value of approximately 7 million square kilometers.

Since 1972, the National Aeronautics and Space Administration has been monitoring sea ice using satellites that detect the small amounts of microwave radiation emitted by the ice. The satellites detect microwave emission through clouds during both day and night, and the resulting grids at 25-km horizontal resolution provide the most spatially-complete, long-term observational record of sea ice concentrations $(0 \le c \le 1)$ over the polar regions in both hemispheres. Unfortunately, the orbit inclination and instrument swath of the passive microwave satellites leave a "polar data gap" around the North Pole where sea ice is not observed (see Figure 1). For many years, researchers assumed that this northernmost region of the Arctic was always covered

with sea ice. However, recent precipitous losses in the polar ice pack [1] call into question this assumption, which can significantly affect overall estimates of Arctic sea ice volume. By way of anecdotal evidence, the past two Decembers (2015 and 2016) have seen freakishly warm temperatures around the North Pole, with periods of almost 50 degrees Fahrenheit above average. Such dramatic changes motivate development of an objective method for estimating unobserved concentrations within the gap.

We propose [6] a partial differential equation-based model with tuned stochastic spatial heterogeneity to estimate the concentrations within a region Ω on Earth's surface:

$f(\theta,\phi) = \psi(\theta,\phi) + W(\theta,\phi),$

where $\theta~$ is longitude and $\phi~$ is latitude, or $f(\vec{r}) = \psi(\vec{r}) + W(\vec{r})$, where $\vec{r} \in \Omega$. We

See See Ice on page 3



Figure 1. The left image is an example of the polar data gap (dark blue disc) on August 30, 2007, with shading outside the disc indicating concentration. The middle and right images show the data fill presented here; the color shading at right is similar to that used by the National Snow and Ice Data Center (http://nsidc.org). Image adapted from [6].

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

4



Cartoon created by mathematician John de Pillis

In the 1990s, there was an effort to provide templates: descriptions of general algorithms that could be customized by the user. SIAM published two books of templates: one on eigenvalue problems [2] and the other on iterative methods for linear equations [3], the latter being accompanied by bare-bones

> Fortran and MATLAB codes. Both books have been very successful.

More recently, a number of SIAM book authors, especially those

writing for the Fundamentals of Algorithms series, have built short, readable codes into their books. Nick Trefethen's Spectral Methods in MATLAB (2000) contains 40 short programs, and he notes that "you can do an astonishing amount of serious computing in a few inches of computer code!" In have recently written a survey of nonlinear eigenvalue problems that includes 12 very short MATLAB programs implementing the main methods discussed [6]. The reader can gain much insight by downloading and playing with the codes. It is also worth noting that some of SIAM Review's most highly cited articles, such as "An Algorithmic Introduction to Numerical Simulation of Stochastic Differential Equations" [7], include short codes.

What is my favorite short program? I offer funm_randomized in Figure 1. This MATLAB function computes f(A)for a square matrix A and a given scalarvalued function f. The built-in MATLAB function funm does the same thing, but is a few hundred lines long and has some restrictions on f. How can funm_randomized be so short? Adding a random perturbation to A produces a matrix that can be "safely" diagonalized. The error in the computed f(A) is typically at or below the level of the square root of the unit roundoff, so the accuracy will generally be quite a bit worse than for funm. Brian Davies proposed and analyzed this "approximate diagonalization" method [4]. Open questions about its behavior remain, and I hope it will be further studied.

The 35-year old "10 print" maze program may seem irrelevant, written in a moribund language. But according to the TIOBE Index for March 2017,³ Basic is still the sixth most popular programming language. As state-of-the-art numerical software grows in length, in response to more

See Short Codes on page 5

http://www.tiobe.com/tiobe-index/

Errata and Clarifications

nomics and the hydrologic cycle. 7 **Dakota Software: Explore** and Predict with Confidence Michael Eldred, Brian Adams, and Laura Swiler describe the Dakota project, which supports a global user community by providing state-of-the-art research and robust, usable software for optimization and uncertainty quantification.



How to Count Fish 9 **Using Mathematics** Bob Pego describes a coagulation-fragmentation model of animal group sizes that addresses resource estimation issues. Pego makes the case that fish school size distribution is highly non-Gaussian, and that ocean fisheries may be overestimating the total population of fish in the sea.

10 Applying Design Thinking to Mathematics Research Jennifer Pearl and Padmanabhan Seshaiyer examine the parallels between design thinking (DT) and mathematical discovery. They introduce readers to DT by demonstrating its successful use in the development of interdisciplinary mathematical approaches to combat animal poaching.



11 Professional Opportunities

nested loops of Gaussian elimination, and go on to implement partial pivoting with just a little more effort. Yet a modern Ax = bsolver must be vastly more complicated than the mathematics suggests if it is to exploit modern computer architectures. Depending on the solver, this might mean employing a panel factorization with an appropriate blocking and use of level 3 BLAS operations,

or using a tile-based factorization with dynamic task scheduling [1]. And exploiting sparsity introduces further complexities. Davis et al. [5] estimate that behind the MATLAB backslash

with a sparse matrix lie about 120,000 lines of code implementing sparse direct methods.

Until the 1970s, it was possible to write practical codes for solving the standard numerical analysis problems within twothree pages; this is what George Forsythe and Cleve Moler did in their book Computer

```
function F = funm_randomized(A, fun)
                     Evaluate general matrix function (randomized).
%FUNM RANDOMIZED
   Randomized approximate diagonalization method of Davies (2007).
%
tol = 8*eps(A(1,1)); % Tolerance for single or double precision A.
E = randn(size(A));
[V,D] = eig(A + (tol*norm(A,'fro')/norm(E,'fro'))*E);
F = V*diag(fun(diag(D)))/V;
```

FROM THE SIAM

PRESIDENT

By Nicholas Higham

Figure 1. MATLAB function funm_randomized.m. This code can be downloaded from https://gist.github.com/higham.

Solution of Linear Algebraic Systems (1967) and later, with Michael Malcolm, in Computer Methods for Mathematical Computations (1977). Moler has said, "One of the biggest reasons these two books were as successful as they were was because the programs in them were not only useful and correct, they were short and readable."²

1 https://nickhigham.wordpress. com/2016/06/29/the-one-line-maze-programin-matlab

a similar vein, his "Ten Digit Algorithms" essay [9] presents algorithms with three constraints: "The program can be at most one page long, and it has to solve your problem to at least ten digits of accuracy on your machine in less than five seconds.'

Providing a short code to help the reader understand the essence of an algorithm in research articles can also be beneficial. Indeed, a good test for an author of a survey paper is to produce simple implementations of the algorithms that are treated. My col-

and Announcements

http://blogs.mathworks.com/ 2 cleve/2013/01/07/george-forsythe/

leagues Stefan Güttel and Françoise Tisseur

Dynamical Systems

Comparison Design Constraints of Constraints of Constraints of Constraints of Constraints of Constraints of Constraints Design Design Des Geometric Design J. Peters, University of Florida Geosciences L. Jenkins, Clemson University Life Sciences T. Kepler, Boston University Imaging Science E. Miller, Tufts University Algebraic Geometry J. Draisma, Technische Universiteit Eindhoven (TUE) Computational Science and Engineering P. Constantine, Colorado School of Mines Applied Mathematics Education P. Seshaiyer, *George Mason University* Nonlinear Wayes and Coherent Structures T. Bridges, University of Surrey Mathematics of Planet Earth H. Kaper, *Georgetown University* Uncertainty Quantification Y. Marzouk, Massachusetts Institute of Technology Optimization Andreas Wächter, Northwestern University

SIAM News Staff

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

Jan/Feb 2017 (Volume 50, Issue 1) In the obituary for Joseph Keller, written by Bernard J. Matkowsky, "Brillouin" is misspelled as "Brioullin" in two places.

March 2017 (Volume 50, Issue 2)

In the article entitled "Modeling Vegetation Patterns in Vulnerable Ecosystems" by Lakshmi Chandrasekaran, Max Rietkerk's name is spelled inconsistently. It should be "Rietkerk," not "Reitkerk."

In Jim Case's book review of Calculating the Cosmos: How Mathematics Unveils the Universe, symplectic integrators, numerical methods specifically designed for the integration of ordinary differential equations in Hamiltonian form, should be $\dot{p} = H_{a}(p,q), \ \dot{q} = -H_{p}(p,q),$ not $\dot{p} = -H_{q}(p,q), \ \dot{q} = -H_{p}(p,q)$

siam news

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

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

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

Printed in the USA.

siam is a registered trademark.

Editorial Board

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

Representatives, SIAM Activity Groups

Linear Algebra

R. Renaut, Arizona State University Discrete Mathematics D. Hochbaum, University of California, Berkeley Mathematical Aspects of Materials Science I. Fonseca, Carnegie Mellon University Supercomputing L. Grigori, INRIA Paris-Rocquencourt, France Control and Systems Theory F. Dufour, INRIA Bordeaux Sud-Ouest, France

Obituaries

By Sarah M. Taylor, Robert J. Taylor, and Douglas W. McMillan

Mathematician Brockway McMillan passed away in Sedgwick, Maine on December 3, 2016. Born in Minneapolis, Minn. on March 30, 1915, he was the only child of Franklin Richardson McMillan, a civil engineer, and Luvena Lucille Brockway McMillan, a school teacher. After living briefly in Philadelphia, Pa. and Brooklyn, N.Y., the McMillans returned to Minneapolis for several years, finally settling in Hinsdale, Ill. in 1925. There Brockway graduated from high school and studied for two years at the Armour Institute of Technology (which later merged with the Lewis Institute to become the Illinois Institute of Technology), before transferring to the Massachusetts Institute of Technology in 1934. He received his B.S. in 1936 and his Ph.D. in 1939, both in mathematics. His thesis, "The calculus of discrete homogeneous chaos," was supervised by Norbert Weiner.

In the fall of 1939, Brockway moved to Princeton University as a Charlotte Elizabeth Proctor Fellow; a year later he was appointed Henry B. Fine Instructor. In June 1942, a mutual friend introduced him to mathematician Elizabeth Audrey Wishard at the Institute for Advanced Study. They married in September.

Soon after his marriage, Brockway entered the Navy, where he served as an ensign at

Sea Ice

Continued from page 1

suggest prescribing the scalar field ψ to be a solution of Laplace's equation

$$\Delta \psi = 0$$

in spherical coordinates with boundary conditions taken from observations on the boundary $\partial\Omega$ of the polar data gap. A unique solution for ψ exists if $\partial\Omega$ is sufficiently smooth and the concentration is a continuous function along $\partial\Omega$. One can numerically obtain this solution by expressing the Laplacian as a second-order finite difference operator. The stochastic term Wprovides realistic deviations from ψ , and was tuned by collecting samples W_s of the difference between observed concentrations and ψ in three circular regions, C_j , j = 1, 2, 3, around the polar data gap,

$$\begin{split} W_{_{s}}(\vec{r}) &= f_{_{\rm obs}}(\vec{r}) - \psi(\vec{r}), \\ \vec{r} &\in C_{_{i}}, \quad j=1,2,3, \end{split}$$

where $f_{\rm obs}$ denotes observed concentrations. Based on analysis of thousands of samples, we formulate a seasonally varying amplitude for *W* and introduce realistic spatial autocorrelation by convolution of spatially uncorrelated noise with a Gaussian function. Figure 1 (on page 1) shows an example of this model applied to the polar data gap in map view for August 30, 2007. Figure 2 below shows this same example with concentrations represented by a third vertical dimension. Tests in regions around the polar data gap reveal observation-model correlations of 0.6 to 0.7 and absolute deviations of order 10^{-2} or smaller. the Naval Proving Grounds in Dahlgren, Va., testing weapons and studying their ballistics. In December 1945, Brockway was reassigned to the Manhattan Project in Los Alamos, N.M., where his daughter

Sarah was born. After his discharge from the Navy as a first lieutenant in 1946, Brockway joined the Mathematical Research Group at Bell Telephone Laboratories in Murray Hill, N.J. His son Douglas was born in 1947 in nearby Summit, where-except for two assignments with the federal government in Washington, D.C.--the McMillans lived until 1979. His son Gordon was born in Boston, Mass. in 1952 while Brockway attended the

Lincoln Summer Study Group. In Summit, Brockway served on the Board of Education, eventually becoming Board president.

At Bell Labs, Brockway's research produced papers and theorems on information theory, in collaboration with Claude Shannon and John Tukey. Other technical interests included electrical network theory and random processes. In later years he fondly recalled his time at Murray Hill, the intellectual stimulation of like-minded colleagues, their noontime experiments with boomerangs and word games, singing in the Murray Hill Chorus, and playing the "wobble organ"¹—a DIY elec-

> tronic musical instrument invented by Larned Meachem, Brockway's Bell Labs colleague. In 1955, Brockway left the research group to become Assistant Director of Systems Engineering and, in 1959, Director of Military Research.

By the late 1950s, Brockway's expertise in communication systems research and development was in demand at the National Security Agency and the Department of Defense. During the winter of 1958-59, Brockway

served as assistant to James Killian, President Dwight D. Eisenhower's science advisor. In 1961, President John F. Kennedy appointed Brockway as Assistant Secretary of the Air Force for Research and Development. Two years later, he became Under Secretary of the Air Force and concurrently the second director of the National Reconnaissance Office

¹ http://120years.net/the-wobble-organlarned-ames-meacham-usa-1951/ (NRO). As director, he advocated maintaining the NRO as the primary U.S. agency in space reconnaissance, and presided over the development of a second-generation, highresolution imaging satellite system.

Brockway returned to Bell Labs in 1965, serving as Vice President for Military Systems from 1969 until his retirement. In 1967, the McMillans bought an 1820s farmhouse overlooking the Benjamin River in Sedgwick, where they summered regularly until retiring there in 1979.

During retirement, Brockway continued his research and correspondence with fellow scientists and mathematicians, consulted for the U.S. government and Eastern Airlines, and stayed active in the American Mathematical Society and SIAM. He served as president of SIAM from 1959 to 1960. Brockway was a fellow of the Institute of Electrical and Electronics Engineers, a fellow of the American Association for the Advancement of Science, and a member of the National Academy of Engineering.

He and Audrey traveled extensively in the U.S. and Europe, spending one winter in Berkeley, Calif., to give a series of invited lectures at the University of California. At home in his Sedgwick darkroom, Brockway developed and printed thousands of pictures, which he exhibited locally. He served as president of the Sedgwick-Brooklin Historical Society and chairman of the

See Obituaries on page 5



Figure 3. 3a. For September 29, 2010, pack ice is shaded gray, the marginal ice zone is shown in white, sparse ice and open ocean are shaded blue, land is shaded black, and islands over which concentrations were interpolated are outlined in black. Image adapted from [7]. **3b.** The solution ψ to Laplace's equation within the marginal ice zone (MIZ) is shaded, and the black curves are examples of streamlines through ψ whose arc lengths define MIZ width. Image adapted from [7]. **3c.** Colored curves are examples of streamlines of a solution to Laplace's equation on a cross-section of the cerebral cortex of a rodent brain, the arc lengths of which are used to objectively measure cortical thickness. Image adapted from [4].

Our formulation of the data fill was motivated by our prior work [5] using Laplace's equation to approximate sea ice concentrations within the marginal ice zone (MIZ), the region where sea ice concentrations transition from dense pack ice $(c \ge 0.8)$ to open ocean $(c \le 0.15)$ (see Figure 3a). The MIZ is important from both climatic and ecological perspectives, and is characterized by strong ocean-ice interactions where waves penetrate the sea ice pack. By adapting medical imaging techniques for measuring non-convex shapes and volumes in the human body [3], we define the width of the MIZ as the arc length of a streamline through the solution to Laplace's equation (see Figure 3b). Spatially averaging the widths reveals a dramatic 39% widening of the MIZ over the satellite record [7]. Figure 3c illustrates an example of the Laplace method applied to measuring the thickness of a rodent cerebral cortex. In the formulation for filling the polar data gap, a least-squares linear function could replace the solution to Laplace's equation, but at the expense of observationmodel agreement along $\partial \Omega$. One could think of the function ψ more generally as the solution to a Poisson equation, or a more general elliptic equation incorporating a local conductivity or diffusivity $D(\vec{r})$,

$$\nabla \cdot (D\nabla \psi) = 0,$$

thereby accommodating local extrema precluded by Laplace's equation. By further increasing the complexity and computational expense, the polar data gap could also be filled by sophisticated numerical models of sea ice evolution, which incorporate dynamics and thermodynamics. In any event, developing methods to objectively fill this critical data gap is a worthy mathematical challenge and will impact our understanding of Earth's rapidly-changing climate. trends, 1979-2010. *The Cryosphere*, *6*, 881-889.

[2] Intergovernmental Panel on Climate Change. (2013). Summary for Policymakers. In *Climate Change 2013: The Physical Science Basis* (pp. 1-30). New York, NY: Cambridge University Press.

[3] Jones, S.E., Buchbinder, B.R., & Aharon, I. (2000). Three-dimensional mapping of cortical thickness using Laplace's equation. *Hum. Brain Mapp.*, *11*, 12-32.

[4] Lee, J., Kim, S.H., Oguz, I., & Styner, M. (2016). Enhanced cortical thickness measurements for rodent brains via Lagrangian-based RK4 streamline computation. *Proc. SPIE Intl. Soc. Opt. Eng.*, 9784, 97840B.

[5] Strong, C. (2012). Atmospheric influence on Arctic marginal ice zone position and width in the Atlantic sector, February-

Brockway McMillan, 1915-2016.

References

[1] Cavalieri, D.J., & Parkinson, C.L. (2012). Arctic sea ice variability and



Figure 2. The example in Figure 1 (on page 1) with concentration indicated by shading and surface elevation. Panels show the polar data gap (left), the solution to Laplace's equation within the gap (middle), and the solution with realistic spatial heterogeneity added (right). Image adapted from [6].

April 1979-2010. *Climate Dynamics*, 39, 3091-3102.

[6] Strong, C., & Golden, K.M. (2016). Filling the polar data gap in sea ice concentration fields using partial differential equations. *Remote Sensing*, 8(6), 442-451.

[7] Strong, C., & Rigor, I.G. (2013). Arctic marginal ice zone trending wider in summer and narrower in winter. *Geophys. Res. Lett.*, 40(18), 4864-4868.

Courtenay Strong is an associate professor of atmospheric sciences at the University of Utah. A substantial component of his research focuses on modeling and analysis of the cryosphere, which includes sea ice and snow. Kenneth M. Golden is a distinguished professor of mathematics and an adjunct professor of bioengineering at the University of Utah. His research is focused on developing mathematics of composite materials and statistical physics to model sea ice structures and processes.

Building Sustainable Decision Tools for a Sustainable Environment

By Kathleen Kavanagh, Lea Jenkins, and Shawn Matott

R esource management, like most things in life, is an optimization problem. When resources grow particularly scarce, their allocation becomes part of national and global news. Efficient water use is increasingly vital as periods of sustained drought, increased activity in previously-undeveloped regions, and overuse of water supplies place long-term water availability in peril. Recent examples include water shortages in the agriculturally-intense states of California and Kansas, where underlying aquifers could be pumped completely dry in our lifetime.

The crises are heightened when there are disparate uses for the resource. In agricultural regions, for instance, farmers, residents, and native environments all compete for access to the same shared water source. Our efforts are intended to help solve challenging resource allocation problems through meaningful dialogue. This requires us to be mindful of all perspectives, and to help resource managers model and balance these perspectives—using trusted, validated solution components—for synergistic, sustainable solutions. As world populations continue to grow, we constantly need to do more with less; our ability to support existing and future populations is dependent on our ability to sustain, and even supplement, available resources. Local governments, including water development boards, are required to set policy to govern the efficient use of resources. As decision-makers, their recommendations must be supported by quantitative analysis that attempts to balance the interests of the competing users.

Addressing these resource crises requires significant collaboration between applied mathematicians with expertise in computer simulation, optimization, and uncertainty; hydrologists; economists; computer scientists; members of the farming community; and water control boards that can define and simulate the relevant problems. We have taken advantage of the workshop program available through the American Institute of Mathematics (AIM) to gather researchers with expertise in different aspects of water resource issues. Funding through the AIM in 2015 allowed us to connect researchers from these disciplines for a week-long discussion of these issues. We aim to model and simulate water resource problems in agricultural sectors of California by developing a user-friendly and open-source software framework to facilitate rational stakeholder decisions in agricultural settings where water availability is of concern (see Figure 1, on page 6).

Our goal is to develop and make easily available an integrated modeling system for exploring water policy alternatives using a linked set of existing models of farming economics and the hydrologic cycle. We chose to meet this objective by making extensive use of existing software tools, in part because repeated studies by a wide range of users have validated these tools. We use the MODFLOW One Water Hydrologic Model (MF-OWHM), created by the United States Geological Survey, to model water resource management and agricultural production in our regions of interest, and we use the Dakota¹ software suite developed at Sandia National Laboratories to handle the optimization.

Our initial attempt, along with farmers from Reiter Affiliated Companies,² to address concerns about water usage in the Pajaro Valley berry-growing region of California generated multiple competing objectives. Preliminary results from an optimization study that did not use an underlying simulation tool have already yielded changes in farming techniques [1, 4]. The ability to represent the farming cycle's impact on water resources and the environment with state-of-the art modeling software will further advance sustainable farming practices.

Researchers have developed, enhanced, and implemented MF-OWHM over decades as an industrial simulation tool meant to

See Sustainable Environment on page 6

¹ Read an in-depth article on page 7 by Michael Eldred, Brian Adams, and Laura Swiler about the Dakota software suite's features ² http://www.berry.net/

Global Food Security

Continued from page 1

on maximizing crop yield has obscured the extent and vulnerability of globalized and regionalized food delivery systems: large parts of the world no longer do—and presumably no longer can—feed themselves. Crop failures or food system interruptions, especially due to multiple major events in a single annual growing cycle in either North or South America, could bring large parts of Europe and Asia to the brink of starvation (see Figure 1). Interruption of ocean transport, a cyber disaster, or major telecommunication networks could do the same. How great, one wonders, are the risks of such disasters?

Food security is inalterably connected to other forms of security, including energy, water, physical (infrastructure), environmental, economic, and human (personal) security. New intelligence paradigms involving multiscale tools that distinguish between, for instance, slow and fast-moving trends are altering our understanding of these interconnections and the way that shocks propagate through the system.

The CSACC has issued a series of seven recommendations for achieving global food security. Some are fairly predictable, including #2: Significantly raise the level of global investment in sustainable agriculture and food systems in the next decade, and #4: Develop specific programmes and policies to assist populations and sectors that are most vulnerable to climate changes and food insecurity. However, Jahn focused on the last one, recommendation #7: Create comprehensive, shared, integrated information systems that encompass human and ecological dimensions [of agricultural and food systems]. this question, Jahn presented two maps of India with brightly colored areas indicating irrigated lands. One map showed some 279 million acres of irrigated land, while the other displayed little more than half as many. Jahn said that the representations were from two mainstream institutions in the country, reinforcing the limitations of such visualizations. Which figure should be included in an integrated information system intended to inform the policy process?

Integrated (and interactive) near-realtime information systems already exist. Figure 2 shows the homepage of one such system, which can track production sites, transport vessels, weather conditions, infrastructure, and more. Yet it reflects only currently-available data, including dubious estimates of many important quantities and no estimates at all of some others.

Information concerning the demand for food is particularly fragmented and incomplete. Ultimately, displays like the one in Figure 2 will depict the flow of energy, including that of human beings, from place to place. Current available representations, however, fail to portray energy flows with sufficient clarity. Might it one day be possible to produce a dynamic and comprehensive display—akin to a weather map of energy flows throughout the global food delivery system, with an indication of the level of uncertainty?

As matters stand, the world has a severely incomplete understanding of risks that could result in food system instability or breakdown. A number of unconventional partnerships have recently formed to address the issue – by assembling trustworthy bodies of information suitable for planning purposes and making them available to the public. Jahn spoke of a nascent collaboration between Oak Ridge National Laboratory and the International Maize and Wheat



Figure 2. Near-real-time interactive maps track vessels, weather conditions, and infrastructure. Image credit: Thomson Reuters Eikon.

Improvement Center (better known by its Spanish acronym, CIMMYT), aided by Thomson Reuters' platform Eikon and the Multi-Agency Collaboration Environment. She also mentioned the work of a group of insurance practitioners, who convened at Lloyd's of London in 2015 to assess the cascade of impacts that could result from a plausible scenario (developed by the Jahn Research Group of UW-Madison, in conjunction with the U.K./U.S. Task Force on Resilience of the Global Food Supply Chain to Extreme Events) of a shock to the worldwide production of certain staple food crops. The group concluded that food insecurity will be among the largest risks to global society over the next ten years, and that climate change will be one of the most important supply-side drivers of that insecurity. They

with economic models other than the "supply-side" model so favored by the Ronald Reagan administration. It differs in name only from the long-dominant "neoclassical model" of economic behavior. Jahn quoted Ha-Joon Chang, a gadfly in the economics profession, whose book [1] furnishes an eminently readable (if somewhat incomplete) guide to alternative schools of economic thought. Because the dominant model favors inaction in almost every circumstance, mathematicians can hasten Jahn's "needed change" by contributing to the development of more reliable economic models. Yet the incorporation of unfamiliar models in the policy process will likely take decades.

A quicker way for mathematicians to enter the fray against food insecurity is by improving the quality and utility of available information through enhanced data mining techniques, the resolution of conflicting data, and interpolation where gaps occur. Though a great deal of information is already being collected in or near real time, much of it is fragmented and disorganized, possibly delaying recognition of credible threats. Even small contributions to the campaign against food insecurity could significantly impact human wellbeing.¹

Why, she asked, does this recommendation deserve special attention? To answer



Figure 1. Main trade flows of corn, wheat, soybean complex, and palm oil. Image credit: Rabobank

quantified the economic impact of the shock in question as follows: U.S. stocks lose 5% of their value, E.U. stocks lose 19% of their value, global rice production falls 7%, maize production falls 10%, soybean production falls 11%, and rice prices rise 500%.

These and related factors create both risk and opportunity for certain types of businesses. For example, food and beverage companies are painfully exposed to supply risks, which have grown with the extension of their supply chains. To reduce such risks, certain features of the global food delivery system will need to change. Global conditions will force governments to prohibit some currently-profitable activities, such as the depletion of fossil water reserves in the mighty (but non-regenerating) Ogallala Aquifer to grow grain for sale in Southeast Asia. In so doing, they will incur the wrath of those whose profits diminish, in league with a swarm of supply-side economists.

Mathematicians can help improve global food security by familiarizing themselves

References

[1] Chang, H.-J. (2014). *Economics: The User's Guide*. New York, NY: Bloomsbury Press.

James Case writes from Baltimore, Maryland.

¹ In an article on page 5, Hans Kaper and Mary Lou Zeeman illustrate how mathematical and computational skills can help model food systems.

Modeling Food Systems

By Hans G. Kaper and Mary Lou Zeeman

A s applied mathematicians and computational scientists, we don't normally think of food systems as a potential research topic. Yet as explained in the accompanying article on page 1 about Molly Jahn's (University of Wisconsin) public lecture at the 2016 SIAM Conference on Mathematics of Planet Earth, many questions related to food systems and food security can challenge our mathematical and computational skills.

Computational models of food systems are essentially economic models (i.e., inputoutput models, computable general equilibrium models). These are *process models*, accounting for as many actors and processes as possible to simulate actual food systems. They are carefully calibrated to match available data and designed to find equilibrium states subject to constraints, by minimizing costs or energy, for example.

From a mathematical perspective, food systems are *complex systems*. They have their own internal dynamics, subject to external forces and stochastic variations; in that sense, they are similar to Earth's climate system. But there are several significant differences. While climate processes ture in mathematical terms. Lastly, *conceptual models*—highly simplified models that focus on a particular phenomenon, with just enough detail to identify critical parameters or highlight underlying mechanisms—are lacking for food systems.

A Safe and Just Space for Humanity

Food systems impact both natural and societal wellbeing. What does it take to achieve a balance between biodiversity and sustainability on the one hand, and fairness and social justice on the other?

Planetary Boundaries. In 2009, a group of Earth system and environmental scientists proposed measuring stress to the Earth system in terms of planetary boundaries [3]. They suggested nine such boundaries and presented measurable control variables (indicators) for seven of them. Their proposal led to the concept of a safe operating space for human existence on the planet. Exceeding the critical value of a control variable would risk triggering abrupt or irreversible environmental changes - a tipping point in the parlance of dynamical systems. Examples of planetary boundaries and their control variables are climate change and the atmospheric CO₂ concentration (in ppm), freshwater use and global consumption by humans (in km³/yr), and land-



Figure 2. Estimated status of the control variables for eight of the social boundaries. Image courtesy of [2].

are governed by the laws of physics and chemistry, the processes that make up the food system don't seem to follow any such laws, except possibly the law of supply and demand. Additionally, agents in the food system make choices based on cultural and societal norms, which are difficult to cap-

n are difficult to capagement and environr [4] Davies, E.B.

Short Codes Continued from page 2

complicated computer architectures, "10 print" serves as a reminder that we need to keep providing simple demonstrators that make the key ideas underlying our algorithms and software accessible. Not every algorithm can be as concisely described as funm_randomized.m, but simplifying down to the core of an idea is a great exercise to improve one's understanding.

converted to crop use (in %). [4] provides an update to the original proposal, while [1] offers a scholarly discussion of boundaries and indicators. Figure 1 (on page 1) shows the current status of the control variables for seven of the planetary boundaries. Given our limited

system change and the

fraction of land surface

understanding of the fundamental processes controlling each planetary boundary, one could argue that it is impossible to present reasonable numbers, or the borders

are much more malleable than the boundaries suggest, or, with better or worse management, boundaries could be moved. The concept of planetary boundaries, however, is now generally accepted and has since been adopted. For example, the United Nations (UN) utilizes it for ecosystem management and environmental governance.

[4] Davies, E.B. (2007). Approximate diagonalization. *SIAM J. Matrix Anal. Appl.*, 29(4), 1051-1064.

[5] Davis, T., Rajamanickam, S., & Sid-Lakhdar, W. (2016). A Survey of Direct Methods for Sparse Linear Systems. *Acta Numerica*, *25*, 383-566.



Figure 3. A safe and just space for humanity. Image courtesy of [2].

Social Boundaries. Planetary boundaries represent the existence of biophysical and ecological constraints to the Earth system. They define an "environmental ceiling," beyond which lie unacceptable degradation and potential tipping points. Similarly, there exist generally-accepted social priorities, which imply unacceptable human deprivation if unmet. A set of 11 priorities, together with their indicators, was proposed to guide discussion at the 2012 UN Conference on Sustainable Development (Rio+20). Example priorities include education levels, the fraction of children not enrolled in primary school, and illiteracy rates among 15-24 year-olds; income and the fraction of the population living on less than \$1.25 per day; and food security and the fraction of the population that is undernourished. Together, these social boundaries define a "social foundation" for a just operating space for humanity.

Figure 2 presents estimates of the current status of indicators for eight of the social boundaries. The indicators are measured from the center, and social justice is achieved when all sectors reach the outer green boundary. The orange sectors indicate not only that we are falling short on social justice at the global level, but also that significant discrepancies exist among the various indicators.

Doughnut Economics. By inserting the social boundaries at the center of the planetary boundaries disc, Kate Raworth [2] presents a visual representation of an *environmentally safe and socially just space* for humanity (see Figure 3). In this space, it is possible to attain inclusive and sustainable economic development. If we imagine this image in three dimensions we have a torus, which is reminiscent of a doughnut; hence, the term *doughnut economics* is appropriate.

ciple for a formal approach to sustainable development, and the concept of doughnut economics can serve as a blueprint for the creation of mathematical models. Though one must adapt the blueprint to the particular question under study, it provides a framework for both qualitative and quantitative analysis that includes the human value system. The online version of this article outlines some preliminary ideas.¹

References

[1] Garver, J., & Goldberg, M.S. (2015). Boundaries and Indicators: Conceptualizing and Measuring Progress Toward an Economy of Right Relationship Constrained by Global Economic Limits. In P.G. Brown & P. Timmerman (Eds.), *Ecological Economics for the Anthropocene: An Emerging Paradigm* (pp. 149-190). New York, NY: Columbia University Press.

[2] Raworth, K. (2012). A safe and just space for humanity: can we live within the doughnut? Oxfam Policy and Practice: Climate Change and Resilience (pp. 1-26).

[3] Rockström, J., Steffen, W., Noone, K., Persson, Å., Chapin, F.S., Lambin, E.F.,...Foley, J.A. (2009). A safe operating space for humanity. *Nature*, *461*, 472-475.

[4] Steffen, W., Richardson, K., Rockström, J., Cornell, S.E., Fetzer, I., Bennett, E.M....Sörlin, S. (2015). Planetary boundaries: Guiding human development on a changing planet. *Science*, *347*, 1259855.

Hans Kaper, founding chair of SIAG/ MPE and editor-in-chief of SIAM News, is an adjunct professor of mathematics at Georgetown University. Mary Lou Zeeman, founding vice-chair of SIAG/ MPE and co-director of the Mathematics and Climate Research Network, is the Wells Johnson Professor of Mathematics at Bowdoin College.

References

[1] Abdelfattah, A., Anzt, H., Dongarra, J., Gates, M., Haidar, A., Kurzak, J.,...YarKhan, A. (2016). Linear Algebra Software for Large-Scale Accelerated Multicore Computing. *Acta Numerica*, 25, 1-160.

[2] Bai, Z., Demmel, J., Dongarra, J., Ruhe, A., & Van der Vorst, H. (Eds.). (2000). *Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide*. Philadelphia, PA: Society for Industrial and Applied Mathematics.

[3] Barrett, R., Berry, M., Chan, T., Demmel, J., Donato, J., Dongarra, J.,... Van der Vorst, H. (1994). *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*. Philadelphia, PA: Society for Industrial and Applied Mathematics. [6] Güttel, S., & Tisseur, F. (2017). The nonlinear eigenvalue problem. To appear in *Acta Numerica*. MIMS EPrint 2017.7, Manchester Institute for Mathematical Sciences, The University of Manchester.

[7] Higham, D.J. (2001). An Algorithmic Introduction to Numerical Simulation of Stochastic Differential Equations. *SIAM Review*, 43, 525-546.

[8] Montfort, N., Baudoin, P., Bell, J., Bogost, I., Douglass, J., Marino, M.,...Vawter, N. (2012). *10 PRINT CHR\$(205.5+RND(1));* : *GOTO 10*. Cambridge, MA: MIT Press. Freely available as a PDF from http://nickm. com/trope_tank/10_PRINT_121114.pdf.

[9] Trefethen, L.N. (2005). *Ten Digit Algorithms* (Report Number 05/13). Oxford University Computing Laboratory. Retrieved from https://people.maths.ox.ac. uk/trefethen/tda.html.

Nicholas Higham is the Richardson Professor of Applied Mathematics at the University of Manchester. He is the current president of SIAM. The proposition of a safe and just space for humanity provides an organizing prin-

Obituaries

Continued from page 3

Sedgwick Board of Appeals, and regularly attended the "Lunch Bunch" in nearby Blue Hill. Brockway and Audrey joined the Wednesday Painters—she painted while he sketched—and sang for many years with the Bagaduce Chorale. In the summer, they sailed to the islands around Eggemoggin Reach, often with children and grandchildren in tow. Brockway was a passionate lover of music, coffee, and chocolate.

After Audrey died in 2008, Brockway continued to live at his farm with help from his son Gordon, where he enjoyed good health until last October, when he was https://sinews.siam.org/Current-Issue

placed under hospice care. He fell just after Thanksgiving, breaking his hip, and passed away at home one week later. He was 101 years and eight months old. Brockway is survived by his three children—Sarah Taylor and her husband Robert Taylor, Douglas McMillan and his wife Molly McMillan, and Gordon McMillan, all of Sedgwick—plus seven grandchildren and eight great-grandchildren. The family will announce a time this summer to meet, remember Brockway, and celebrate his life.

A version of this obituary previously appeared in The Ellsworth American. Brockway's daughter, son, and son-in-law contributed to the content.

Measuring Curvature with a Bike

he following nice fact can be found in [1] (in a slightly different formulation than here): The center C of curvature of a bike's rear track (see Figure 1) lies at the intersection point of the two axles' extensions, i.e., of the normals to the front and rear tracks.

I speak here of a mathematician's bike, namely of a fixed length segment RF whose front F moves along a prescribed path and whose rear R has velocity vector constrained to the line RF.

[1] posed the problem of finding a geometrical proof for this neat fact. I offer such a proof/explanation here, along with a few additional observations.





To see without calculation why this curious fact holds, imagine first locking the steering angle α to a fixed value, as in Figure 2. With the steering locked, the wheels will trace out two concentric circles with the center at the intersection point of the two axles, thus proving/explaining¹ the claim for $\alpha = \text{const.}$

¹ Proofs which also explain *why* probably deserve a special name, something like "exproof."

Sustainable Environment

Continued from page 4

fully analyze water usage in a large-scale region and provide reliable representations for decision-makers. It incorporates every major component of the water cycle, including subsurface flow, precipitation events, streamflow routing, surface-water routing, seawater intrusion, and riparian evapotranspiration. This allows for accurate tracking of the water balance throughout the domain of interest. Such accounting is especially useful when applying the model to regions that are subject to water rights, usage restrictions, and other regulatory controls. Ultimately, the MF-OWHM model has the potential to be a key linkage point for agricultural economic modeling if paired with the appropriate computational models within that regime. For example, shifts in the supply and demand of water within the economic model will trigger changes in the water balance within the MF-OWHM model.

Dakota is a widely-used and well-supported optimization suite; it contains a

Stakeholders	\M/ator
(Citizens Farmers	vvater

RFigure 2.

It remains to remove the constancy assumption, i.e., to explain why curvature κ does MATHEMATICAL not in fact depend on the variation of α but only on α itself (and on the length l = RF). Referring to Figure 3, where

R moves with speed 1 (treating the arc length *s* as the time), we have

$$\kappa = \frac{d\theta}{ds} = \frac{v\sin\alpha}{l} = \frac{\tan\alpha}{l}, \quad (1)$$

proving the independence of κ on $d\alpha/ds$



Figure 3. Proving (1) by applying " $\omega = v/r$ " to compute the angular velocity of RF, i.e., the curvature at R.

variety of derivative-free optimization methods and is thus well suited to handle "black box" simulation-based problems. Optimization algorithms in Dakota allow us to consider single- and multi-objective formulations of the problem, meaning that we can acknowledge competing viewpoints of different members of the community. Our team wrote Python wrappers to connect the I/O streams between Dakota and OWHM. The wrappers write the appropriate input (i.e., decision variables) to Dakota-formatted data files, read the output from an OWHM simulation, and compute the associated values for the objective functions and constraints required by the optimization algorithm in Dakota. Thus, we can consider any model parameter in OWHM as a decision variable and use any output from OWHM to define an objective function that captures the priorities of the various stakeholders in a given agricultural region. This flexible approach, using welltrusted software tools, lets us focus our efforts on defining appropriate objective functions, constraints, and design spaces.

and thus justifying the original claim. Actually, the claim also follows directly from (1), which yields $\kappa^{-1} = l \cot \alpha$ and coincides with $RC = l \cot \alpha$ from Figure 1.

I was planning to stop here while writing this note, but then began to wonder if there is a way to see the curvature κ itself, rather than the radius of curvature $RC = 1/\kappa$. Figure 4 answers this question:

$$\kappa = KR,$$

CURIOSITIES

By Mark Levi

assuming l=1 for simplicity. Indeed, the triangles ΔFRC and ΔKRF are similar, so that (taking l = RF = 1),

$$\frac{KR}{1} = \frac{1}{RC}, \text{ i.e.},$$

 $KR \cdot RC = 1.$



tion point of the rear axle with the direction line of the front wheel. Here, l = RF = 1.

Thus, $KR = RC^{-1} = (\kappa^{-1})^{-1} = \kappa$, as claimed.

The complexity of coupled modeling frameworks like Dakota/MF-OWHM presents challenges of usability and computational cost. In this regard, several recent efforts have attempted to link these types of modeling frameworks with user-friendly graphical interfaces and high-performance computing resources. For example, Michael Fienen and Randall Hunt describe an opensource appliance (HTCondor) that runs on a remote cluster of distributed computers and is readily adapted to support wide-ranging environmental applications [2]. The underlying software stack is capable of supporting a variety of simulation-based optimization and model assessment (e.g., parameter estimation and sensitivity and uncertainty analysis) approaches. Additional customizable frameworks for providing webbased parallel computing portals include AWESIM³ and HubZero.⁴ For instance, the Virtual Infrastructure for Data Intensive Analysis (VIDIA)⁵ project customizes the HubZero framework to provide access to HPC-enabled data analytics software like R/RStudio⁶ [3], RapidMiner,⁷ and Orange.⁸ One could similarly adapt HubZero to support water resources management and the aforementioned Dakota/MF-OWHM deci-

Eyeballing κ while riding the bike would force one to look backwards (and with Kpassing from one side of the line RF to the other, doing so becomes particularly difficult and embarrassing). Here is a safer



Figure 5. Measuring the curvature of the rear track with the bike light.

way, which avoids twisting the neck (or breaking it, if v is large). Imagine mounting a light-or better, a laser pointer-on the handlebars; then the deviation d of the light spot cast on the ground (see Figure 5) determines κ (for l=1) via

$$\kappa = d/\rho + O(d^3).$$

From now on I will probably always think of κ when riding a bike at night.

The figures in this article were provided by the author.

References

[1] Alexander, J.C. (1984). On the Motion of a Trailer-Truck. SIAM Review, 26(4), 579-580.

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

that using existing open-source software frameworks-coupled through user-friendly, accessible interfaces-is the path forward for resolving these difficult problems.

References

[1] Bokhiria, J., Fowler, K., & Jenkins, E. (2014). Modeling and optimization for crop portfolio management under limited irrigation strategies. Journal of Agriculture and Environmental Sciences, 2, 1-13.

[2] Fienen, M.N., & Hunt, R.J. (2015). High-Throughput Computing versus High-Performance Computing for Groundwater Applications. Groundwater, 53(2), 180-184.

[3] Ihaka, R., & Gentleman, R. (1996). R: A Language for Data Analysis and Graphics. Journal of Computational and Graphical Statistics, 5(3), 299-314.

[4] Kupec, I.F. (2014, July 1). Strawberries with a thirst. National Science Foundation. Retrieved from https://www.nsf.gov/discoveries/disc_summ.jsp?org=NSF&cntn_ id=131827.

Further Reading

[1] Adams, B., Bauman, L., Bohnho, W., Dalbey, K., Ebeida, M., Eddy, J.,... Vigil, D. (2009). Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 5.4 User's Manual. Technical Report SAND2010-2183. Albuquerque, N.M.: Sandia National Laboratories. [2] Hanson, R.T., Boyce, S.E., Schmid, W., Hughes, J.D., Mehl, S.M., Leake, S.A.,...Niswonger, R.G. (2014). One-Water Hydrologic Flow Model (MODFLOW-OWHM). Techniques and Methods 6-A51, U.S. Geological Survey. Retrieved from http://dx.doi.org/10.3133/tm6A51.



Figure 1. A collaborative approach using integrated software tools to aid decision-makers and stakeholders in agricultural communities. Image credit: Kathleen Kavanagh, Lea Jenkins, and Shawn Matott.

sion tool.

Ultimately, the success of our efforts will be measured by our ability to build on our existing collaborations to develop and deploy a truly interactive modeling framework that is useful for and used by real, existing stakeholders in a region - and not just in academics. To achieve this, we rely on our fellow researchers in modeling, simulation, and optimization, and on the software and computational tools they have developed and already applied to a wide range of challenging, real problems. We have been fortunate to work with experts who are generous with their time and knowledge. Our team's success is attributable in part to effective communication and open collaboration. In addition, we believe

- www.awesim.org
- https://hubzero.org/
- http://vidia.ccr.buffalo.edu/ 5
- 6 https://www.rstudio.com/
- https://rapidminer.com/
- 8 http://orange.biolab.si/

Kathleen Kavanagh is a professor of mathematics at Clarkson University. Lea Jenkins is an associate professor in the Department of Mathematical Sciences at Clemson University. Shawn Matott has a B.S. in computer engineering and a Ph.D. in environmental engineering. He is a computational scientist at the Center for Computational Research at the University at Buffalo, where he also serves as industry outreach coordinator.

Dakota Software: Explore and Predict with Confidence

By Michael Eldred, Brian Adams, and Laura Swiler

The Dakota software project¹ serves the mission of Sandia National Laboratories and supports a worldwide user community by delivering state-of-the-art research and robust, usable software for optimization and uncertainty quantification (UQ). These capabilities enable advanced exploration and risk-informed prediction with a wide range of computational science and engineering models [1].

In its simplest mode, Dakota automates iterative analysis using a general-purpose interface to a computational model, as shown in Figure 1. Its fundamental strength is a broad suite of algorithmic techniques facilitating parameter exploration, global sensitivity analysis, design optimization, model calibration, UQ, and statistical inference. These core algorithms provide a foundation for more advanced, multicomponent solution approaches, including hybrid optimization, surrogate-based optimization, multi-fidelity UO and optimization, mixed aleatory-epistemic uncertainty analyses, and optimization under uncertainty. By integrating these capabilities within a single software tool, users can easily transition between different types of studies when exploring a computational model - from identifying to calibrating influential parameters and from characterizing the effect of uncertainties to performing design optimization in their presence.

Dakota's development activities span a spectrum from algorithm research and prototyping to production application deployment, with the goal of delivering exploration and prediction capabilities for all kinds of computational models. Efficient computing is also a central goal, with support ranging from desktops to the latest supercomputers.

Algorithm Research and Development

The Dakota project started in 1994 as an internal research and development effort, and has retained this emphasis throughout its history. Research in new algorithms is guided by challenges in deploying methods to complex, high-fidelity engineering and science applications where parameter spaces may be high-dimensional, quantities of interest may be nonsmooth or unreliable, and simulation budgets may be severely constrained.

In the case of optimization methods, we have primarily addressed these issues through surrogate-based approaches relying on data fit, multi-fidelity, or other approximations. We mitigate simulation defects and accelerate local and global search processes through the use of adaptive model management approaches.

For UQ, we seek scalability by exploiting anisotropy, sparsity, and low-rank structure using spectral expansion methods. Dovetailing multilevel multi-fidelity efficiency gains. Moreover, these forward UQ techniques enable scalable statistical inversion; we are presently crafting inference approaches that leverage dimension reduction, emulator acceleration, and multi-fidelity modeling.

Building on these optimization and UQ investments, we tailor model managementbased optimization algorithms to the capabilities of specific UQ approaches, enabling efficient optimization under uncertainty. This allows for the design of statistically robust and reliable engineered systems.

Persistent investment in algorithm research allows us to deploy the latest algorithmic approaches and evolve and mature them alongside time-tested and production-hardened methods. This continuous influx and maturation of novel capabilities is essential for supporting new challenges within our mission space.

Enabling Architecture

Dakota's object-oriented C++ architecture empowers developers to effectively craft and deliver algorithm capabilities and enables users to productively apply them. Supported by software engineering infrastructure and processes, the architecture facilitates the concurrent research, development, production, and deployment necessary to meet diverse Department of Energy (DOE) program goals.

Iteration is a central theme that inspires the C++ class abstractions in Dakota. *Models* manage the mapping of *variables* (parameters) through an *interface* to *responses* (quantities of interest). Model instance types support mappings based on computational simulations, surrogate approximations,

formulation recastings, and nested recursions. *Method* classes implement iterative analysis algorithms, which are broadly grouped into parameter exploration and

design of experiments, non-deterministic methods for UQ and inference, and minimization for optimization and calibration. These classes are both composable and extensible, allowing developers to prototype new algorithms and users to flexibly configure them in Dakota studies.

Dakota supports parallel computing from desktops to supercomputers. We use multilevel parallel computing (comprised of message passing, asynchronous local, and hybrid approaches) to utilize coarse-grained parallel concurrency within a recursive scheduling approach in order to augment and amplify fine-grained simulation parallelism. A new Dakota graphical analysis environment aims to help users interface to simulations, create/execute studies in parallel, and interpret Dakota results.

To facilitate greater interactivity, we are transforming Dakota's software architecture into a more modular and extensible system of components with an increasingly flexible integration layer. Additional fine-grained C++ application program interfaces (APIs) will ease library integration of Dakota into



Figure 2. Dakota supports a variety of mission areas, including problems related to climate (Greenland ice sheet model), energy (¼ core model of a nuclear reactor), and defense (thermal load on a weapon). Defense and climate images courtesy of Sandia National Laboratories, energy image courtesy of the Consortium for Advanced Simulation of Light Water Reactors, www.casl.gov.

simulation codes for a better-integrated user experience. Developers and end users alike will be able to directly access individual components and orchestrate them with Python, or perhaps with a domain-specific language. Essentially, Dakota's architecture is evolving to support larger order-ofmagnitude problems (in terms of parameter/ response dimension), effectively span the spectrum from black box to embedded methods, and scale to next-generation extremescale hybrid computer architectures.

Impact

Dakota is open source and distributed under the GNU Lesser General Public License (LGPL). More than 25,000 users worldwide have downloaded the software since January 2010. It has hundreds of users at DOE laboratories and is widely used across government, industry, and academ-

> ic sectors. Dakota runs on Linux, Mac, and Windows operating systems, including high-performance computing clusters. Software downloads (source and binary), system requirements, and

installation details are available on the Dakota website. Given Dakota's active research efforts, accompanying release notes indicate emerging capabilities and their corresponding maturity.

Computational science and engineering practitioners use Dakota across many disciplines and in conjunction with a wide variety of computational models, some of which are shown in Figure 2. For example, Dakota has been used to support the following DOE mission applications:

• Optimization of the performance of neutron generators to ensure that designs meet specifications in terms of voltage, current, and space

• Establishment of a simulation model's credibility for thermal battery performance through a detailed verification and validation/UQ analysis

• Sensitivity analysis of nuclear reactor fuels performance to understand parameter influence in pressurized water reactors ver-

Community

The Dakota team strives to cultivate an active worldwide user community that contributes to collaborative research, software development, requirements definition, and user support. Research collaborations currently span dozens of universities and labs, and are essential for advancing the state of the art in model-based prediction and decision-making. Publicly-accessible repositories facilitate joint software development. Contributors can implement algorithms, help Dakota scale to next-generation computing platforms, improve architecture, develop adapters or interfaces, and improve quality through software engineering infrastructure. Developer resources are continually improving to expedite such cooperation.

Dakota users come from diverse science and engineering domains, business sectors, and geographies, thus mandating that we nurture a self-sustaining user community. Members support each other via a public mailing list and (soon-to-come) web-based forums, and users can contribute bug reports, enhancement ideas, and case studies. Domain- or simulation code-specific topical groups might integrate Dakota with popular simulation codes and workflows, sponsor-focused user group meetings or training sessions, or contributed tutorials. A vibrant and engaged user community is central to sustaining Dakota as a leading open-source optimization and UQ tool. We invite your participation!

References

[1] Adams, B.M., Bohnhoff, W.J., Dalbey, K.R., Eddy, J.P., Ebeida, M.S. Eldred, M.S.... Wildey, T.M. (2016, November). *Dakota, a Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.5 User's Manual.* Technical Report SAND2014-4633. Albuquerque, N.M.: Sandia National Laboratories. Retrieved from http://dakota.sandia.gov/documentation.html.

Michael Eldred (mseldre@sandia.gov), Brian Adams (briadam@sandia.gov), and Laura Swiler (lpswile@sandia.gov) develop Dakota in the Optimization and Uncertainty Quantification Department in the Center for Computing Research at Sandia National Laboratories. Eldred, a Distinguished Member of Technical Staff and aerospace engineer by training, founded Dakota in 1994 and now leads its algorithm R&D activities. Adams, a Principal Member of Technical Staff, is the Dakota Project Lead and has been a team member in various roles since completing his applied mathematics degrees. Swiler, a Distinguished Member of Technical Staff, applies her operations research and engineering training to Dakota research, development, and applications.

SOFTWARE AND PROGRAMMING

model hierarchies further amplifies their

http://dakota.sandia.gov



Figure 1. Interaction between Dakota and a parameterized simulation. Image credit: Sandia National Laboratories.

sus boiling water reactors

• Calibration of parameters governing thermal-hydraulic models that simulate cooling flows within a reactor core

• Abnormal thermal safety analysis using sparse grids, compressed sensing, and mixed aleatory-epistemic UQ methods

• Analysis of circuit performance and circuit variability given radiation damage to electrical components

• Quantification of the performance of vertical axis wind turbines subject to uncertain gust conditions

• Inference of uncertain basal conditions underlying the Greenland ice sheet, based on available observational data

• Estimation and propagation of uncertain atomistic potentials to quantify material performance

These applications motivate both our stewardship of time-tested production methods and our investment in new algorithms to support growth in problem scale and complexity. Sandia National Laboratories is a multimission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.



Engineering Mathematics Around the World

By Aaron Hagström

The term "engineering mathematics" comes from an era when physics, mechanics, and mathematics were more closely tied together. With the dawn of high-powered computing, larger data sets, and new mathematical methods, engineering mathematics departments have begun to branch out into more exotic interdisciplinary realms, leaving students with ever more compelling career options.

Engineering mathematics covers "a huge spectrum that runs from theoretical applied mathematics to strong, industrially-driven computations," said Margot Gerritsen,

to build data mining and machine learning applications in-house, so they need to understand the engines involved."

To prepare students for industry, Stanford encourages internships through its industrial affiliate programs and participation in large projects through the Army High Performance Computing Research Center and the Predictive Science Academic Alliance Program II Center, among others. These projects cover a broad range of topics, including genomics, physiology, and Earth sciences.

"Students are consulting with companies on a regular basis and founding companies," Gerritsen said. "We are in the midst of



Margot Gerritsen (right) acknowledges students who made special contributions to the community at "ICME Xtravaganza," Stanford University's year-end celebration with the Institute for Computational and Mathematical Engineering community, in May 2016. Photo credit: Ana Santos.

who leads the Institute for Computational and Mathematical Engineering (ICME) at Stanford University. "What one calls 'engineering mathematics' might be called 'applied mathematics' elsewhere. Everyone has their own flavor and different heroes, depending on where they sit on the spectrum."

Housed within the Stanford University School of Engineering, ICME is a multidisciplinary graduate-level institute with about

200 students and roughly 60 faculty members. The institute interacts with 20 academic departments across the university, including engineering, Earth sciences, and medicine.

"That sort of model, which is more university-wide, is not so common in Europe, where most institutes are organized by department and by definition

are a bit more insular," Gerritsen said. "We try to be the web that glues all these people together, connecting mathematics to the applied sciences and engineering."

Founded in 2004, ICME has a long history of association with Stanford's Department of Computer Science. Before ICME, George Forsythe and Gene Golub created the "Numerical Analysis Group," which later became known as the Scientific Computation and Computational Mathematics Program. Nonetheless, even while Gerritsen was studying at Stanford in the early 1990s, the university was already considering the establishment of a separate institute that took a broader, more interdisciplinary approach to computational mathematics. ICME has moved beyond the traditional engineering mathematics discipline and offers a Ph.D and a two-year M.S. degree, which includes specialized tracks in computational geosciences, data science, imaging science, and mathematical and computational finance. The institute makes a point of training its graduates in both the theoretical and technical aspects of computational mathematics. "We place students in computational groups in larger companies," Gerritsen said. "Companies want

Silicon Valley, which is computationally extremely heavy. Our students therefore must be good team players, excellent mathematicians, pretty good programmers, and have engineering sense."

Former Stanford Ph.D. student Ryan Lewis works at Ayasdi, a venture-backed machine intelligence software company that provides data analysis to the financial services and healthcare industries. His professor, Gunnar Carlsson-also a Stanford grad-

uate-cofounded Ayasdi to commercialize his own foundational work in pure topology. Carlsson appreciates how ICME transcends the traditional approaches to engineering mathematics.

"A lot of engineering mathematics has been about certain computational paradigms in linear algebra and differential equations," Carlsson said. "But ICME is moving beyond that to all kinds of stochastics and combinatorial and more discrete mathematics, so I think what you are seeing is a math program that is broadening what applied math means and doing a really good job of it."

Graduates of Stanford's related departments of computer science and mathematics have founded companies and become educators. 2013 Ph.D. graduate Reza Zadeh

established his own machinelearning company called Matroid. Nick Trefethen studied computer science at Stanford and now heads the University of Oxford's Numerical Analysis Group. Google founders Larry Page and Sergey Brin both studied computer science at Stanford, and Gerritsen speculates that their grounding in numerical linear algebra may have played a role in their discoveries, including that of the page-ranking algorithm.

Founded in 2003, the University of Texas's Institute of Computational Engineering and Science (ICES) includes about 160 faculty and 70 students. A key professor in the institute, Mary Wheeler, works on the theoretical side of engineering mathematics in the oil and gas industry. "Companies don't want to prove theorems," Wheeler said. "Generally in engineering, you see more of applying the research and invalidating or verifying it."

The interdisciplinary Computational Science, Engineering, and Mathematics (CSEM) program at ICES offers M.S. and Ph.D. degrees and includes concentrations in numerical analysis and mathematical modeling. Students work with researchers from diverse departments, performing field tests and experiments to create predictive mathematical models, such as the injection of CO_2 into demonstration sites.

Wheeler also leads an Industrial Affiliates Program to help students better understand industrial challenges. The program has connections to roughly 10 companies, including IBM and various oil and environmental corporations.

On the other side of the Atlantic, the University of Bristol's Department of Engineering Mathematics is also seeking to broaden the definition of engineering mathematics. The department, which is within the Department of Engineering, comprises roughly 220 undergraduate students and plans to establish an M.Sc. in engineering mathematics next year. Director Alan Champneys considers the title "engineering mathematics" to be sort of a misnomer, given its emphasis on mathematical and data modeling.

See Engineering Math on page 9

The following is a list of some of the institutions worldwide that offer programs in engineering mathematics:

<u>U.S.A.</u>

California Institute of Technology, Department of Computing and Mathematical Sciences

- Applied and Computational
- Mathematics (B.S.)
- Applied and Computational Mathematics (Ph.D.)
- Computing and Mathematical Sciences (Ph.D.)

Columbia University, Applied Physics and Applied Mathematics with Materials Science and Engineering

- Applied Mathematics (B.S.)
- Applied Physics, Materials Science &
- Engineering (B.S./M.S./Ph.D.) Harvard University, John A. Paulson School of

Engineering and Applied Sciences

- Applied Mathematics (A.B., A.B./S.M.)

- Applied Mathematics (Ph.D.)

Johns Hopkins University, Applied and **Computational Mathematics**

- Applied and Computational
- Mathematics (M.S.)

- Post-Master's Certificate

New York University, Courant Institute of Mathematical Sciences

- Scientific Computing (M.S.)

Princeton University, The Program in

- Applied and Computational Mathematics - Applied and Computational Mathematics (Certificate)
- Stanford University, Institute for
- Computational & Mathematical Engineering - Computational and Mathematical
 - Engineering (M.S.)
- Computational and Mathematical Engineering (Ph.D.)

University of Texas at Austin, Institute for

- Computational Engineering and Sciences - Computational Engineering and Sciences (M.S.)
 - Computational Engineering and Sciences (Ph.D.)

<u>ENGLAND</u>

- Oxford University, Mathematical Institute
 - Mathematical Modeling and Scientific Computing (M.Sc.)
 - Industrially Focused Mathematical Modeling (Doctoral Training)

University of Bristol, Department of

Engineering Mathematics - Engineering Mathematics (B.Eng.)

- Engineering Mathematics (M.Eng.)

<u>EUROPE</u>

Chalmers University of Technology

- Engineering Mathematics and Computational Science (M.Sc.)
- Advanced Engineering Mathematics (Licentiate)

Ecole Polytechnique

CAREERS IN MATHEMATICAL and applied computational SCIENCES



Ryan Lewis (right) represents Ayasdi at "ICME Xtend," a two-day recruiting and networking event organized at Stanford University in November 2016 for partners and students. Photo credit: Chris Arson Photography.

- Applied Mathematics (Bachelor's/ Master's/Ph.D.) KTH Royal Institute of Technology in Stockholm - Applied and Engineering Mathematics (N5TeAM) Lund University - Engineering Mathematics (M.Sc.) **Technical University of Budapest** - Research University Program **Technical University of Denmark** - Applied and Engineering Mathematics (Nordic M.Sc.) **Technical University of Munich** - Computational Science and Engineering (M.Sc.) Uppsala University - Master's Program in Computational Science (M.S.)

<u>CHINA</u> Tsinghua University, Department of Mathematical Sciences

How to Count Fish Using Mathematics

By Bob Pego

ow many fish are in the sea? Fields Medalist Charlie Fefferman asked at the end of my talk about a coagulationfragmentation model of animal group sizes during a workshop held in Princeton, N.J., in September 2015. Fefferman's naïvesounding question cut to the heart of the resource estimation issues that the model was designed to address. My work on this model, with collaborators Pierre Degond (Imperial College London) and Jian-Guo Liu (Duke University) [1], began with our interest in Japanese fisheries scientist Hiro-Sato Niwa's investigation of the frequency distribution of school sizes for pelagic fish - fish that roam in the mid-ocean.

Niwa analyzed a large amount of observational data and found that, when scaled by an expected school size, it collapses well onto a single, highly non-Gaussian curve. Niwa worked under the hypothesis that simple rules for random merging and splitting of schools could explain the observed size distribution. He modeled this situation with a stochastic differential equation and performed merging-splitting simulations to estimate variance. Impressively, he then used Itô calculus to find an explicit solution of the model, in the form

$$f(s) = s^{-1} \exp(-s + \frac{1}{2}se^{-s}).$$
 (1)

Remarkably, this expression has no fitting parameters yet fits the data rather well (see Figure 1). For this distribution to be consistent with Niwa's scaling, the distribution sf(s) (of population in groups of size *s*) and its first moment should agree:

$$\int_0^\infty sf(s)ds = \int_0^\infty s^2f(s)ds$$

Niwa mentions that he checked this numerically to an accuracy of 128 digits! (Proving this with elementary calculus is quite a nice challenge.)

Our own work [1] involves solving and analyzing a more faithful model of Niwa's

Engineering Math

Continued from page 8 $\,$

"It doesn't really conjure up an image of who we are," Champneys said. "Going back 40 or 50 years, it was about process modeling—about modeling mechanics and fluid flow—the traditional engineering mathematics. Now we are more into cool technology."

Some of these innovative technologies are in the subdisciplines of dynamical systems, artificial intelligence, biological modeling, and robotics. Senior lecturer Nathan Lepora, once a theoretical physicist and children's author, works at the cutting edge of neuroscience and robotics in a discipling called swarming behavior simulated merging-splitting process. He was very aware of the type of coagulationfragmentation model that we study, but its mathematical treatment turns out to require new developments in complex function theory related to Laplace transforms. One result of our analysis is that the coagulationfragmentation equation has an exact solution that takes the form

$$f_{\star}(s) = g(s) \exp\left(-\frac{8}{9}s\right)$$

where g(s) is a *completely monotone* function—a smooth positive function that is decreasing, convex, and has derivatives that alternate in sign indefinitely—that behaves as

$$\begin{split} g(s) &\sim c_0 s^{-2/3} \text{ as } s \to 0, \\ g(s) &\sim c_\infty s^{-3/2} \text{ as } s \to \infty. \end{split}$$

Moreover, the profile f_{\star} is computable in terms of a series in powers of $s^{1/3}$, namely

$$f_{\star}(s) = (6s)^{-2/3} \sum_{n=0}^{\infty} rac{2(-1)^n}{\Gamma(rac{4}{3} - rac{2}{3}n)} (6s)^{n/3}.$$

Niwa's prefactor s^{-1} has exponent -1 that interpolates nicely between the $-\frac{2}{3}$ and $-\frac{3}{2}$ that we find valid in the small and large limits, respectively. Furthermore, the distribution f_{\star} differs minimally from Niwa's f (less than 20%, hardly noticeable on the scale of Figure 1) in the shoulder region of the log-log plot. The crossover in powerlaw behavior seems likely to complicate the fitting of exponentially-truncated power laws to empirical data on animal group size, as has been attempted by a number of researchers since the mid-1990s.

The coagulation-fragmentation model is essentially a simple kind of Boltzmann equation from the kinetic theory of gases. Instead of modeling collisions and the scattering of gas molecules, it models the merging and splitting of clusters. Prominent Polish physicist Marian Smoluchowski first derived coagulation equations a century ago.

Scientists have since used them to model cluster-size distributions in a wide variety of physical systems, from soot and smog particles in aerosol physics to planetesimals and dark-matter galactic halos in astrophysics. In the case of pelagic fish, Niwa argued that the collision and splitting rates would not permit detailed balance, and that no analog Boltzmann's of H-theorem could explain equilibrium. Consequently, studying the dynamics posed a novel problem.



Figure 1. Empirical school-size distribution of six types of pelagic fish. Data types and sources are listed in Table 1 of [3]. Data is scaled by empirical average. The solid line corresponds to (1). Figure reprinted from [3], with permission from Elsevier.

Degond, Liu, and I made progress by rewriting the equations using what we now call *Bernstein transforms*. Though these are "just" antiderivatives of familiar Laplace transforms, they have a number of distinctive properties that make them a worthy subject of a recent book by René Schilling, Renming Song, and Zoran Vondracek [5]. For example, the composition of two Bernstein transforms is a Bernstein transform, and so is the inverse to a Bernstein transform's antiderivative.

In the case of the Niwa-motivated model in the continuum limit of large populations, the Bernstein transform of the size distribution, given by

$$\varphi(q,t) = \int_0^\infty (1 - e^{-qs}) f(s,t) \, ds,$$

turns out to satisfy an attractive integropartial differential equation, namely

$$\frac{\partial \varphi}{\partial t} = -\varphi^2 - \varphi + \frac{2}{q} \int_0^q \varphi(r, t) dr. \quad (2)$$

ment-sponsored doctoral training program that has about 50-60 students completing Ph.Ds., with roughly half receiving supervision from engineering math faculty.

It was once common for graduates of the Bristol program to enter careers in financial services, Champneys said, but in the last several years they have begun to gravitate more toward technical consultancy, especially in renewable energy. Some of his students now work for Frazer-Nash Consultancy, a British technical consulting firm.

"There is a lot of work in defense and software," Champneys said. "There is a niche market for essentially being consultants who do mathematical modeling, and it doesn't matter what the domain is."

Every engineering math student has a

The steady states of this equation have a scale-invariant shape φ_{\star} , determined implicitly by the simple algebraic relation

$$\varphi_{\star} = q(1 - \varphi_{\star})^3.$$
 (3)

To recover information about the equilibrium size distribution f_{\star} from its Bernstein transform, we use a curiously strong theorem in Bernstein function theory involving global analyticity properties. This theorem states that f_{\star} itself is a Laplace transform (and thus completely monotone) if and only if its own Bernstein transform φ_{\star} is a Pick function – a globally-complex analytic function on the upper half plane \mathcal{H} , mapping \mathcal{H} into \mathcal{H} . This turns out to be true for the φ_{\star} given by (3).

We can also prove that f_{\star} is a global attractor for the model's dynamics. This is derived from (2) by improving the classical continuity theorem for Laplace transforms to demonstrate that pointwise convergence of Bernstein transforms corresponds to

See Fish on page 11

"If you study at Chalmers, you really become an engineer," director Håkan Andreasson said. "It is required that you really receive some skills associated with engineering. We have students at the software company Ericsson doing electronics, and a number of students end up doing statistics or mathematical biology at AstraZeneca."

Jacob Leander studied engineering mathematics, graduating with an M.S. in engineering mathematics and a licentiate (half of a Ph.D) in advanced engineering mathematics after a combined five years. He wrote his thesis on the optimal design of clinical studies for drugs while interning two years at AstraZeneca in Gothenberg and working in collaboration with the Fraunhofer-Chalmers Centre for Industrial Mathematics, where he completed his licentiate project on data analysis and algorithm development. After graduation, Leander worked on car GPS systems at Volvo and later as a clinical pharmacometrician at AstraZeneca, where he now creates mathematical models to describe the effects of drugs that treat respiratory, inflammatory, and autoimmune diseases. He relies heavily on dynamical systems, statistics, and ordinary differential equations. "I use my engineering background in a setting where most people don't have that sort of detailed knowledge about the mathematics," Leander said. "So I really enjoy it."

which may prove useful in drug delivery and drone applications.

Academic options include a three-year B.Eng., a four-year M.Eng. (an integrated undergraduate and postgraduate program), and an M.Sc. (one year + summer program after B.Sc.) in robotics and autonomous systems. The program has four core areas: mathematics, computational science, general engineering, and hands-on mathematical modeling. Champneys says the program distinguishes itself from a standard engineering track with its advanced mathematics courses. He plans to launch a one-year M.Sc. in engineering mathematics next year.

Related to the Bristol Engineering Mathematics Department is the Bristol Centre for Complexity Science, a govern-

in a discipline called swarming behavior, Centre for Complexity Science, a gov



Alan Champneys (second from left) interacts with students at the Agri-Food Mathematical Science Study Group with Industry at the University of Bath this past January. Photo credit: Matt Butchers.

Every engineering math student has an industrial tutor from some company with which Bristol has connections. Thomas Melvin, who earned his Ph.D. from Bristol, works as a research scientist for the U.K. Meteorological (Met) Office, where he creates numerical models for weather prediction by starting with a very simplified mathematical model that he gradually augments based on ground, balloon, airplane, and ship observations.

To the north, Sweden is known as a powerhouse in the theory of engineering mathematics, through such universities as the Royal Institute of Technology (KTH) in Stockholm and Chalmers University of Technology in Gothenburg. Around 2005, Lund University began the first engineering mathematics program in Sweden. In 2008, Chalmers established a combined bachelor's and master's degree program in engineering mathematics and computational science with three tracks: computational science, mathematical statistics, and general mathematics.

Aaron Hagström is a Manhattan-based journalist and graduate of the Annenberg School of Journalism at the University of Southern California. He mainly writes on mathematics and technology.

Applying Design Thinking to Mathematics Research Developing an Interdisciplinary Method to Combat Poaching

By Jennifer S. Pearl and Padmanabhan Seshaiyer

T n recent years, design thinking (DT) has L become a widely-used methodology to generate innovative solutions to so-called "wicked problems" - problems plagued by incomplete information or complex interdependencies, often with a human factor. DT has been used in product design and urban planning, as well as more theoretical or policy-based settings. Upon learning about DT, we were immediately struck by its parallels with the process of mathematical discovery. Although design thinkers come from various backgrounds, it is hard to find many that are trained as research mathematicians. We hope to introduce DT to the SIAM community and offer an example of its successful use in helping students develop interdisciplinary mathematical approaches to eliminate animal poaching.

DT is a human-centered approach to problem solving that employs an iterative process of discovery, ideation, and experimentation to address and innovatively solve real-world challenges that focus on human needs. Companies like IDEO and Stanford University's d.school have extensively used and popularized the technique. Jeanne Liedtka, Tim Ogilvie, and Rachel Brozenske present a particularly nice formulation of DT [2], denoting the DT steps with four questions:

What is? What if? What wows? What works?

We see parallels between the DT steps "What is?," "What if?," and "What works?" and the steps that many research mathematicians employ in their jobs. "What wows?" is not as critical to mathematicians and falls under "What works?;" if it works for us, it wows. While some proofs are more elegant or insightful and some algorithms are faster, cheaper, and more optimal than others, we only wish to show what is true.

The first step, "What is?," focuses on a thorough comprehension of particular examples from the problem under study. The emphasis is not on sifting through large volumes of data, but rather understanding key examples very, very well. DT literature provides various techniques-often lowtech and involving direct observationto help do this. In a famous example, a group of students at Stanford aimed to solve mortality problems of premature and low-birthweight babies in developing countries. These babies seldom had access to incubators, so the thinking at the time revolved around the development of lowercost incubators. Instead of jumping on this bandwagon, the students visited Nepal to observe births in Kathmandu and the surrounding villages. By taking the time to carefully understand many birth situations, they found that most of the premature and low-birthweight babies were born in rural areas and would never make it to a hospital. Thus, cheaper incubators would not solve the problem. They realized they had to "reframe" the problem, a key step in the "What is?" stage of DT. This reframing mirrors the way a mathematician might attack a problem. Mathematicians first generate many examples to get a sense of the phenomenon under study, and then attempt to identify and categorize those that are significant, determining which aspects are crucial to interpreting the underlying structure. Mathematician Arnold Ross famously said, "Think deeply of simple things." Understanding a few key examples often yields real insight, but determining which examples are key is not easy. Furthermore, mathematicians are familiar with the crucial moment when they realize that the problem they are solving is actually not the right one to tackle. This notion is parallel to the aforementioned "reframing."

In the "What if?" step, design thinkers utilize tools to generate creative possibilities in a carefullyarticulated way. The idea is to "push beyond simplistic expressions of new possibilities" [2] by following brainstorming rubrics that build on the observations in the "What is?" stage and do not allow for premature judgment. Mathematicians also formulate theories or hypotheses by looking at examples and attempting to generalize the specific behavior they observe. They draw pictures to



See Design Thinking on page 12 Figure 1. Nonlinear dynamics and control of a quadcopter. Image courtesy of [1].

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

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 bttp://www.cityu.edu.bk/lbj/







Fish

$Continued \ from \ page \ 9$

weak convergence of corresponding measures on the compactified half-line $[0, \infty]$.

A further twist in the story pertains to discrete size distributions, to which Niwa's merging-splitting model leads for finite total population. We were unable to solve this model with Niwa's original postulated splitting rates, namely equal rates for a group of size *s* splitting into two groups of size *j* and s-j for j=1 to s-1. However, we noticed that if we modify the model slightly to include the trivial cases j=0 and j=s, the Bernstein transform again solves the same integro-differential equation (2) after a change of variables!

The curiously strong Bernstein theorem doesn't work to describe equilibrium in the discrete-size case, but we discovered a discrete analog. This analog explains which sequences $(c_j)_{j=0}^{\infty}$ are sequences of moments of measures on positive intervals [0, T]. The characterization is in terms of simple global analyticity properties of the generating function

$$F(z) = \sum_{j=0}^{\infty} c_j z^j.$$

For example, one characterization says zF(z) is a Pick function analytic on $(-\infty, T^{-1})$. Through generating functions, discrete equilibria in Niwa's model are related to the classical *Fuss-Catalan* numbers of combinatorics, given by

$$A_n(p,r) = \frac{r}{pn+r} \binom{pn+r}{n},$$

as well as sequences of moments of random matrix ensembles, infinitely divisible probability distributions on the natural numbers, and convolution semigroups of completely monotone sequences. The connections are laid out in [2]. An unusual detail, related to the fact that the map $r \mapsto (A_n(p,r))_{n \ge 0}$ is a convolution semigroup, is the formula

$$\sum_{n=0}^{\infty} {pn \choose n} z^n = \int_0^1 rac{1}{1-f_p(u)z} \, du,$$

where

$$f_p(u) = \frac{\sin \pi u}{\sin(\frac{1}{p}\pi u)\sin^{p-1}(\frac{p-1}{p}\pi u)}$$

 $\sin^p \pi u$

This formula was discovered due to Tewodros Amdeberhan's use of the amazing *Zeilberger algorithm* [4], which derives and proves combinatorial formulas, and a striking integral expression for binomial coefficients, namely

$$\binom{n}{k} = \frac{1}{\pi} \int_0^{\pi} \frac{\sin^n x}{\sin^k (\frac{k}{n} x) \sin^{n-k} (\frac{n-k}{n} x)} dx$$

I would like to know a simple proof, but please don't assign this as a calculus problem! It follows from results mentioned in [6].

Returning to Fefferman's question about the number of fish in the sea, I didn't have such a number handy. However, I could mention something about data collection methods, such as the use of sonar-measured thickness as a proxy for school size. Pelagic fish schools can extend over several kilometers in diameter and be tens of meters thick.

A central conclusion of Niwa's modeling and data analysis is that the fish school size distribution is highly non-Gaussian. It is not characterized by a normal distribution about a mean, but instead has exponential-like tails that are much 'fatter' than Gaussian ones. Thus, observations of large schools are likely to be much more frequent than Gaussian statistics suggest. This indicates that the use of familiar Gaussian models may easily overestimate the total population.

Our work provides a mathematically consistent foundation for this line of thought. One hopes that the scientists involved in resource estimation are aware of the unsuitability of Gaussian models for this purpose, and that the management of ocean fisheries is not based on inaccurate models and estimates.



TALKS:

Measure, Understand, Control: Applications of Mathematics to Zika Virus Disease Dr. Marc Lipsitch, Harvard University

When Will I Ever Use This: How Scientists Use Math to Model and Understand Hurricane Storm Surges Dr. Talea Mayo, University of Central Florida

References

[1] Degond, P., Liu, J.-G., & Pego, R.L. (2017). Coagulation-fragmentation model for animal group-size statistics. *J. Nonlinear Sci.*, *27*(2), 379-424.

[2] Liu, J.-G., & Pego, R.L. (2016). On generating functions of Hausdorff moment sequences. *Trans. Amer. Math. Soc.*, *368*, 8499-8518.

[3] Niwa, H.S. (2003). Power-law versus exponential distributions of animal group sizes. *J. Theo. Biol.*, 224, 451-457.

[4] Petkovšek, M., Wilf, H.S., & Zeilberger, D. (1996). A = B. Wellesley, MA: AK Peters, Ltd.

[5] Schilling, R.L., Song, R., & Vondracek, Z. (2010). *Bernstein Functions*. Vol. 37 of *De Gruyter Studies in Mathematics*. Berlin, Germany: Walter de Gruyter & Co.

[6] Simon, T. (2014). Comparing Fréchet and positive stable laws. *Electron. J. Probab.*, 19(16), 1-25.

Bob Pego is a professor of mathematical sciences at Carnegie Mellon University.

The JOHN VON NEUMANN Lecture

TUESDAY, JULY 11, 2:30 - 3:30 pm

David Lawrence Convention Center Pittsburgh, Pennsylvania

• SIAM ANNUAL MEETING •

SINGULAR PERTURBATIONS IN NOISY DYNAMICAL SYSTEMS Bernard J. Matkowsky

Northwestern University

Consider a deterministic dynamical system in a domain containing a stable equilibrium, like a particle in a potential well. The particle, independent of initial conditions, eventually reaches the bottom of the well. But if the particle is subjected to white noise, a dramatic difference occurs in its behavior; it can exit the well. The natural questions then are (1) how long will it take for the particle to exit, and (2) where on the boundary of the domain of attraction will it exit? Matkowsky computes the mean first passage time to the boundary and the probability distribution of boundary points being exit points. When the noise is small, each quantity satisfies a singularly perturbed deterministic boundary value problem.

Matkowsky will treat the problem by the method of matched asymptotic expansions (MAE) and generalizations thereof. Although MAE has been

used successfully to solve problems in many applications, there are problems for which it does not suffice, including those exhibiting boundary layer resonance. Matkowsky will present a physical argument and four mathematical arguments to modify MAE and make it successful. Finally, he will discuss applications of the theory.



SOCIETY for INDUSTRIAL and APPLIED MATHEMATICS 1-800-447-SIAM • meetings@siam.org • www.siam.org

Professional Opportunities and Announcements

Send copy for classified advertisements and announcements to: marketing@siam.org; For rates, deadlines, and ad specifications visit www.siam.org/advertising.

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

Math, Tipping Points, and Planet Earth Dr. Mary Lou Zeeman, Bowdoin College, festival representative for Math of Planet Earth

ALL DAY HANDS-ON ACTIVITIES:

Climate, Math, Ice Cores, and You: Hands-On Data from Planet Earth

Dr. Mary Lou Zeeman and the Mathematics and Climate Research Network (MCRN) and the Computational Sustainability Network (CompSustNet).

Real Science, Real Data, You: Scientific Exploration with NOVA Labs Games NOVA Labs

Math Climate Research Network

Ocean Prediction Postdoctoral Positions Naval Research Laboratory, Stennis Space Center, MS

The Naval Research Laboratory is seeking postdoctoral researchers to push forward the frontiers of ocean forecasting. The work covers a wide scope of physics including surface waves, thermohaline circulation, nearshore circulation, and ocean/atmosphere coupling from global to nearshore scales. This challenging work includes processing and analysis of satellite and in water observations, construction of numerical model systems on high performance computing systems and assimilation for predicting the ocean environment. For a quick overview of some of the research work within the NRL oceanography division at Stennis Space Center, visit the web site:

https://www7320.nrlssc.navy.mil/pubs.php



Applicants must be a US citizen or permanent resident at time of application. Applications will be accepted until positions are filled. Please e-mail a resume and description of research interests: Gregg Jacobs: gregg.jacobs@nrlssc.navy.mil

Design Thinking

Continued from page 10

explain the ideas to others (or to themselves) and further their thinking processes. Many hypotheses are typically generated, nearly all of which are wrong. But the process helps hone in on the underlying structure they seek to uncover.

In the "What works?" stage of DT, practitioners test conceived possibilities by developing rough prototypes and using tools and games to understand assumptions and limitations. Mathematicians often behave similarly, employing strategies to determine which hypotheses might be true or which algorithms will work. Looking for counterexamples is one strategy, while another is proof by contradiction. These two widelyused mathematical approaches are reflected in two tools described in [2]: "Worst Idea" and "Contra-Logic." After discarding several alternatives or prototypes, the real problem's essence begins to show. It is often at this stage that we return to the original problem and reframe it again. Determining the "correct" problem statement is generally the crux of the whole issue, and the answer comes easily after this is done. The Stanford students investigating infant mortality with DT techniques reframed their problem to focus on keeping babies warm without reliable electricity. This led them to design Embrace,¹ a cheap, portable, and reusable baby sleeping bag that has been used by over 200,000 babies to date.

Since DT steps closely mirror our thought processes as mathematicians, it seemed natural to formally introduce some DT techniques in a multidisciplinary student research project. In 2015, a group of researchers including faculty, graduate and undergraduate students, and high school teachers and students from the U.S. and Tanzania investigated the poaching of elephant tusks and rhino horns. This collaborative project, led by co-author Padmanabhan Seshaiyer and supported² in part by the National Science Foundation, helped participants engage in the discovery phase for "What is?," "What if?," and "What works?" The "What is?" stage consisted of directly talking to all stakeholders, including students, teachers, faculty, park rangers, and the broader community, about the problem of poaching. Using written and online surveys and pre- and post-assessments, students developed a needs assessment for poaching and helped us (as problem solvers) empathize-by observation and review-with the audience for whom we wish to design solutions.

We then identified several problems during the "What *if*?" step, including the purpose, process, logistics, and current approaches for poaching. From these, we *defined* a specific problem that involved developing new engineering, mathematical, and scientific approaches to stop poaching. In the next phase of "What *if*?," the team brainstormed using a variety of *ideation* approaches to develop an early-warning alarm consisting of an intelligent sensor-based tracking system combined with a mobile and satellite

¹ http://embraceglobal.org/

network that game rangers can employ for tracking and monitoring. The "What works?" process then allowed us to prototype and test unmanned air vehicles, such as quadcopter drones, that the tracking system could utilize to understand the process of illegal poaching.

The DT framework also provides an exciting opportunity for an integrated science, technology, engineering, and mathematics (STEM) experience for faculty and students at all levels. Specifically, the poaching project allowed the team to address the following questions: How does one build a drone? What mathematics and physics

are involved? What types of engineering concepts and control processes must be employed? What kinds of mathematical calculations should be performed? What type of next generation technology should be incorporated? How do we promote awareness of this project's integrated STEM education to the next generation of students?

Understanding the quadcopter dynamics and simulation requires the development of mathematical relations to describe inertial and rotational equations of motion for the rigid body dynamics. For example, one can employ Newton's laws of motion to describe the relationship between the displacements of the quadcopter, given in terms of the various forces \mathbf{F} and the mass m. These equations must be solved with rotational equations of motion that express the rotation about the center of the quadcopter. The rotational components of angular acceleration ω are expressed as a function of components of the inertia matrix I and torque τ . One may also consider a suitable Proportional Derivative (PD) control, with the component proportional to the error between our desired and observed trajectories and its derivative (see Figure 1, on page 10).

Additionally, mathematicians can tackle the search problem associated with the drone's decision-making on whether the target is present in the search region, and if so, where exactly it is located. They can study the associated search problem using a Bayesian framework with the objective of improving the decision as the search pattern continues through the evolution of a belief function. One could consider a binary detection random variable in the analysis, representing whether a specific target in a given cell has been detected. Combining this with a given sequence of observations allows for the computation of individual cell belief probabilities to iteratively identify target location. Figure 2 depicts a summary of a target detection algorithm, along with a closed formula obtained as part of our research for the belief function of a specific case.



Figure 2. Probabilistic approaches to target detection algorithm for the quadcopter. Image courtesy of [1].

steps carry over to mathematics. Although mathematics can model human behavior in critical ways, the problems mathematicians solve are not always human-centric. And although mathematicians tend to value succinct communication and can often be found scribbling equations on the backs of napkins, we don't write formal "napkin pitches" like design thinkers do. However, we do think that the ideas of "What *is*?," "What *if*?," and "What *works*?," along with the mantras of empathize, define, ideate, prototype, and test, carry over quite nicely and can be useful both in the research and teaching of mathematics.

Disclaimer: Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

References

[1] Baez, A., Mclane, K., & Pradyuta, P. (2016, April). *Council on Undergraduate*

Research: 20th Annual Posters on the Hill. Washington, D.C.

[2] Liedtka, J., Ogilvie, T., & Brozenske, R. (2014). *The Designing for Growth Field Book (a step-by-step project guide)*. New York, NY: Columbia Business School.

Jennifer S. Pearl is a program director in the Division of Mathematical Sciences at the National Science Foundation (NSF). She learned about design thinking through coursework at the University of Virginia and the Brookings Institution, and tries to use it to develop creative solutions for the NSF. Padmanabhan Seshaiyer is a professor of mathematical sciences at George Mason University and currently serves as a program director in the Division of Mathematical Sciences at the NSF as well as chair of the SIAM Diversity Advisory Committee. He has developed a course titled DICE: Design Thinking, Innovation, Creativity and Entrepreneurship in STEM, which has helped foster student and teacher interest in solving global challenges using STEM tools.

Mathematics of Planet Earth Explained

Mathematics of Planet Earth (MPE) views our planet through these themes:

- Planet Earth as a physical system: e.g., climate dynamics, oceans, atmosphere, cryosphere, Earth, and space
- Planet Earth as a system supporting life: e.g., mathematical ecology, carbon cycle, food systems, natural resources, and sustainability
- Planet Earth as a system organized by humans: e.g., land use, energy, communication, transportation, and socio-economics
- Planet Earth as a system at risk: e.g., global change, biodiversity, water, food security, epidemics, and extreme events



² https://nsf.gov/awardsearch/ showAward?AWD_ID=1407087 Comparison of DT processes and mathematical research has limits. Not all of the DT

SIAM Supports the March for Science

On Earth Day, April 22, 2017, scientists worldwide will participate in numerous activities that promote science, science education, and the use of scientific evidence to inform policy. A March for Science¹ is scheduled in Washington, D.C., with numerous satellite marches in other locations throughout the U.S. and around the world. SIAM supports the goals of the March for Science² and encourages its members to help make the event a success.

SIAM's support for the march is based on the recognition that mathematics is an integral part of the scientific enterprise. Science offers the public an open pathway to discovery. It has deepened our understanding of the world and advanced innovations that have yielded significant economic benefits. The March for Science is a unique opportunity to communicate the importance, value, and beauty of science to the public in a nonpartisan manner.

We hope that many of our readers will choose to join us on the National Mall on April 22, or participate in a march closer to home. We welcome your suggestions on how to continue to engage and promote the value of science following the march. The SIAM Activity Group on Mathematics of Planet Earth (SIAG/MPE) provides a forum for mathematicians and computational scientists to study our planet, its life-supporting capacity, and the impact of human activities.

Join the SIAG!

http://www.siam.org/activity/mpe/

*SIAM Photo/Officers of SIAG/MPE

www.marchforscience.com

² https://sinews.siam.org/Details-Page/siam-supports-goals-of-march-for-science