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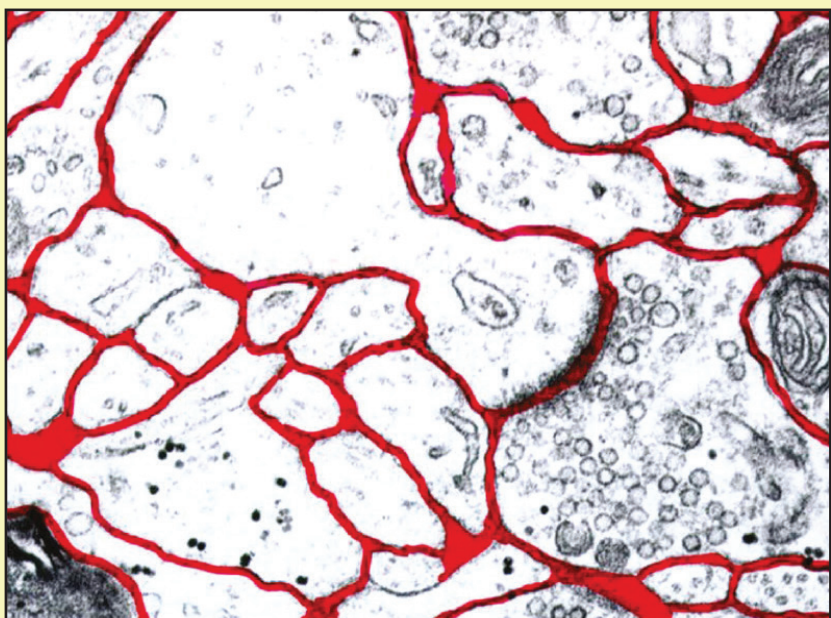


Figure 2. Cells in the brain lie in extracellular fluid. The fluid is coloured red. Image courtesy of [3].

In the article “Modelling Drug Dynamics in the Brain” on page 3, Vivi Rottschäfer presents a mathematical model that helps study the processes that govern the concentration profile of drugs in the brain.

Combining Data and Models to Study Woody Plant Encroachment

By Nathaniel A. Brunsell and Erik S. Van Vleck

Woody plant expansion into grasslands and savannas, which is accelerating worldwide, often affects ecosystem processes. Understanding and predicting the environmental and ecological impact of encroachment has led to a variety of methodologies for assessing its onset, transition, and stability. These methods generally rely on dynamical systems approaches.

We seek to understand the competition between alternate stable states of grasses, trees, or shrubs and the influence of climate, fire, precipitation, and livestock grazing. Of particular interest to us are climate and fire interactions occurring worldwide (both naturally and due to fire suppression), especially the impact of woody encroachment on prairie grasslands in the central U.S. The Konza Prairie Biological Station (KPBS) is a native tallgrass prairie preserve located in the Flint Hills of northeastern Kansas, a grassland region of steep slopes overlain with shallow limestone soil unsuitable for cultivation. The Flint Hills region encompasses over 1.6 million hectares and is the largest remaining area of unplowed tallgrass prairie in North America.

The KPBS is divided into various watersheds, each with distinct enforced conditions. These conditions include different rates at which each watershed is burned and possible grazing by cattle or bison. The station is an ideal place to blend data acquisition and utilization with models to understand phenomena such as woody encroachment.

Our research on woody encroachment combines both data and models, and our initial work builds upon the development of simple low-dimensional stochastically-forced models [4-5, 7-8]. A low-dimensional model with stochastic precipitation and fire disturbance can examine the complex interactions between precipitation and fire as mechanisms that may suppress or facilitate increases in woody cover [1].

To analyze the impact of fire and precipitation frequency and intensity, we employ local in-time Lyapunov exponents or so-called Steklov averages [2-3, 6] that assess convergence/divergence over different divergence timescales as a measure of relative stability or instability. Lyapunov exponents calculate the perturbation sensitivity of time-varying solutions of dynamical systems. By varying the parameters that

See **Plant Encroachment** on page 4

Self-organization in Space and Time

By Matthew R. Francis

Self-organization is an important topic across scientific disciplines. Be it the spontaneous flocking of birds or dramatic phase transitions like superconductivity in materials, collective behavior without underlying intelligence occurs everywhere.

Many of these behaviors involve synchronization, or self-organization in time, such as activation in heart cells or the simultaneous blinking of certain firefly species. Others are aggregations, or self-organization in space, like swarming insects, flocking birds, or the alignment of electron spins in magnetic material.

Despite their conceptual similarity, self-organization in space and time have largely been treated separately. “I was curious about whether the two fields had been wedded, and it turns out they hadn’t, at least not fully,” Kevin O’Keeffe, a postdoctoral researcher at the Massachusetts Institute of Technology, said. “I knew all these tricks and mathematical tools from synchronization, and I was looking to cross-fertilize them into the swarming world.”

O’Keeffe, along with Hyunsuk Hong of Chonbuk National University in South Korea and Steven Strogatz of Cornell University, developed a simple mathematical model for simultaneous spatially-coordinated and synchronous behavior [1]. They designed their “swarmalator” model to be as simple as possible in order to understand general principles before applying it to more realistic physical or biological systems.

“We came across these Japanese tree frogs that had exactly the right ingredients,” O’Keeffe said. “If you observe a bunch of frogs in a field, they not only synchronize their calling but also move around and form swarms, so they have both spatial and temporal degrees of freedom.”

The team also considered sperm, which move collectively and beat their tails synchronously, triggered by certain chemical reactions. Despite its simplicity, the swarmalator model exhibits multiple distinct complex behaviors, depending on the

interactions of the individual elements of the oscillating swarms.

The mathematical study of synchronization began about 50 years ago, when nonlinear dynamics pioneer Arthur Winfree¹ developed a simple model for circadian rhythms based on interacting oscillators. A few years later, physicist Yoshiki Kuramoto simplified Winfree’s model and solved it exactly. Researchers have created many variations of the Kuramoto model to address everything from firefly flashes to superconductivity; it is also similar in mathematical form to several physics-based models of magnetism.

O’Keeffe and his team based the swarmalator model on the simplest form of the Kuramoto model: a system of coupled ordi-

nary differential equations (one for every oscillator). Each oscillator interacts with all others at the same strength — there is no falling off with distance or communication time lag, for example. A single (scalar) parameter sets both the strength of the interaction and the system’s preference as to whether all the oscillators are in or out of phase. The systems cycle freely when the parameter is zero, much like the minute hand of a clock revolving at a steady rate of one cycle per hour.

As a general rule, swarming is much more complicated than synchronization. It is easy to see why: there are three directions in space but only one in time. If the swarming bodies are free to move in all three directions, they have many possible ways to self-organize.

See **Self-organization** on page 3

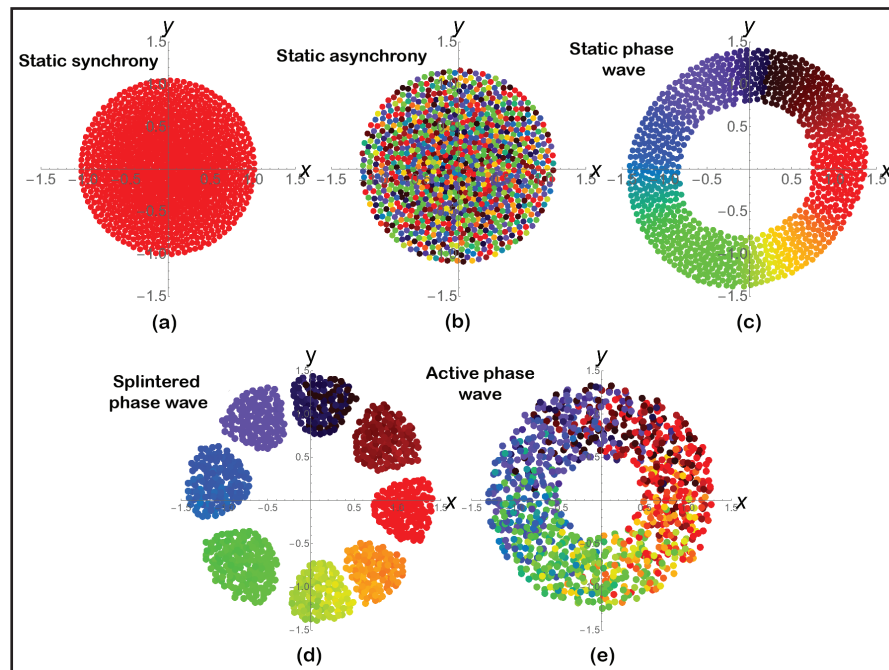


Figure 1. The five major ending states of the simulated “swarmalator” system on the x - y plane. Like colors are synchronized with each other, while the full rainbow indicates varying degrees of asynchronization. **1a.** All swarmalators are synchronized and want to be close to each other. **1b.** Swarmalators exhibit maximum asynchronization, but still swarm. **1c.** Swarmalators group with in-phase oscillators but repel those out of phase, making “the wave.” **1d.** Swarmalators behave similarly to **1c**, but with abrupt gaps between groups of in-phase oscillators. **1e.** Groups of oscillators revolve in opposite directions. View accompanying animations in the online version of this article. Image courtesy of Kevin O’Keeffe, adapted from [1].

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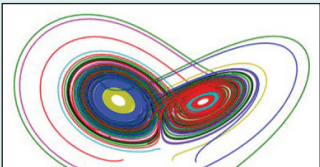
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Somebody Else’s Dream
Bonita Saunders gives an inspiring account of her road to a career as a research mathematician at the National Institute of Standards and Technology. As a young African American student, she experienced the complicated aftereffects of school integration firsthand.
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Research Software Engineer: A New Career Track?
Chris Richardson and Mike Croucher outline a U.K. initiative spearheaded by the Software Sustainability Institute to improve academic software reliability and reusability. By encouraging better software practices and pushing for a unique research software engineering career track, the institute is enhancing research software in academia.
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Jupyter: Tools for the Life Cycle of a Computational Idea
Min Ragan-Kelley, Carol Willing, and Jason Grout provide an overview of Project Jupyter, which offers tools—from interactive exploration and experimentation to publication and communication of results—for the life cycle of a computational idea.
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The Underlying Laws Binding Cities, Companies, and Living Systems
James Case reviews *Scale: The Universal Laws of Growth, Innovation, Sustainability, and the Pace of Life in Organisms, Cities, Economies, and Companies* by Geoffrey West, who argues that one can apply the basic mathematical laws that define growth in the physical world to the biological, political, and corporate realms.
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Reservoir Computing: Harnessing a Universal Dynamical System
While artificial intelligence algorithms are in great demand, learning a deterministic dynamical system is useful for applications such as weather forecasting and radio transmitter fingerprinting. Daniel J. Gauthier describes how a reservoir computer can train a “universal” dynamical system to predict the dynamics of a desired system.
- 

It’s a Matter of Style

Does your writing have a noticeable style? Is there something characteristic about your use of vocabulary, punctuation, voice, and the many other ingredients of written composition?

Style is likely not foremost on your mind when you are writing a paper. Refining and verifying the technical content and completing the paper are usually of higher priority.

Although the format of an academic paper is quite rigid and confining, there is still plenty of scope for writing it your own way. A trivial example is the explanation of a paper’s organization, which usually appears at the end of the introduction. Many authors write, “The contents of this paper are as follows,” or “The rest of this paper is organized as follows.” But there are ways to avoid these clichéd phrases. For example, one can write, “We begin, in the next section, by ...” The ensuing sentences are typically of the form, “In section 2 we investigate ...” — you could rewrite these more compellingly to sound less like a table of contents.

How you cite other work is also very much a matter of style. Compare

Jones’s analysis was extended in [1], [2].

with

Smith extended Jones’s analysis to semisimple eigenvalues [1], and Walker subsequently treated the general case of defective eigenvalues [2].

The second version adds a human interest element and saves the reader from having to turn to the bibliography to determine the gist of the extensions.

Especially for those of you starting out in academic writing, it is good exercise to identify authors whose style you like and analyze what it is about their writing that attracts you. Donald Knuth’s writing has always inspired me, and I learned a lot from his book on mathematical writing [2]. As with all of us, Knuth’s writing style has evolved over time. In one of the volumes collecting his papers on particular subjects, he writes, “I first wrote nearly all of these chapters long before the copy editors of *TAOCP* [*The Art of Computer Programming*] taught me how to write better sentences. I cannot be happy now with stylistic errors that I would no longer tolerate in the writing of my students, so I have tried to remove them, together with all the technical errors that have come to my attention” [1].

Software for checking style goes back at least as far as Unix utilities of the 1970s. At their crudest, these tools compute readability indices or check for commonly used “waffle words.” Microsoft Word reviews both grammar and spelling as you type. I am not aware of many tools that integrate with other editors, though a variety of web-based services are available. It seems reasonable to expect that future artificial intelligence-based tools will offer useful analysis of one’s text.

FROM THE SIAM PRESIDENT

By Nicholas Higham



Cartoon created by mathematician John de Pillis.

A different aspect of style is the house style of journals. Most reputable journals have a prescribed submission style for uniformity. Copy editors edit for this style and correct grammatical and formatting errors in manuscripts. SIAM is well known for the quality of its copy editing. Less well known is the *SIAM Style Manual*, which is freely available.¹ SIAM style is not too prescriptive and largely follows standard guidelines, such as those in the *Chicago Manual of Style*, though with more detail on how to format mathematics. Although primarily aimed at documenting SIAM style for copy editors, the *SIAM Style Manual* is also an informative read for authors. You might as well try to adhere to the style guidelines if you are writing for a SIAM journal, as this will minimize the copy editing changes made to your manuscript. What’s more, simply thinking about style issues may help you improve your paper’s readability.

Less experienced authors who submit to SIAM may benefit from improved wording provided by SIAM copy editors — as many of us have over the years, and as Knuth did from the *TAOCP* copy editors. Likewise, my articles always benefit from improvements suggested by *SIAM News* copy editors, who apply *SIAM News*’s own house style.

Another aspect of style concerns the LaTeX style file used to produce SIAM papers. This has evolved over the years, with a major modernization in 2016.² The most recent version is dated December 17, 2017, and is thoroughly documented. It comes with a BibTeX style file `siamplain.bst` that formats your bibliography in SIAM style, and will include DOIs if they are present in the BibTeX database. By using `siamplain`.

¹ <http://www.siam.org/journals/auth-info.php>
² <https://sinews.siam.org/Details-Page/qa-tamara-kolda-on-siam-journal-macro-update>

`bst`, you can produce a neatly formatted, DOI-linked bibliography and save a great deal of copy-editing time.

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[1]

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[2]

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Modelling Drug Dynamics in the Brain

By Vivi Rottschäfer

While scientists have devoted much research to models of neural activity in the brain, they have paid little attention to modeling drugs that target the brain. Development of this class of drugs is very challenging and necessitates an understanding of the highly complex processes that govern the concentration profile of a drug in the brain over time. Since access to the brain for measurement purposes is very limited, a mathematical model is a helpful tool. But before we present a model, we must introduce some of the brain's physiology and the processes that occur after medicine consumption.

The brain is interlaced with a network of blood capillaries (see Figure 1). Following intravenous or oral administration and subsequent intestinal absorption, the drug in question begins to circulate in the blood and primarily enters the brain from the arterial network by crossing the blood-brain barrier (BBB). One of the BBB's principal functions is to limit transport into the brain and protect it from harmful substances, thereby preventing brain damage. When the drug does enter the brain through the BBB it circulates in brain fluids, such as the extracellular (ECF) and cerebrospinal fluids. It then binds to receptors on cells in ECF (see Figure 2, on page 1). When a drug binds to a receptor, it leads to an

effect in the body. Here we will focus on drug transport in ECF and the subsequent binding to receptors.

Compartmental models are widely used in pharmacology, and have also been developed to model drug concentration in the brain. For example, [5] presents a general compartmental model of the central nervous system. Unfortunately, these models do not account for drug transport in ECF and other tissues, which mainly occurs via diffusion and bulk flow. Moreover, compartmental models do not consider receptor binding. A diffusion-advection equation can model drug transport where the drug is administered directly into the brain [2]. As a first step towards a full model of the brain, our model incorporates diffusion and flow in ECF, inflow through the BBB, and receptor binding.

Though the brain is three-dimensional, we start by creating a model on a two-dimensional domain, which represents a tissue unit of brain ECF. This square domain is surrounded by brain capillaries and can be considered the smallest building block of the brain, in terms of drug distribution (see Figure 3). In the human brain, the distance between capillaries is on average 50 μm . Cells with receptors are located inside the domain. We model drug transport in the unit by diffusion and bulk flow, assuming that the latter occurs in the x -direction. One can consider ECF a porous medium, as it is filled

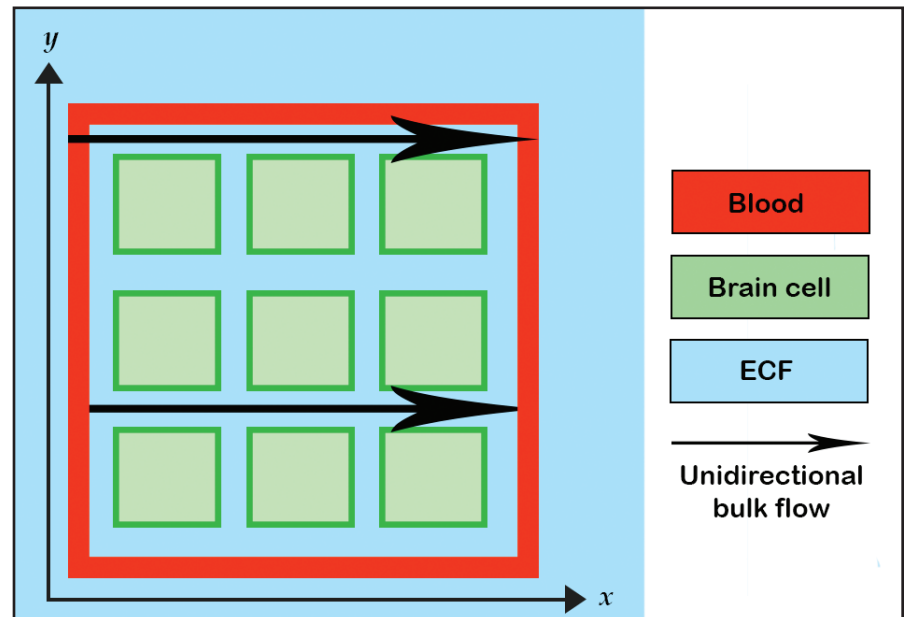


Figure 3. The two-dimensional unit of extracellular fluid, which contains cells with receptors and is bounded by blood capillaries. Concept for figure provided by Vivi Rottschäfer.

with many obstacles—such as cells and proteins—that limit diffusion. This leads to an effective diffusion smaller than normal (in a medium without obstacles). We model this with the so-called tortuosity λ , thereby dividing the normal diffusion d by λ^2 , which results in a smaller diffusion coefficient. Tortuosity differs between drugs due to their varying sizes and deformabilities.

To formulate the model, we denote the concentration of free (unbound) drug by D

and the concentration of receptor-bound drug by B . This yields

$$\begin{aligned} \frac{\partial D}{\partial t} &= \frac{d}{\lambda^2} \Delta L - v \nabla L \\ &\quad - k_{on} D(B_{max} - B) + k_{off} B, \\ \frac{\partial B}{\partial t} &= k_{on} D(B_{max} - B) + k_{off} B, \end{aligned}$$

where v is the speed of the flow. When a drug binds to a receptor, it forms a drug-receptor complex until it dissociates (unbinds) into drug and receptor again. We model this by the final terms in the D -equation, which represent receptor binding with a rate k_{on} and unbinding with a rate k_{off} . The maximum concentration of receptors B_{max} limits the binding.

We assume that no drug is present in the brain at $t=0$, and hence $D(t=0)=0$ and $B(t=0)=0$. We use boundary conditions to model the concentration of the drug in the blood and its crossing through the BBB. While drugs can cross the BBB via several mechanisms, including passive

See Drug Dynamics on page 5

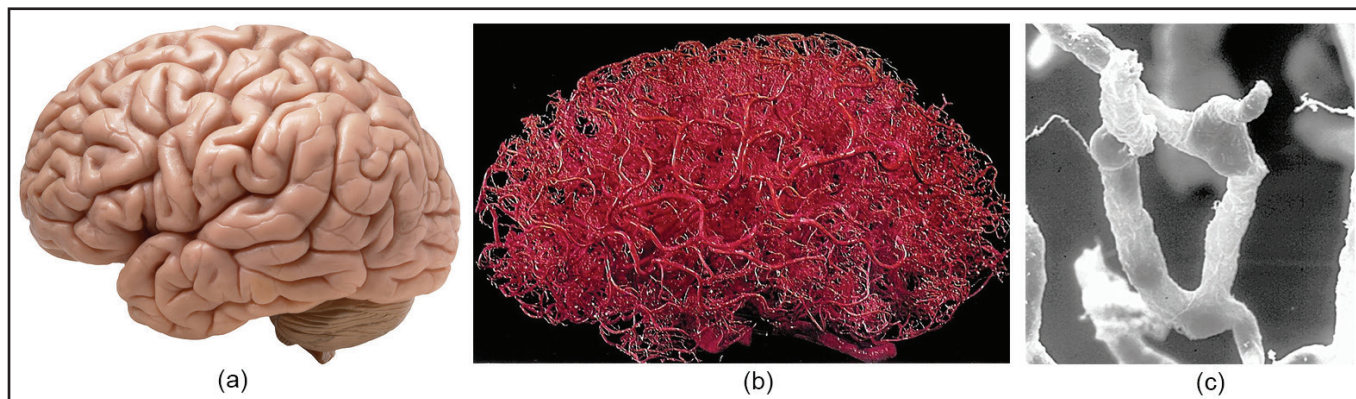


Figure 1. The brain and its interlacing capillary network. **1a.** The brain. **1b.** The network of capillaries that intertwines the brain. **1c.** Brain capillaries from the human cerebellar cortex. 1a and 1b are public domain images, and 1c is courtesy of [1].

Self-organization

Continued from page 1

Moreover, unlike synchronization, “swarming” is not a clearly-defined mathematical concept. “You have an intuitive understanding of swarming,” O’Keeffe noted. “You can imagine flocks and stuff, but when you get to the mathematical axioms, there aren’t many.”

This is because swarming behavior is relative to the system under consideration. For many real-world systems, the orientation of the objects within the swarm is important to the overall dynamics. There is also the question of how close the swarming objects want to get to each other, which can theoretically be considered a force that switches from attractive to repulsive when the distance gets too small. After all, maximization and minimization of population density within a group are both forms of self-organization.

The swarmalator formulation uses the so-called aggregation model, which ignores complications like orientation and utilizes power laws to model attraction and repulsion. The model is restricted to two spatial dimensions, which sacrifices some realism for geometric simplicity. Two state variables characterize each swarmalator: a phase angle θ —representing the temporal oscillator state—and the two-dimensional vector $\mathbf{x}=(x,y)$, describing the position. The authors also looked at the three-dimensional version and found many of the same basic behaviors, though the systems were understandably more complicated and harder to interpret.

The equations for N swarmalators are

$$\begin{aligned} \dot{x}_i &= \frac{1}{N} \sum_{j \neq i}^N \left[\frac{x_j - x_i}{|x_j - x_i|} \right] \\ &\quad \left(1 + J \cos(\theta_j - \theta_i) \right) - \frac{x_j - x_i}{|x_j - x_i|^2}, \\ \dot{\theta}_i &= \frac{K}{N} \sum_{j \neq i}^N \sin \left(\frac{\theta_j - \theta_i}{|x_j - x_i|} \right), \end{aligned}$$

where the dot indicates an ordinary derivative with respect to time. Because the swarmalators begin in a state with no oscillations or motion in space, the initial conditions for the system are static.

The coupling parameter K , modulated by the distance between the swarmalators, determines how strongly the oscillator state variables interact. When K is positive, the oscillator states minimize their phase differences. When K is negative, they maximize them. This connection weakens with large separation between swarmalators. When the parameter J is positive, swarmalators are attracted to others with the same phase. When J is negative, they are attracted to those with opposite phases.

Varying the values of J and K produces a phase diagram (see Figure 1, on page 1), based on whether the swarmalators synchronize, clump, or produce more complicated behaviors. O’Keeffe, Hong, and Strogatz identify five major classes of swarmalator activity, which correspond to Figure 1 (view accompanying animations in the online version of this article).

(a) When $K > 0$, the swarmalators synchronize and settle into a static configuration, regardless of the value of J . This is a mathematically-boring configuration but potentially important for many real-world applications, such as the aforementioned tree frogs.

(b) When both J and K are negative, or when K is negative and J is positive but small, the swarmalators prefer to be next to those whose phases are maximally different from theirs, and settle into another static spatial arrangement. This is also mathematically uninteresting.

(c) When $K=0$ and $J > 0$, the swarmalators behave like “the wave” at sports games; oscillators group with like oscillators, but the phase difference grows with distance across the swarm. The swarmalators settle into a static ring pattern in space. This is qualitatively similar to the behavior of colloidal particles on a surface, where the oscillator variable corresponds to the electric dipole of the particles.

(d) Keeping $J > 0$ and looking at small negative K values produces something O’Keeffe jokingly calls a “pizza” configuration or “splintered phase wave.” This is like a sports wave, with significant divisions between each group of fans’ motion.

(e) The transitional state between phases (b) and (d) creates a system of groups of counter-rotating swarmalators. This is qualitatively similar to sperm behavior, where the wiggling tail represents the oscillation. The cells tend to stick to surfaces and create clusters in which all the sperm wiggle their tails synchronously, but neighboring clusters have slightly different oscillation phases.

Despite its simplicity, the swarmalator model exhibits enough complex behavior to be interesting. Simplicity often means

generality, and extending the original model can provide ways to restore any lost specificity. “You want the simplest model that gives the right physics,” O’Keeffe said. “That is why the Kuramoto model took off and became so popular — just because it was simple.”

There is still much to learn from the model as it stands. For instance, the equations give ambiguous answers for the lines of transition between various phases. Since these transitions determine how one behavior switches to another—analogue to water freezing or a material becoming magnetized—knowledge of them is important for understanding the function of swarmalator groups.

O’Keeffe hopes other researchers will further study the system. “The dream would be to get some experimentalists or physicists interested in this, who could engineer real swarmalator systems,” he said. “If someone could go out there and come up with something tangible, that would be brilliant.”

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Further Reading

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Winfree, A.T. (1967). Biological rhythms and the behavior of populations of coupled oscillators. *J. Theo. Bio.*, 16, 15.

Matthew R. Francis is a physicist, science writer, public speaker, educator, and frequent wearer of jaunty hats. His website is BowlerHatScience.org.

Plant Encroachment

Continued from page 1

control fire and precipitation, and comparing the dependence of quantities analogous to the largest Lyapunov exponent as a function of these parameters, we ascertain the relative control exerted on woody encroachment through these mechanisms.

Researchers have successfully employed the largest Lyapunov exponent in different areas of biology and ecology as an indicator of chaos (i.e., sensitivity to the initial state) and a measure of the relative sensitivity of parameterized systems. For example, Lyapunov exponents are indicative of a dynamical system's exponential rate of change either away or toward a particular state of the system, such as a grass or woody state. A positive exponent illustrates an exponential rate away from the current state, i.e., an unstable state and transition to a stable one. A negative exponent indicates a trajectory toward the initial state, meaning that the state is stable. Therefore, if a given precipitation environment results in a negative Lyapunov exponent for woody fraction, the particular rainfall regime is stable for the expansion of woody species; a positive exponent signals an unstable regime.

Figure 1 displays the divergence time i versus the logarithm of divergence distance $\tilde{y}(i)$'s time-averaged logarithm, defined by

$$\tilde{y}(i) = \langle \log(d_j(i)/d_j(0)) \rangle \approx \lambda_1(i) \cdot i,$$

where the average is over j and $d_j(i)$ denotes the divergence of the j th difference over a fixed length of time i . $\lambda_1(i)$ (analogous to the largest Lyapunov exponent) denotes the average divergence rate over time intervals of length i . The algorithm in [6] allowed for computations using an appropriate delay coordinate embedding. Figure 1 illustrates the behavior of the normalized local Lyapunov exponents for a subset of the precipitation magnitudes, frequencies, and burn considered in [1] that corresponds to a 16-year fire frequency and high annual precipitation.

Figure 1 also shows that these local type Lyapunov exponents produce an annual pattern with seasonal variations for some parameter configurations. Grass assimilation (A), woody transpiration (Tr_t), and top layer soil moisture (θ) have two peaks per year while other variables—such as bare soil evaporation (E_s)—have one peak per year. Two peaks in these plots correspond to instability (sensitivity with respect to perturbations in that variable) over divergence times of zero-three months, six-nine months, 12-15 months, etc.; one peak per year corresponds to instability over divergence times of zero-six months, 12-18 months, etc. Perturbations are amplified by approxi-

mately $e^{\tilde{y}(i)}$, so that they grow with time when the slope in Figure 1 is positive and decay when the slope is negative.

The results in [1] indicate that precipitation frequency is more significant than the intensity of individual precipitation events when controlling woody encroachment. Fire, however, has a much more dominant impact on limiting encroachment. These results suggest that fire management—in the form of more frequent burns—may be an effective strategy to slow the onset of woody species into grasslands. While climate change might predict a reduced potential for woody encroachment in the near future, these findings imply that a reduction in woody fraction may be unlikely when considering anthropogenic fire suppression.

Our next steps involve the incorporation of data into more complex land surface models (LSMs). Noah-MP is an LSM that employs multiple options for key land-atmosphere interaction processes. It contains a separate vegetation canopy defined by a canopy top and bottom; crown radius; and leaves with prescribed dimensions, orientation, density, and radiometric properties. The Noah-MP model prescribes both the horizontal and vertical density of vegetation using either ground- or satellite-based observations. It utilizes a dynamic vegetation model that allocates carbon to various parts of vegetation (leaf, stem, wood, and root) and soil carbon pools (fast and slow). The model distinguishes between C3 photosynthesis pathways (used by most plants) and C4 pathways (used more by semi-arid grasses), and defines vegetation-specific parameters for plant photosynthesis and respiration.

To understand transitions between these competing stable states, we are interested in quantifying several coupling metrics from Ameriflux¹ data, remotely-sensed atmospheric profiles, atmospheric boundary layer height and soil moisture, and output from both a low-dimensional model and the Noah-MP model. These factors will help identify the coupling state and relationship to available energy and partitioning, vapor pressure, and temperature gradients to quantify each state's stability and determine the underlying data and model sensitivity. Ultimately, this will increase our understanding of the physical mechanisms responsible for coupling dynamics in the central U.S.

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¹ <http://ameriflux.lbl.gov/>

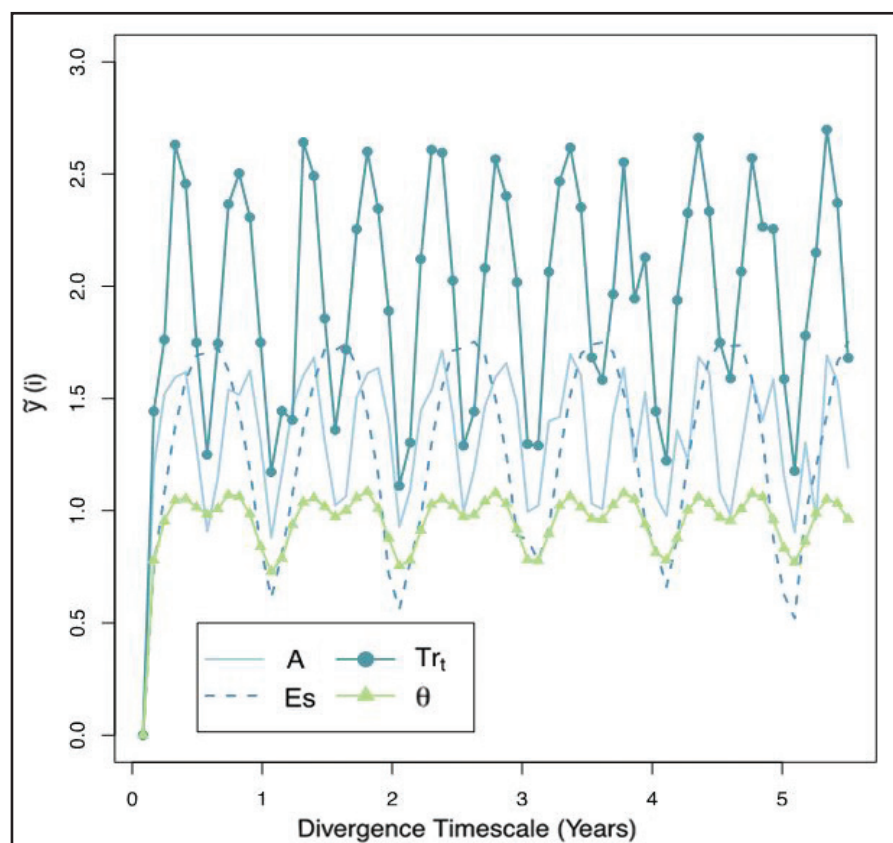


Figure 1. Normalized divergence as a function of the divergence time scale i (in years) for parameter values that correspond to a 16-year fire frequency and high annual precipitation for grass assimilation, woody transpiration, top layer soil moisture, and bare soil evaporation. Figure credit: Nathaniel A. Brunzell and Erik S. Van Vleck.



From left: Yuxin Chen (Northwestern University), Mary Silber (University of Chicago), Nate Brunzell (University of Kansas), and Erik Van Vleck (University of Kansas) visit the Konza Prairie Biological Station. Photo credit: Karna Gowda.

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Recent Advances in Dimensionality Reduction with Provable Guarantees

The following is a short introduction to an invited lecture to be presented at the upcoming 2018 SIAM Annual Meeting (AN18) in Portland, Ore. from July 9-13. Look for feature articles by other AN18 invited speakers introducing the topics of their talks in future issues.

Researchers have used *dimensionality reduction* for over a hundred years — first Francis Galton, then Karl Pearson, and later Harold Hotelling in the late 19th and early 20th centuries. Pearson and Hotelling developed principal component analysis (PCA); the formation of a number of methods, including multidimensional scaling, kernel PCA, and isometric feature mapping, soon followed. One can employ these methods in statistics, data mining, machine learning, and many other areas after approximately fitting high-dimensional data to low-dimensional models by extracting a few variables that “explain” most of the data.

Orthogonal but complementary is the study of dimensionality reduction from the perspective of low-distortion embeddings into low-dimensional normed spaces. Researchers utilize such methods in high-dimensional computational geometry, signal processing, algorithms for large-scale linear algebra problems, identification of motifs in computational biology, machine learning, etc. Algorithms used in high-dimensional computational geometry problems typically suffer from the *curse of dimensionality*, wherein the running time and/or memory usage of the best-known algorithms scale poorly (even exponentially) with dimension. Such problems include nearest neighbor search and various clustering problems. The idea is that, given some input set of data points $X = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$, one can quickly compute some $f: X \rightarrow \mathbb{R}^m$ for $m \ll d$, such that $f(X)$ has roughly the same geometry as X (e.g., preservation of pairwise distances, angles, volumes of simplices defined by subsets of points, etc.). A cornerstone result in this line of work is the so-called Johnson-Lindenstrauss (JL) lemma, proven in 1984:

Lemma 1 (JL lemma). For any $X \subset \ell_2$ and any $0 < \varepsilon < 1$, there exists an embedding $f: X \rightarrow \mathbb{R}^m$ with $m = O(\varepsilon^{-2} \log |X|)$, such that

$$\forall x, y \in X, \quad (1 - \varepsilon)\|x - y\|_2 \leq$$

$$\|f(x) - f(y)\|_2 \leq (1 + \varepsilon)\|x - y\|_2.$$

That is, the JL lemma preserves pairwise Euclidean distances, and the embedded dimension depends only on the number of points (and only logarithmically) and not on their original dimension! Furthermore, all known proofs of the JL lemma provide an f that is *linear*, and even chosen at random from an appropriate probability distribution, oblivious of the actual point set X to be embedded. Thus, one defines f as the map $x \mapsto \Pi x$ for a random matrix $\Pi \in \mathbb{R}^{m \times d}$, chosen from an appropriate distribution. Both facts have proven useful for a variety of applications.

Since the introduction of the JL lemma and its use in computer science applications beginning in the mid-1990s, a variety of questions concerning the lemma have been asked and recently answered, either optimally or near-optimally. These include the optimal dimension m that can be achieved by a Euclidean dimensionality-reducing map in terms of $\varepsilon, |X|$ (i.e., is the m achieved in the JL lemma optimal?), and whether one can choose the aforementioned Π in such a way that the map $x \mapsto \Pi x$ can be computed quickly. Researchers have also found new generalizations of the JL lemma and its applications, such as speeding up low-rank approximation computations for the PCA method and other large-scale linear algebra problems, like approximate least squares regression. They have used a generalization of the JL lemma called subspace embeddings—pioneered by Tamás Sarlós in 2006—to achieve these.

My talk at the 2018 SIAM Annual Meeting will touch on recent developments in dimensionality reduction.

—Jelani Nelson, Harvard University



Jelani Nelson, Harvard University

Somebody Else's Dream

By Bonita Saunders

I once told a colleague that I sometimes feel like I'm living somebody else's dream. Sure, I'll admit to the standard "grow up, get married, have kids, and live in a nice home" dream, but I also wanted a career. As a young girl growing up in Portsmouth, Va., in the 1960s and 70s, that meant emulating my superb elementary and junior high school teachers. Some might find that surprising, since my schools were essentially segregated and all-black: black students and black teachers. However, teaching was considered a prestigious and lucrative career to which most African Americans could aspire, and it attracted some of the best and brightest minds.

I was born shortly after the landmark *Brown vs. Board of Education* Supreme Court decision, which declared laws specifying a separate but equal education for blacks and whites unconstitutional. But school integration was more theory than application during the first decade or so after the ruling. In the early 60s, Portsmouth implemented "Freedom of Choice," a policy that allowed

students to attend any public school in the city. This typically meant that a few black students attended white schools, but no white students attended black schools. Like most black students, I continued to attend black schools. But by the early 70s, the threat of court cases pressured many school systems—including Portsmouth—to abandon their failed integration policy and implement forced busing.

Being bused across town to Cradock High School was socially devastating, separating me from my closest friends. Still, I was fortunate. Black kids in my neighborhood were assigned to the same high school all four years, while most of my junior high friends were bused to multiple high schools as battles raged over what to do with the black high school. My friends excelled despite the turmoil, but one brilliant student suffered a mental breakdown a few years later. Today I'm still haunted by the possibility that her experience during those years caused or hastened her distress.

I began my first year at Cradock with some apprehension about the transition to an integrated environment. My academic fears, at least, dissipated once I received my first report card with 5 As and a B (in chorus). By the next report card even that lonely B had become an A, and at the end of four years I graduated as valedictorian.

I applied to a small number of colleges, both black and white, and eventually chose the College of William and Mary (W&M). From earlier visits, I knew that black enrollment at W&M was small, but the sparsity of African American students still surprised me when I arrived for orientation—only 23 blacks in a freshman class of around 1,000 students.

W&M had only two black professors in the 70s, but almost all of the housekeeping staff, bus drivers, and food service

workers were black. On many days, just a wave, smile, or kind word from one of them was a big comfort. On one occasion a friend and I, busy talking as we walked back to our dorm after class, barely noticed the campus bus roll by. At the very next meeting of the Black Student Organization, the president suggested that some of us were becoming a little "uppity" because bus drivers were complaining that we weren't waving back at them!

I majored in mathematics, intent on becoming a high school math teacher. For the most part, my professors seemed knowledgeable and fair, but recent con-

versations with other black alumni suggest that my STEM major offered me some protection against subjectivity and bias. Still, I heard the occasional "off-color joke" from a professor who apparently "forgot"

that his class included black students, and watched a troubling behavioral science film concerning human-imprinting in monkeys that never should have seen the light of day.

One of the worst college incidents that I recall happened my junior year. Upon returning from a holiday break, I found my roommate, a young black woman, staring blankly into space. She and a white friend had planned to ride back to school together, but the joint trip was scrapped after her friend's mother told her daughter that it wasn't socially acceptable to be friends with blacks.

Fortunately, my recent visits to campus indicate that much has changed since then. Minority enrollment has increased significantly, and the university is currently celebrating the 50th anniversary of the first three African Americans to live on campus. Two new dorms were also recently named in honor of blacks, one of which—Lemon Hall—is named after an 18th-century slave owned by the univer-

sity. Like many U.S. universities, W&M is making an effort to atone for its ownership and exploitation of slaves.

After graduation, I pondered an offer to teach in the Portsmouth public school system and an acceptance letter from the graduate Department of Mathematics at the University of Virginia (UVA). The lure of tackling challenging mathematics at UVA eventually won out.

I enjoyed theoretical mathematics at UVA, but harbored a fascination—inspired by earlier classes at W&M and a high school summer program at Old Dominion University (ODU)—with writing computer codes to solve practical mathematical problems. Once I blurted out to my classmates, "What's this stuff good for?" A fellow student laughed and said, "Bonita, you're not supposed to ask that question!" These concerns, and a professor's insight on job opportunities in numerical analysis and applied science, convinced me to wait before pursuing a Ph.D. After graduating with a master's thesis in commutative algebra, I accepted a teaching offer from Norfolk State University.

However, an ad for a new master's program in computational and applied mathematics at ODU drew me back to school. I enrolled part time to pursue a second master's degree while continuing to teach at Norfolk State, and later Hampton University. When ODU's math department was approved for a doctoral program, I received a letter congratulating me on my admittance. Upon questioning my acceptance into a program to which I hadn't even applied, the director said with a sneaky smile, "Oh, we put all of our promising students into the Ph.D. program!" I decided to stay.

It was a great decision. Philip Smith, my dissertation advisor, helped me obtain an internship with an aerospace engineer

See *Somebody Else's Dream* on page 6

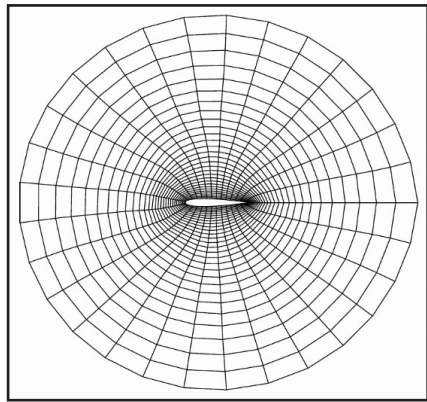


Figure 1. A two-dimensional grid around an airfoil, or wing cross section. The area near the wing looks dark because of the large concentration of grid points needed to solve the equations close to the wing's boundary. Farther away from the wing, the airflow is less affected and fewer grid points are needed. Figure credit: Bonita Saunders.

Drug Dynamics

Continued from page 3

and active transport, we only analyse passive transport resulting from diffusion. At $x = 0$, this leads to

$$d \frac{\partial D}{\partial x} = P(D - D_{\text{blood}}(t)),$$

and similar conditions at the other boundaries [4]. P is a measure of the permeability—transport through the BBB—and $D_{\text{blood}}(t)$ describes the drug concentration in the surrounding capillaries' blood. This can and will vary with time since the drug enters the blood and is thereafter eliminated from it.

The time dynamics of the concentrations is of interest, and this presents an important mathematical challenge as it differs from the "standard" question of behaviour of solutions as t becomes large; at larger t , all of the drug is eliminated from the brain.

We perform simulations, study the free drug concentration and the bound complex concentration in the domain over time [4], and choose all coefficients in physiologically-relevant ranges. Many of the coefficients vary widely among different drugs; therefore, we examine the influence of changing various parameters on the concentration. As an example, we show results of the impact of changing the BBB's permeability P on the concentration. After fixing the rest of the parameters and only changing P , we plot the concentrations of the free drug D and bound drug B versus time in the middle of the domain (see Figure 4). We also plot the concentration of drug in the blood $D_{\text{blood}}(t)$ (in red).

We vary P from the lowest possible physiological value to an intermediate, followed by a larger value. The lowest value of P corresponds to drugs that have diffi-

culty crossing the BBB. When P is larger, the drug easily moves through the BBB and D 's profile strongly follows the profile of $D_{\text{blood}}(t)$. In contrast, D increases and decreases more slowly when P is smaller because the drug both enters and leaves brain ECF more slowly. In Figure 4 (right), we plot B and observe that when P is of higher value, B rapidly increases to a maximum before quickly decreasing again. This decrease in B starts when there is not enough of the free drug present to bind to all the free receptors because it has flowed back through the more permeable BBB. In contrast, B increases more slowly and limits to a certain value when P is lower. B only decreases after time periods longer than those shown in the simulation.

As a next step, we are currently working on a three-dimensional model for a unit of the brain. We can form an entire brain by combining several of these units. This will yield a simplified model that will allow us to assign non-identical parameter values to different units, thus accounting for brain heterogeneity. For example, receptors are not distributed evenly in the brain; drugs target different

regions, and receptor concentrations can vary per region. A local disease can also greatly influence the parameters.

A broad range of opportunities exists for mathematicians to collaborate with pharmacologists in various areas, even beyond brain modelling. Among the challenges for modelers is the need for a combination of biological processes with drug influence. We strongly believe that this calls for the continued development of mathematical pharmacology.

Acknowledgments: This is based on joint research with Esmée Vendel (Mathematical Institute) and Liesbeth de Lange (Leiden Academic Centre for Drug Research), both of Leiden University.

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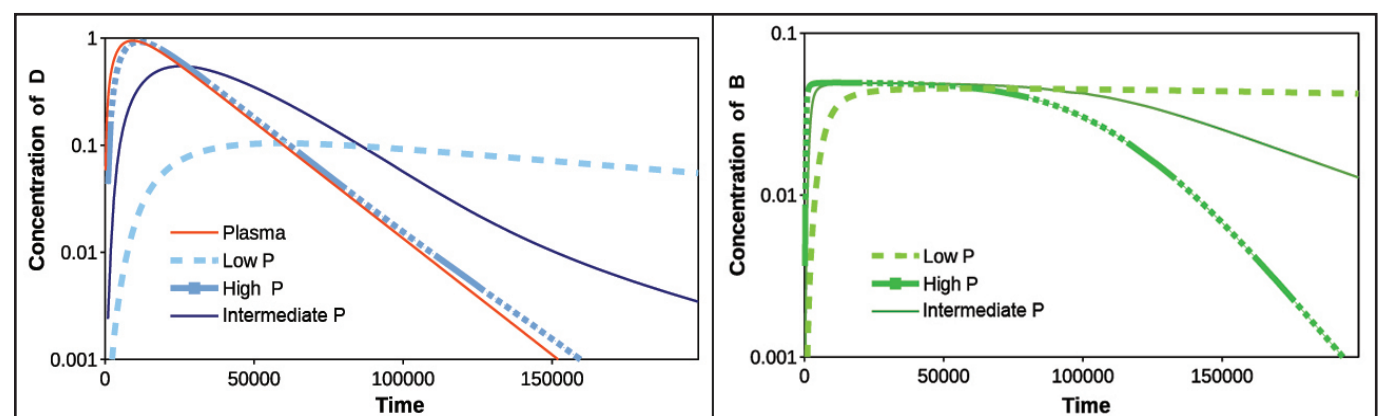


Figure 4. Influence of permeability through the blood-brain barrier (BBB). The effect of changing permeability P on the log concentration-time profiles of D and B for low, intermediate, and high P . Figure courtesy of [4].

Research Software Engineer: A New Career Track?

By Chris Richardson and Mike Croucher

In 1675, Isaac Newton famously wrote in a letter to Robert Hooke, “If I have seen further, it is by standing on the shoulders of giants.” Perhaps he was not being entirely kind to his colleague and rival, but the general idea pervades the sciences to this day: we rely on others’ work to advance our own. This has never been truer than in the world of research software.

Software written for academic purposes has a poor reputation for reliability and reusability. It is not uncommon to hear about a newly-developed software in one’s research area, only to find that it has no documentation, does not compile on all systems, yields errors, or is out of date. Given the lack of incentive for academics to devote precious time to write documentation, test code on other systems, or even keep it working, this is no surprise. Once researchers have found solutions to their specific questions and published a few papers with their code’s outputs, there is little reward in continuing to advance software developed for this purpose.

Recognising this problem, several like-minded individuals at the University of Southampton, the University of Oxford, the University of Edinburgh, and the University of Manchester came together in 2010 to form the Software Sustainability Institute (SSI).¹ With the tagline “better software,

better research,” they have been promoting “software carpentry,” “collaborations workshops,” and specialized software conferences in the U.K. An SSI survey² found that 70 percent of researchers relied on software for their results, and over 50 percent wrote their own software. By advocating for revision control, automated testing, and open-source development, SSI’s founders have significantly impacted research software, both in the U.K. and internationally. However, it soon became clear that encouraging better research software practices could only produce limited results, as most academics had very little time to focus on it. Those that did were failing to advance in their careers because they had spent too much time producing software for everyone else’s benefit. While Newton was able to give up his theological studies to devote himself to the new field of science, most researchers do not have the luxury of abandoning publication to concentrate on software development.

The SSI leadership reasoned that the best way to improve software quality was to invent a new career track with a different set of metrics. The term “research software engineer” (RSE) was coined at an SSI-sponsored event to describe a career track principally devoted to software within the research community. In January 2014, the U.K. Research Software Engineer (UKRSE) Association³ was formed to provide advice and support to anyone who identifies as an RSE. The association is free to members. Around this time,



Attendees at the Second Conference of Research Software Engineers, held in Manchester, U.K., in September 2017.

a few U.K. universities began experimenting with “research software groups” (RSGs) — teams comprised of programmers not dedicated to any specific project, but instead available as resources across the university. Providing a mechanism to interact with academics and conduct the maintenance, testing, and documentation that otherwise would not occur has produced better-quality software. The experiment was a success, and the model has spread across the country.⁴

Of course, nothing happens without funding. The funding model adopted by most research software groups involves overwriting a core set of positions and services with central university funds. Academics can then access this pool of resources by including an RSE element in their grant proposals, which is then charged back to the RSE pool. This model helps universities retain talented RSEs and provides both additional flexibility for academics and a stable career pathway for the RSEs themselves.

¹ <https://www.software.ac.uk>

² <http://dx.doi.org/10.5281/zenodo.14809>
³ <http://www.rse.ac.uk>

⁴ <http://rse.ac.uk/community/research-software-groups-rsgs/>

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Somebody Else’s Dream

Continued from page 5

at NASA’s Langley Research Center. This eventually led to a graduate student research fellowship at NASA that paid more than my teaching position at Hampton.

My research involved boundary-fitted grid, or mesh, generation. Such grids are used in fields where equations are solved over an oddly-shaped domain, such as aerodynamics (aircraft, automobile design), hydrodynamics (ship design), electromagnetics, and materials science. Figure 1 (on page 5) shows a grid constructed via variational methods and tensor product B-splines that may be used to assess the effectiveness of wing design by solving the equations of motion around an airfoil. Both a grid’s shape and the interior points’ distribution can severely affect the accuracy of numerical simulation.

Budget issues limited the number of new positions at NASA, so after earning my Ph.D. I moved to the Washington, D.C. area and spent four years as a programmer analyst with a defense contractor. The work was spotty and somewhat boring, but provided an excellent opportunity to enhance my computer skills. Still, I was

ecstatic when contacts suggested by Smith, my dissertation advisor, led to a job in the Applied and Computational Mathematics Division (ACMD) at the National Institute of Standards and Technology (NIST).

NIST’s broad mission to conduct theoretical and applied research to advance measurement science and promote U.S. innovation offers project flexibility. ACMD allows scientists to design or join projects that align with their research interests within NIST goals.

Such was the case when I joined NIST’s Digital Library of Mathematical Functions (DLMF) Project, created to replace the classic National Bureau of Standards’ *Handbook of Mathematical Functions* [1] with a new, expanded online resource¹ and print companion [2]. Like the original handbook, the DLMF contains definitions and formulas for all types of high-level mathematical functions that solve problems in the mathematical and physical sciences, but also enhances ease of use through the power of the web.

I focused on informative graphs and visualizations for the DLMF Project, realizing that grid generation techniques could facilitate the plotting of function surfaces

containing branch cuts, zeros, poles, and other areas of interest (see Figure 2). I created a sub-project supported by a dedicated team of both NIST computer scientists and mathematicians, and college students employed under NIST’s Summer Undergraduate Research Fellowship internship program.² We created more than 600 graphs and visualizations of complex functions while also advancing research in interactive three-dimensional web graphics. Over a decade of work has led to numerous technical publications and presentations at international conferences. The DLMF Project team has received several awards and honors, including a U.S. Department of Commerce Gold Medal (2011); a cover article in *Notices of the American Mathematical Society* (August 2011); and recently, an invited article in *Physics Today*, the flagship publication of the American Institute of Physics [3].

I serve on the DLMF editorial board and also lead one of several spinoff efforts, the NIST Standard Reference Tables on Demand Project. The project is a collaboration between NIST’s ACMD and the University of Antwerp’s Computational Mathematics

Research Group to build an online testing service where users can generate high-precision tables of special function values with certified error bounds for comparison with their own uploaded function data.³

So why do I feel like I’m living somebody else’s dream? Well, my career bears little resemblance to the dream I initially described. But fortunately, I’ve had some time to reflect on a hasty comment made during a pensive mood.

What was I thinking? Of course I’m living somebody else’s dream! I’m living the dream of *Hidden Figures*’ Mary Jackson, who reluctantly gave up her engineering career to accept a position as an equal employment opportunity manager to advance the careers of other women and minorities; the dream of my excellent first-grade teacher, who longed for the chance to be excellent in another career; the dreams of my parents, who graciously viewed my accomplishments as a fulfillment of their own dreams; the dreams of civil rights legends like Congressman John Lewis, who have lived to see the heirs to their dreams. And may I never forget: the dreams of countless slaves, whose only freedom was their dreams.

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³ <http://dlmfatables.uantwerpen.be>

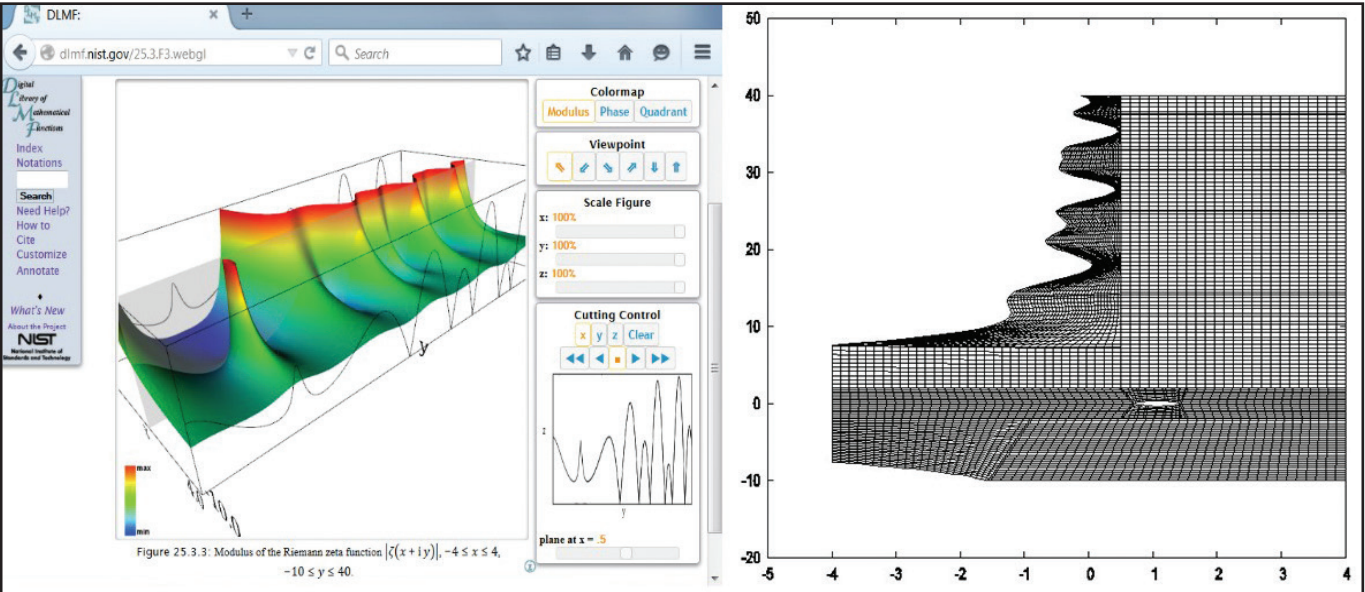


Figure 2. A Digital Library of Mathematical Functions (DLMF) webpage with an embedded visualization of the Riemann zeta function, an important function that arises in the field of number theory (left). Computing the function value at each point on the grid (right) provided the surface data, and computing values along the boundary and around the hole produces a nice clipping—or cutoff—of the function surface and a smooth color map. Figure credit: Bonita Saunders.

Jupyter: Tools for the Life Cycle of a Computational Idea

By Min Ragan-Kelley, Carol Willing, and Jason Grout

Computation is increasingly becoming an integral part of science and education across disciplines. The life cycle of a computational idea typically involves interactive exploration and experimentation, as well as publication and communication of results. Reproducible computation demands open research tools, good software practices, and transparent documentation of research processes and results. Project Jupyter¹ is an open community that builds open-source software tools and protocols for the life cycle of a computational idea. Two core pieces of the project are an open protocol for interactive computation and an open document format with which to record and share computational ideas. The Jupyter Notebook application builds on these to provide a powerful, interactive, computational environment.

The Jupyter Notebook

What Is a Notebook? The Jupyter Notebook is a document composed of a sequence of code cells and markdown cells. A code cell contains a block of code (in any language, including but not limited to Julia, R, and Python) and the output from running the code. Output displayed below a code cell is a rich representation of results and can include text, images, and interactive visualizations. A markdown cell consists of prose text in the markdown format—a lightweight, shorthand syntax for HTML—with added support for LaTeX mathematics. This structure allows authors to interleave formatted narrative and mathematics with blocks of code and their rich outputs, rendering the notebook document a powerful tool for communicating insights and results.

¹ <https://jupyter.org/>

The notebook document format is free, transparent, and understandable, in keeping with its aim to facilitate open and accessible science. It is stored as a single JSON-formatted text file, making it easy to manipulate and understand using standard programming tools, without the need for Jupyter software. The notebook file format is public,² and Jupyter software is open-source under the BSD license.

Many authors communicate using Jupyter Notebook. GitHub hosts 1.4 million notebooks, and some people have written entire books as collections of notebooks, such as Jake Vanderplas’s *Python Data Science Handbook*.³ Because notebook documents preserve their content structure and metadata, they are easily convertible to other formats, including plain scripts in the document’s language of choice. This also makes them easy to integrate into publication pipelines via formats such as LaTeX, Markdown, and reStructuredText via Jupyter’s conversion tool, nbconvert.⁴

Using Notebook Documents. The Jupyter Notebook server is a web-based application for interacting with notebook documents. The server renders a notebook document for the user and begins a persistent interactive “kernel” session in the desired language (such as Julia, R, Python, etc.) for executing user code. A user enters the code in a code cell and runs it (in the kernel session) before viewing the rich output results from the kernel, which may include text, images, and interactive controls. The user continues creating, editing, and executing or re-exe-

² https://nbformat.readthedocs.io/en/stable/format_description.html

³ <https://github.com/jakevdp/PythonDataScienceHandbook>

⁴ <https://nbconvert.readthedocs.io/en/latest/>

cutting code cells in the same persistent kernel session, thus building and exploring a computational idea. The user can also create and interleave markdown cells to explain an idea using formatted text and mathematics (see Figure 1).

Users typically install the notebook application on their local computer, where it functions like a desktop application and works with local notebooks and data. Since it is a web application, the notebook server can also run on a remote computer and provide the notebook application via a browser, with no installation required on the user’s machine.

Administrators of shared computational resources,⁵ instructors,⁶ or companies such as Microsoft can also host and manage these remote Jupyter Notebook servers. The JupyterHub⁷ project provides tools to host and administer remote servers for large numbers of users, without the need for software installation on every user machine. For example, over 1,000 students in the Data Science Education Program at the University of California, Berkeley successfully use Jupyter Notebooks in their classes through a university-wide JupyterHub deployment.

The Jupyter Protocol

The Jupyter Notebook application interacts with a kernel session using the Jupyter kernel protocol — an open, documented message protocol⁸ for communication of the code to execute and the resulting rich

⁵ <https://www.nersc.gov/users/data-analytics/data-analytics-2/jupyter-and-rstudio/>

⁶ <https://jupyter.brynmawr.edu/hub/login>

⁷ <https://jupyterhub.readthedocs.io/en/latest/>

⁸ <https://jupyter-client.readthedocs.io/en/stable/messaging.html>

Software Engineer

Continued from page 6

Several funding councils have supported this model, with the U.K.’s Engineering and Physical Sciences Research Council (EPSRC)⁵ taking the lead. EPSRC provided the initial funding for the SSI (subsequently joined by the Biotechnology and Biological Sciences Research Council and the Economic and Social Research Council), along with funding for a fundamentally different type of research fellowship — the RSE Fellowship.^{6,7}

The EPSRC RSE Fellowship scheme has funded 11 fellows across two funding calls thus far. The programme funds each individual for a five-year period and offers participants a great deal of freedom to develop as leaders in their institutions. Projects are highly varied and include development of specialised software, establishment of RSGs and national RSE networks, exascale and accelerator-based computing, data visualisation, and diverse training programs.⁸

More work must be done in the areas of role definition and job specification. Although many job postings claim to seek RSEs, institutional human resources depart-

⁵ <https://www.epsrc.ac.uk/>

⁶ <https://www.epsrc.ac.uk/funding/calls/rsefellowships/>

⁷ <https://www.epsrc.ac.uk/funding/calls/research-software-engineer-fellowships-ii/>

⁸ <http://www.walkingrandomly.com/?p=6037>

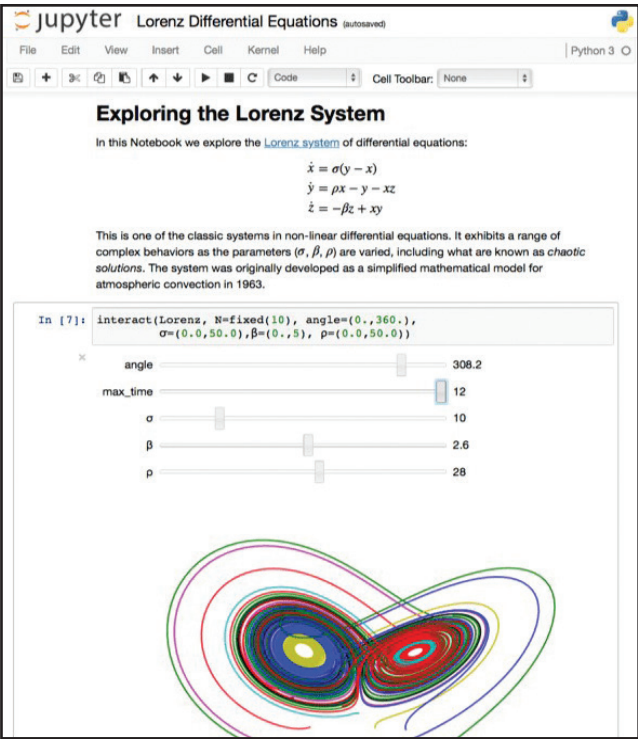


Figure 1. Jupyter notebooks exploring the Lorenz system.

output representations between front ends and language kernels. Many programming language communities provide interactive kernels that understand this message protocol and seamlessly work with applications like Jupyter Notebook.

Open Standards Foster Collaboration

Because the Jupyter message protocol and notebook document formats are open, public standards, a rich community of tools has evolved for interactive computing. Computational environments such as JupyterLab⁹ (the successor of the Jupyter Notebook application, see Figure 2 (on page 9)), the interact¹⁰ desktop application, and hosted environments like Microsoft Azure Notebooks¹¹ and CoCalc¹² all interact with Jupyter kernels and notebook files. GitHub¹³ and nbviewer¹⁴ render notebook files for read-only viewing online. By building on the

See Jupyter on page 9

⁹ <https://github.com/jupyterlab>

¹⁰ <https://interact.io/>

¹¹ <https://notebooks.azure.com/>

¹² <https://github.com/sagemathinc/cocalc>

¹³ <https://github.com/trending/jupyter-notebook>

¹⁴ <https://nbviewer.jupyter.org/>

ments have not yet caught up with the trend and generally pigeonhole applicants as technical support or academics. On the other hand, the RSE job description can sometimes overlap with these existing roles. Finding the right solution may take some time.

Ultimately, RSE advancement in the U.K. has been a great success so far.⁹ The UKRSE Association currently has over 1,000 members and continues to grow, adding about 200 more each year. The association’s second conference was held at the Museum of Science and Industry in Manchester, U.K., in September 2017. The meeting brought together RSEs from 14 different countries, including many in Europe, and as far as Canada and New Zealand.

Chris Richardson has spent time in physics, mathematics, and geosciences departments in the U.K. and Japan, and now works at the University of Cambridge BP Institute as a research software engineer. He is a core developer in the open-source FEniCS finite element code, and an Engineering and Physical Sciences Research Council (EPSRC) Research Software Engineering Fellow. Mike Croucher is also an EPSRC Research Software Engineering Fellow and co-founder of the Research Software Engineering Group at the University of Sheffield. Beginning in April 2018, he will be director of research computing at the University of Leeds.

⁹ <https://zenodo.org/record/495360#.WmH5U5OfJQ>

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The Underlying Laws Binding Cities, Companies, and Living Systems

Scale: The Universal Laws of Growth, Innovation, Sustainability, and the Pace of Life in Organisms, Cities, Economies, and Companies. By Geoffrey West. Penguin Press, New York, NY, May 2017. 496 pages. \$30.00.

As a teenager in London, physicist and author Geoffrey West procured a temporary job in the research labs of International Computers Limited. It was a transformative experience, during which he decided to pursue a career in research. After obtaining an undergraduate degree in physics at the University of Cambridge and a Ph.D. from Stanford University, West eventually moved to Los Alamos National Laboratory and became the founder and group leader of the Elementary Particle Physics and Field Theory Group. He later joined the Santa Fe Institute (SFI), eventually serving a term as president. In 2006, he was listed among *Time*'s "100 Most Influential People in the World."

Among the phenomena that initially piqued West's interdisciplinary curiosity were the extraordinary number of documented power laws $y = x^p$, which reduce to straight lines when both variables are measured on a logarithmic scale. He possesses a physicist's appreciation of scaling arguments, and traces the development thereof from Galileo—who argued that the heights to which certain animals can grow is limited by the fact that areas increase as the square of height while volumes increase as the cube—to William Froude—who discovered the importance of the ratio¹ gV^2/L for ship design—to Lord Raleigh, who explored the advantages of

expressing physical laws in terms of dimensionless variables.

Scale's main story line—from which West digresses early and often—begins with four striking power law examples, illustrated by scatter plots of the following: the basal metabolic rates of animals against their body mass, the number of heartbeats in an animal's lifetime (also against body mass), the number of patents held by residents of particular cities against their populations, and the income and/or assets of corporations against the number of their employees.

The basal metabolic rate of an organism is simply the rate at which it consumes energy while at rest (for such, $p \approx 3/4$). For heartbeats in a lifetime, $p \approx 0$, indicating that the hearts of virtually every known species beat roughly one billion times between birth and death.

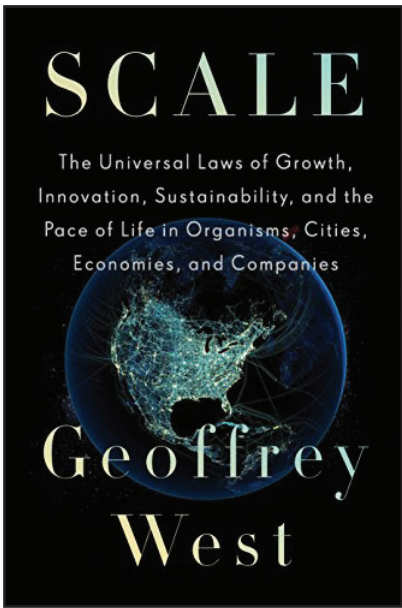
Small animal hearts beat much faster than human hearts, while large animal hearts beat more slowly. Thus, dogs and cats live only a few short years, while whales and elephants survive significantly longer than humans. The fact that $p \approx 3/4$ for metabolic rates implies an economy of scale whereby an animal weighing 100 times as much as another consumes only 32 times as much energy while both are at rest. For patents held by city residents, as for income and/or assets of corporations, p exceeds unity, meaning that a

city or firm that is 100 times as large as another consumes more than 100 times as many resources. Therein, says West, lies a fundamental difference between biophysical and socioeconomic growth.

As intriguing as the ubiquity of power laws themselves is the tendency of the observed exponents p to cluster, at least in the biophysical realm, around multiples

BOOK REVIEW

By James Case



SCALE: The Universal Laws of Growth, Innovation, Sustainability, and the Pace of Life in Organisms, Cities, Economies, and Companies. By Geoffrey West. Courtesy of Penguin Press.

¹ Where g is acceleration due to gravity, V is velocity, and L is the length of the vessel of interest.

See *Underlying Laws* on page 10

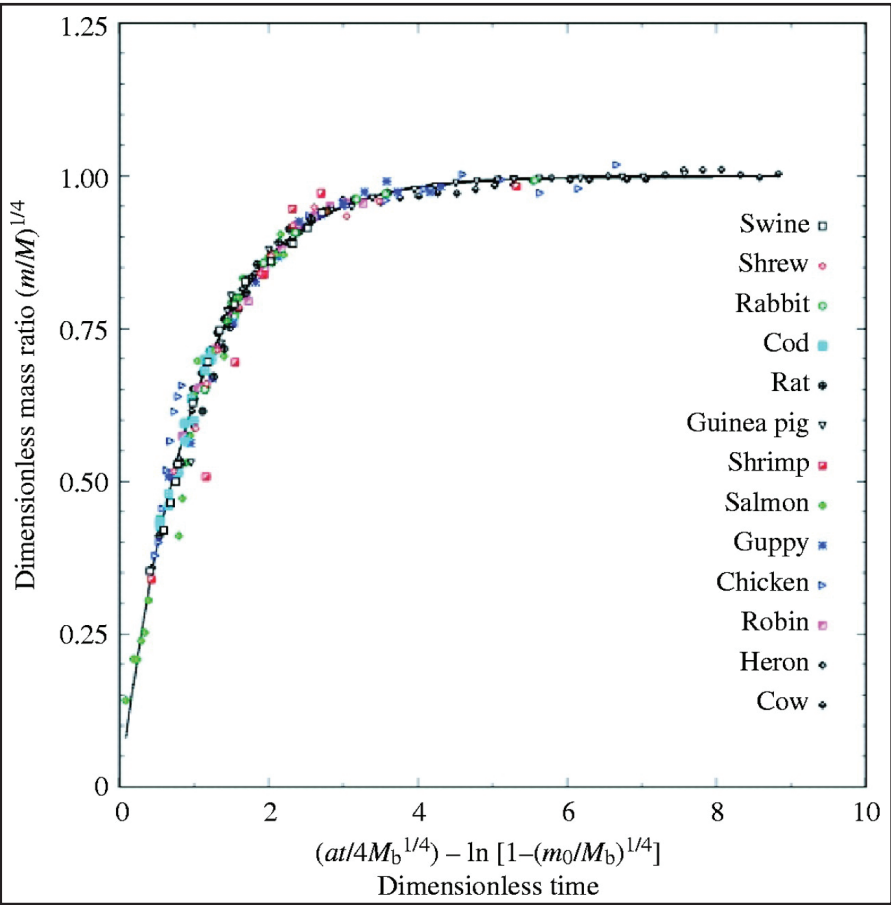


Figure 1. Geoffrey West's universal growth curve. Courtesy of Penguin Press.



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The Mathematics of Wrinkles and Folds

The following is a short introduction to an invited lecture to be presented at the upcoming 2018 SIAM Annual Meeting (AN18) in Portland, Ore., from July 9-13. Look for feature articles by other AN18 invited speakers introducing the topics of their talks in future issues.

The wrinkling and folding of thin elastic sheets is familiar to most: our skin wrinkles, a crumpled sheet of paper folds, and a flat sheet stretched over a round surface must wrinkle or fold. Similar patterns occur in a wide variety of settings. Their study is important for a number of reasons:

(a) In some situations, wrinkling patterns are highly ordered and reproducible. Such patterns can be useful when measuring the physical properties of sheets or designing templates for self-assembly, for example.

(b) Wrinkled configurations are local minima of a variational problem—the elastic energy of the sheet—with a rather special structure. Understanding their

properties is a problem in energy-driven pattern formation, a current frontier in the calculus of variations.

(c) We would like to understand the features of low-energy configurations in specific settings; this will help us separate universal phenomena from those that depend, for example, on the history of loading.

(d) Strong analogies exist between the wrinkling of elastic sheets and pattern formation in other physical systems, such as liquid crystals, ferromagnets, and superconductors. Progress in any of these areas has the potential to yield insight for the others.

What kind of mathematics is this? The elastic energy of a thin sheet consists of



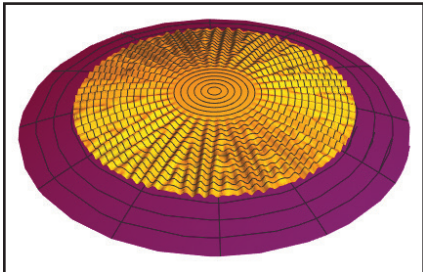
Robert V. Kohn, New York University

a nonconvex *membrane energy* (which prefers isometry) plus a small coefficient times *bending energy* (which penalizes curvature). The bending term is a *singular perturbation*; its small coefficient is the sheet thickness squared. The patterns and defects in thin sheets arise from energy minimization — but not in the same way that minimal surfaces arise from surface area minimization. Rather, analysis of wrinkles and folds involves the *asymptotic character* of minimizers in the limit as the sheet thickness tends to zero.

What kind of methods are useful? Simulation is of limited utility, since the problems are highly nonconvex and very stiff. Bifurcation theory is also of limited utility, because the configu-

rations of interest lie deep in the bifurcation diagram. Instead, focusing on the *energy scaling law*—the minimum energy’s dependence upon the thickness of the sheet (and other relevant physical parameters)—has been fruitful. Optimizing the energy within a particular ansatz gives an *upper bound* on the minimum energy. Obtaining ansatz-free *lower bounds* is a key mathematical challenge. The lower and upper

See *Wrinkles and Folds* on page 12



When a disk-shaped flat sheet is wrapped around a sphere, it wrinkles to avoid compression in the longitudinal direction. Image courtesy of [1].

Jupyter

Continued from page 7

same Jupyter formats and protocols, the aforementioned variety of interoperable tools enables interdisciplinary collaboration and communication among researchers, students, and others.

Reproducible Scientific Results

Jupyter provides useful tools for communicating scientific results. At its base level of reproducibility, a notebook is a single, shareable document containing a prose explanation of an idea, code for its implementation, and the output and figures illustrating the results. To accurately reproduce another researcher’s findings, a reader needs access to a similar computational

environment, including the applicable data and software libraries. Binder¹⁵ provides a service for sharing a reproducible computational environment. For example, the LIGO/Virgo collaboration (see Figure 3) uses Binder to enable interaction with its Nobel Prize-winning research, observing gravitational waves with a single click.¹⁶

Enhancing Education

Due to its strength in exploratory research and scientific communication, Jupyter has found a welcome home in education. As computation becomes more prominent in ever-widening fields—including computational biology, digital humanities, and data literacy—almost every student will need to

apply programming in some form. Several open-source tools for education have developed around the Jupyter Notebook.

RISE,¹⁷ a plugin for the Jupyter Notebook application, displays notebooks as presentations by stepping through interactive content cells. These presentations are live notebooks, so instructors can pause to answer questions and run code demonstrations.

The nbgrader project¹⁸ is another example of a tool that is useful to educators. It allows instructors to automatically distribute Jupyter Notebook assignments and students to submit completed notebooks. Since notebook cells sometimes have associated metadata, instructors can mark submissions efficiently by selecting certain notebook cells to be automatically graded and others to be graded by hand.

munication of insights and results, and enable a flourishing ecosystem to support collaboration and reproducibility in science and education.

Acknowledgments: The authors wish to recognize the following people for their contributions to this article: Fernando Perez, Paul Ivanov, Brian Granger, Jessica Forde, Matthias Bussonier, and Damian Avila, as well as the Project Jupyter team on whose combined work this report is based.

Min Ragan-Kelley has been working on interactive computing tools as part of the IPython and Jupyter teams since 2006. She now works primarily on JupyterHub as a postdoctoral researcher at Simula Research Laboratory in Oslo, Norway. Carol Willing is a Python Software Foundation Fellow and former director, a core developer for CPython and Project Jupyter, and a research software engineer at California Polytechnic State University. She is also geek-in-residence at Fab Lab San Diego, and co-organizes PyLadies San Diego and San Diego Python. Jason Grout is a Jupyter developer at Bloomberg. He received his Ph.D. in mathematics from Brigham Young University and has been helping develop open-source scientific software platforms, such as SageMath and Jupyter, since 2007.

Conclusion

Project Jupyter provides open, documented protocol and notebook file format standards, in addition to a wide variety of interoperable open-source tools for the life cycle of a computational idea. These open standards and tools range from early exploratory interactive research to com-

¹⁷ <https://damianavila.github.io/RISE/>
¹⁸ <https://nbgrader.readthedocs.io/en/stable/>

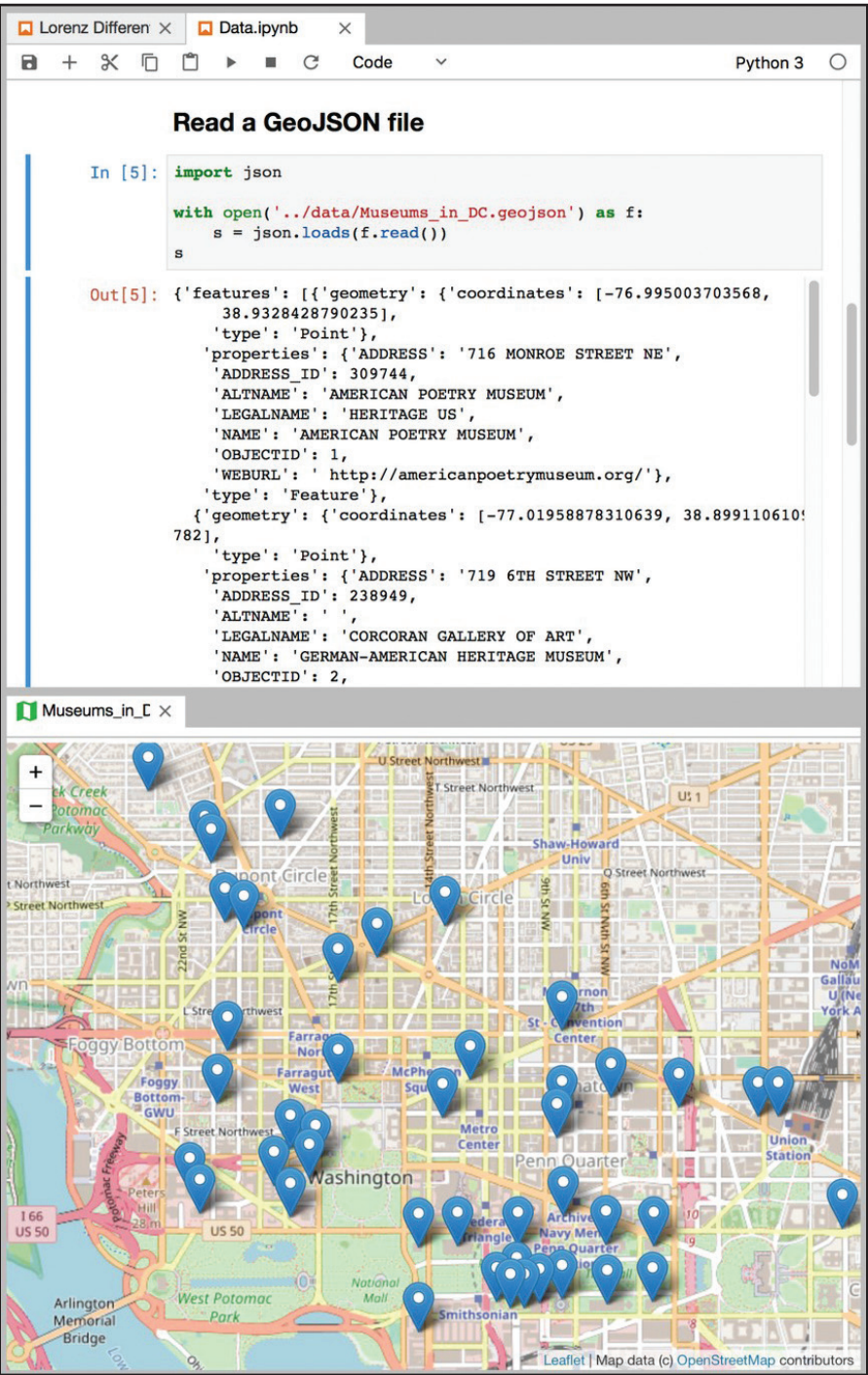


Figure 2. View of a notebook and GeoJSON file in JupyterLab.

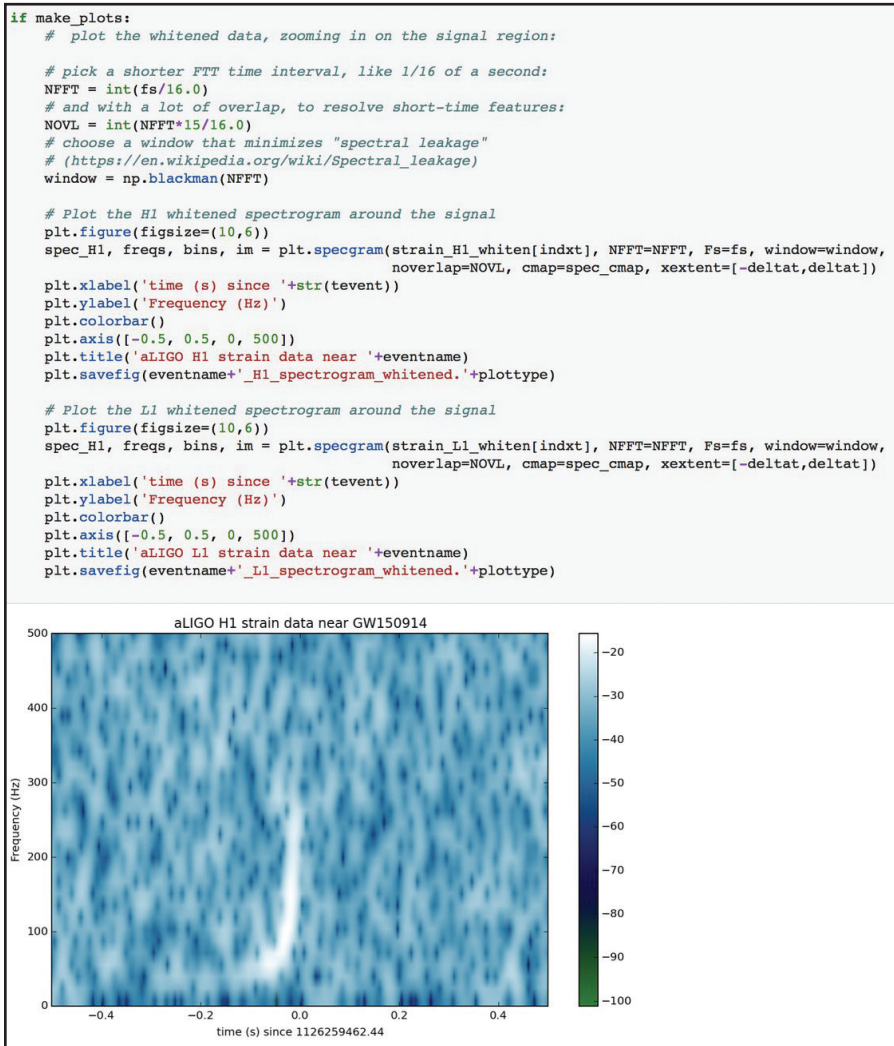


Figure 3. Excerpt from LIGO tutorial notebook, run on <https://mybinder.org>. Via <https://losc.ligo.org/tutorials/>.

SIAM Committee on Science Policy Discusses Federal Priorities

By Eliana Perlmutter, Miriam Quintal, and Ben Kallen

The SIAM Committee on Science Policy (CSP) meets twice a year to review the society's science policy priorities and engage with federal agency leaders in positions relevant to computational and applied mathematics. In December, the committee met with officials from the National Science Foundation (NSF), Department of Energy (DOE), Department of Defense (DoD), and National Institutes of Health to discuss the applied mathematics community's perspective on current and future agency priorities. Committee members also spoke with budget examiners in the Office of Management and Budget to convey the critical importance of federal funding for applied mathematics in future presidential budget requests.

Lewis-Burke Associates, SIAM's government relations consultants and Washington, D.C. office, opened the meeting with a presentation on the federal funding and policy landscape. Despite challenges in 2017, the science community engaged in successful advocacy on key issues. Congressional champions also stepped up to safeguard the research ecosystem from proposed funding and tax changes.

The meeting consisted of general discussion and presentations from federal officials. Tie Luo, acting director of the NSF's Division of Mathematical Sciences (DMS), talked about department programs and initiatives relevant to the applied mathematics community. He provided an overview of "10 Big Ideas for

Future NSF Investments,"¹ the strategic framework guiding the agency's future research investments. Luo focused on the three ideas most pertinent to applied mathematics: Harnessing Data for 21st Century Science and Engineering, The Quantum Leap: Leading the Next Quantum Revolution, and Understanding the Rules of Life: Predicting Phenotype. The DMS plans to continue implementing programs as part of these big ideas, such as the Transdisciplinary Research in Principles of Data Science program and the NSF-Simons Research Centers for Mathematics of Complex Biological Systems.

Dawn Tilbury, assistant director of the Directorate for Engineering (ENG), offered an overview of ENG programs and focused much of her presentation on the need to address challenges inherent to the ENG community, including diversity enhancement and inclusion and adjustment to flat or decreasing budgets. To that end, ENG is piloting an Advanced Placement engineering class to broaden student access to engineering inside the classroom. ENG is generating the program's curriculum with plans for implementation. To help with tight budgets, the Division of Civil, Mechanical and Manufacturing Innovation (CMMI) is heading the Leading Engineering for America's Prosperity, Health, and Infrastructure (LEAP HI) program, which involves partnerships with industry, government, and international collaborators.

Robin Staffin, who at the time of the meeting was weeks away from retiring as

¹ https://www.nsf.gov/news/special_reports/big_ideas/

Director of Basic Research at the DoD, spent much of his session reflecting on his tenure and initiatives to promote and ensure the future sustainability of basic research at the agency. He also discussed his efforts to leverage his position to help foster engagement between industry and academia, most recently through the new Defense Enterprise Science Initiative (DESI). DESI seeks to incentivize use-inspired basic research programs by partnering universities with industry to solve key defense challenges and address capability gaps.

Patricia Brennan, director of the National Library of Medicine (NLM), spoke about her vision for the NLM to catalogue and make data and models usable, similarly to how PubMed Central has made scientific publications accessible to researchers. The committee gave Brennan extensive feedback on the challenge of cataloguing models.

Barbara Helland, associate director of Advanced Scientific Computing Research (ASCR) at the DOE's Office of Science, gave an update on ASCR's budget outlook and programs, noting that its budget continues to grow as it implements the Exascale Computing Project. Helland outlined recent ASCR focus areas in machine learning and quantum computing, and presented several upcoming opportunities for the applied mathematics community, including a new Mathematical Multifaceted Integrated Capabilities Center solicitation. Additionally, she reaffirmed ASCR's support for early-career researchers, including through the Computational Sciences Graduate Fellowship program.

David Bressoud, a CSP member and director of the Conference Board of the

Mathematical Sciences, provided an update on Transforming Post-Secondary Education in Mathematics (TPSE Math), an initiative focused on educational reforms for the mathematical community. TPSE Math addresses students' lack of persistence to complete mathematics degrees and helps improve the success of traditionally under-represented students. The committee conversed about whether external advisory boards to engineering departments could inform departmental offerings to better match workforce needs.

The CSP will meet again with federal agency representatives this April. Additionally, the committee will engage with delegation offices and committee staff on Capitol Hill to advocate for increased funding for critical agencies and discuss the importance of applied and computational mathematics to areas of national importance, such as health, economic development, and national security. The CSP is also welcoming an inaugural class of Science Policy Fellowship² recipients, who will be joining the spring meeting and assisting with advocacy. These recipients will have opportunities to hone their science policy skills and act as additional ambassadors for SIAM's science policy engagement.

Eliana Perlmutter is a Legislative Research Assistant, Miriam Quintal is SIAM's Washington liaison, and Ben Kallen is a government relations associate, all at Lewis-Burke Associates LLC.

² <https://sinews.siam.org/Details-Page/siam-science-policy-fellowships>

Underlying Laws

Continued from page 8

of 1/4. In collaboration with various SFI colleagues, West found an explanation for this propensity in the structure of so-called "vital networks," the most obvious examples being the mammalian network of veins and arteries and the fiber bundle structure of plants and trees. Cities also rely on vital networks, such as transportation networks, natural gas and electrical networks, water mains, and sewer lines. Corporations have organization charts and communication networks that are often quite different. All such networks appear fractal in the sense that, by zooming in on successively smaller parts of the whole, one discovers a series of remarkably similar branching diagrams.

West and his coworkers soon concluded that vital networks share three essential characteristics: they are (i) space-filling, in that they reach every extremity of the host organism, (ii) equipped to serve their clients through standard interfaces—capillaries for vascular networks, wall plugs for electrical networks, faucets and toilets for water and sewer lines—that vary little from client to client, and (iii) evolved to perform their essential services with notable efficiency. It is in this efficiency that West finds the beginnings of an explanation for the quarter power laws that govern the vascular networks of plants and animals.

At a point where a single channel divides in two, a standard principle of fluid mechanical design decrees that the cross-sectional areas of the downstream branches should sum to that of the upstream branch, lest impeding waves be reflected back toward the source of the flow. This fact is an important part of the rather complex argument by which West and his colleagues are able to account for numerous properties of plant and animal life, including the ability of plants and trees to bend without breaking when stressed by wind. Due to the area-preserving property of vital networks, the

cross-sectional area of a tree trunk must equal the sum of the cross-sectional areas of all the leaf stems (a fact already known to Leonardo da Vinci).

The insight that a 3/4 power law relates basal metabolic rates to body mass leads West to a remarkably simple explanation of the "growth curves" used in industry to predict, among other things, the food requirements of animals being raised for meat as they progress from birth to market weight. Growth is accomplished primarily through cell division, which proceeds at a rate roughly proportional to the number of cells in place, and hence to body mass $m(t)$. West thus concludes that

$$\dot{m} = am^p - bm, \quad (1)$$

where $p = 3/4$.

The first term on the right represents the metabolic rate, while the second represents cell division. One may deduce species-appropriate constants a and b from measurements taken in the field and/or laboratory. Solutions are generally S-shaped, rising first slowly, then steeply from a birth weight m_0 near 0 before leveling off at the maximum sustainable level determined by setting $\dot{m}(t) = 0$. The substitution $m = x^4$ reduces (1) to a linear equivalent.

More remarkably, West has identified dimensionless variables μ and τ , in terms of which many (possibly all) species share the common growth curve $\mu = 1 - e^{-\tau}$. To justify such a universal claim, he assigns specific colors and shapes to different animal species to display their growth histories as shapes scattered along the proposed curve (see Figure 1, on page 8).

West devotes the first part of *Scale* to biophysical growth, concluding with an attempt to parlay his understanding of the metabolic process into an estimate of the longest possible human life span. He points out that aging proceeds at a roughly linear rate beginning at or about the age of 20, and counters the oft-expressed hope that

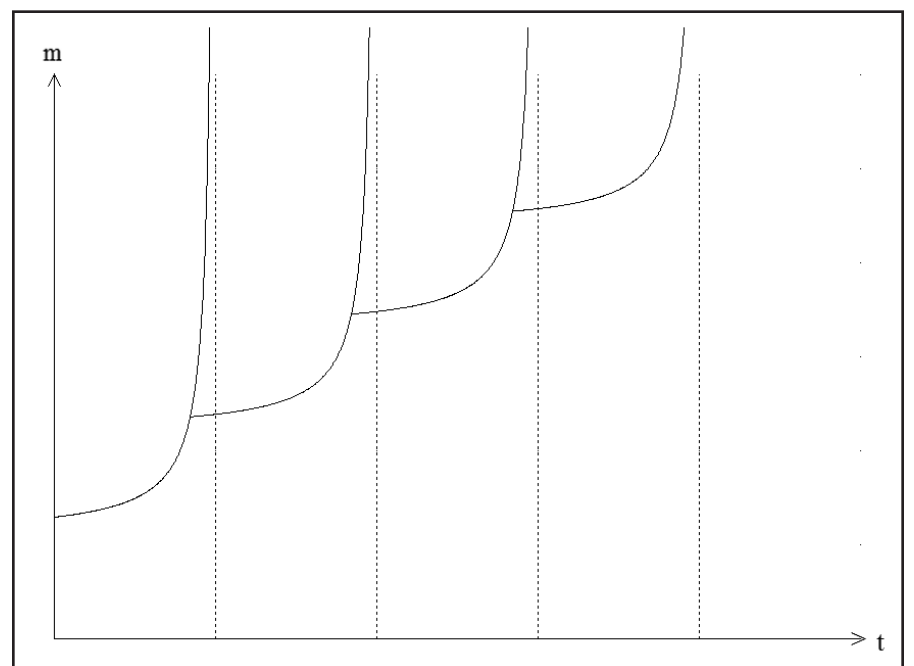


Figure 2. Successive innovations. Figure credit: James Case.

science can extend human life spans much beyond 125 years. While caloric restriction may increase the lifetimes of lab mice by as much as 50 percent, West does not believe that humans are likely to subject themselves to so Spartan a regimen.

In chapters 5-10, West approaches the study of growth in socioeconomic systems—including cities, companies, and economies—similarly to the study of biophysical systems. Since the dawn of the Industrial Revolution, the advancements of such entities has brought rising standards of living to many nations, and most of the population would like to see it continue.

As previously mentioned, the power laws found in the study of socioeconomic phenomena are prone to exhibit exponents p in excess of unity. Accordingly, the solutions of (1) tend to escape to ∞ as t approaches some finite t_0 . If $p = 8/7$, for instance, (1) may be reduced to a simple quadrature via the substitution $m = x^7$. This, says West, need not doom mankind to an imminent apocalypse, because if some new innova-

tion should materialize before the witching hour t_0 , a new (slightly curvilinear) "hockey stick" can succeed the old one. And if that can occur once, it can happen many times, as suggested in Figure 2.

Unfortunately, these progress-preserving innovations must keep growing larger and more frequent, meaning that the gaps between the vertical asymptotes of Figure 2 will narrow with the passage of time. This lends credence to the fear expressed by John von Neumann shortly before his death in 1957: mankind seems to be approaching an "essential singularity" in time, beyond which it may become impossible to prolong the era of rapid progress initiated by the Industrial Revolution.

Geoffrey West's *Scale* is a landmark volume full of interesting ideas and engaging digressions that endow the book with both entertainment and cognitive value.

James Case writes from Baltimore, Maryland.

Measuring Areas with a Shopping Cart

One late night in a deserted supermarket, I was waiting in a check-out aisle for a cashier. With no one around and nothing better to do, I began rolling the shopping cart's front wheel around the outline of a floor tile. The cart ended up rotated after one traversal, as Figure 1 illustrates (for a round "tile" and with a "bike" instead of a shopping cart). It then dawned on me that the angle θ , by which the cart turns in one cycle (see Figure 1), is proportional to the area A of the tile, up to a small relative error if the diameter ε of the curve (not necessarily a circle) is small:

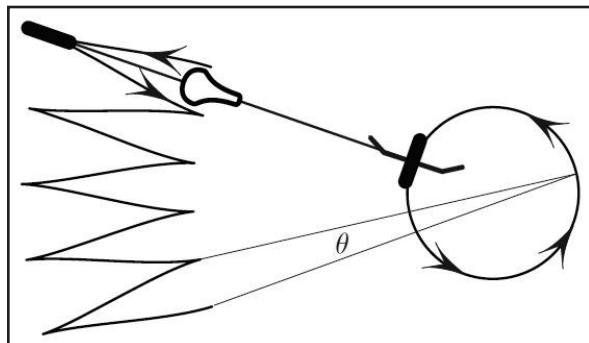


Figure 1. Trajectories of the two wheels as the front one repeatedly circumscribes a closed curve.

$$A = \theta L^2 + O(\varepsilon^3), \quad (1)$$

where L is the length of the "bike."

As happens with nearly every observation, someone noticed this before. Holger Prytz (a Danish cavalry officer) proposed the idea of calculating areas more than 100 years ago, and without the advantage of a shopping cart. One can find a beautiful description of this in [2], along with the discovery that the bike's direction angle

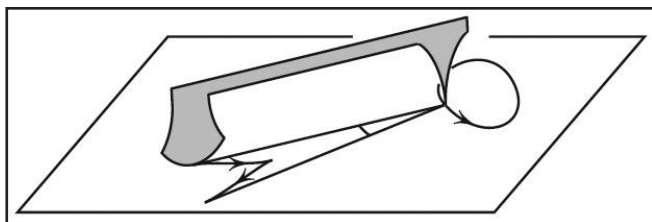


Figure 2. The hatchet planimeter; (1) gives the area.

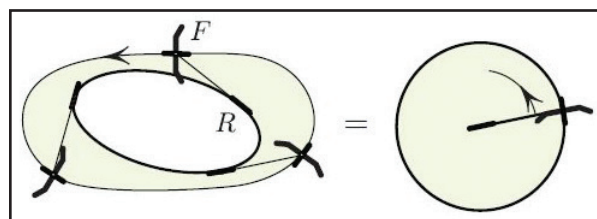


Figure 3. RF is a directed segment with R 's velocity constrained to the line RF .

changes after a cycle according to the Möbius transformation restricted to a circle,

$$z \mapsto e^{i\alpha} \frac{z - a}{1 - \bar{a}z},$$

where α and a are functionals of the front path. The Prytz planimeter, also called the hatchet planimeter, is sketched in Figure 2. The hatchet moves like a rear wheel, not sliding sideways. The needle is guided around the region's boundary, and the angle θ gives

the area according to (1).

A geometrical explanation of (1) rests on two observations of independent interest.

Observation 1

The signed area¹ swept by a moving segment (as described in Figure 3) remains unchanged if the longitudinal velocity is altered (and in particular made to vanish).

This statement is intuitively plausible since the longitudinal motion has no effect on the rate at which RF sweeps the area.

¹ The area counts with the positive sign if the motion is to the left of RF , as it is in Figure 3.

MATHEMATICAL CURIOSITIES

By Mark Levi

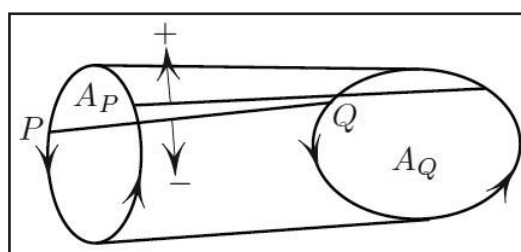


Figure 4. The doubly-swept area contributes zero, leaving $A_Q - A_P$ as the net swept area.

But this area equals $A - A_R$ by Observation 2, so that

$$A - A_R = \theta L^2.$$

It is not hard to show that $A_R = O(\varepsilon^3)$; this completes the outline of the proof of (1).

It is worth noting that if one extends the "bike" to $\mathbb{R}^3$,

Observation 2

A segment PQ executing a cyclic motion in the plane sweeps the signed area $A_Q - A_P$ (see Figure 4).

Proof of Prytz's Formula (1)

Figure 5 shows the motion of RF over one zig-

zag, with F returning to its starting position; the rotation around the start/stop point through θ completes the cyclic motion, bringing RF to its initial position (the rotation violates

the no-slip condition).

During the "sliding" stage, RF sweeps area $\frac{1}{2}\theta L^2$, according to Observation 1. During the "rotating" stage, RF sweeps the sector of area $\frac{1}{2}\theta L^2$. The total swept area is thus θL^2 .

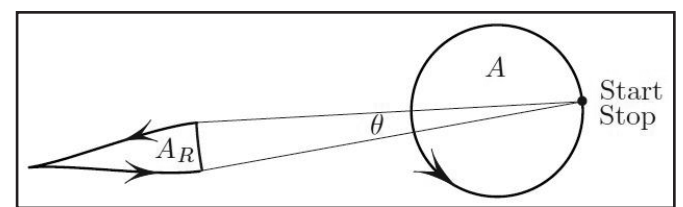


Figure 5. Proof of Prytz's formula (1).

Prytz's formula (1) admits an eye-opening explanation entirely different from the one I just described. This explanation (given in [1]) is similar in spirit to the explanation of the finiteness of the radius of convergence of $1/(1+x^2)$ by extending to the complex domain.

As a concluding remark, choosing a circular annulus in Figure 3 yields another proof of the Pythagorean theorem

(modulo the proof of Observation 1), as Figure 6 illustrates.

The figures in this article were provided by the author.

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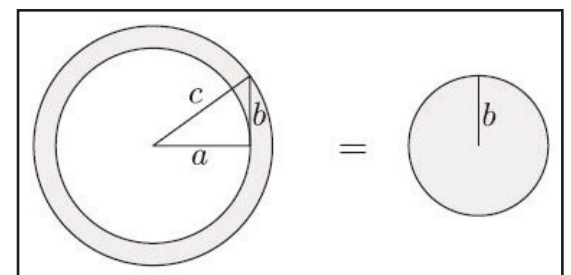


Figure 6. $\pi c^2 = \pi a^2 + \text{ring} = \pi a^2 + \pi b^2$.

2017 SIAG/Analysis of Partial Differential Equations Prize

Scott N. Armstrong (Courant Institute, New York University) and Charles K. Smart (University of Chicago) were awarded the 2017 SIAM Activity Group on Analysis of Partial Differential Equations (SIAM/APDE) Prize for their paper, "Quantitative Stochastic Homogenization of Convex Integral Functionals," published in *Annales Scientifiques de l'École Normale Supérieure* in 2016. They received their awards at the 2017 SIAM Conference on Analysis of Partial Differential Equations, held last December in Baltimore, Md., where Armstrong also gave a talk entitled "Quantitative Stochastic Homogenization by Variational Methods."

The SIAG/APDE Prize is awarded biennially to the author or authors of the most outstanding paper, according to the prize committee, published in a peer-reviewed journal in the three calendar years preceding the award year. The 2017 prize committee states that Armstrong and Smart's work "obtained outstanding results and developed fundamental new techniques that have greatly advanced the field and opened the path to further developments."

Scott Armstrong is currently an associate professor at New York University's Courant Institute of Mathematical Sciences. His research lies at the intersection of probability and analysis, with a recent focus on

stochastic homogenization of partial differential equations (PDEs). Charles Smart is an associate professor of mathematics at the University of Chicago. He is particularly interested in the interaction of nonlinear PDEs and probability, in the form of either scaling limits of statistical physics models or homogenization of PDEs with random coefficients.

Both Armstrong and Smart received their Ph.D.s at the University of California, Berkeley. Their collaboration began after graduation with a "just for fun" project about the infinity Laplacian. This project generated a series of papers, and they have been working together ever since.

They responded collectively to our questions.

Why are you excited to be receiving this prize?

We are deeply honored to win this prize and grateful to the committee for acknowledging our work in this way. There has been a lot of interesting mathematics in the last several

years on the topic of quantitative stochastic homogenization, and we hope that the prize shines a spotlight not just on our paper but also on the work of our collaborators, Tuomo Kuusi and Jean-Christophe Mourrat, as well as the excellent work of

others, such as Antoine Gloria and Felix Otto, who really inspired us.

Can you tell us a bit about the research that won you the prize?

Our research is about the behavior of solutions to certain PDEs with coefficients that are randomly oscillating on very small length scales. These equations model physical properties (like electrical or thermal conductivity) of composite materials. On smaller scales, the solutions behave very erratically since they depend on the equation's ran-

dom oscillations; this is very hard to analyze. Researchers want to be able to rigorously prove that on large macroscopic length scales, the solutions behave in a much simpler way because all of this randomness averages out in some sense. This phenomenon is called "homogenization," and the theory has many similarities to problems in statistical physics and probability theory. There has recently been a lot of focus among researchers on understanding more precisely this homogenization approximation's ability to describe the real solution. In our paper, we introduced some new ideas for obtaining quantitative bounds on the homogenization error, which arose out of the variational formulation of the equations.

The variational interpretation of the equations gives a rigorous way of implementing a "renormalization group" approach to the problem, and in later work our methods subsequently lead to an essentially optimal quantitative theory for this specific model.

What does your research mean to the public?

We hope that our research, and that of others working on similar topics, will yield new mathematical approaches for understanding other equations with random coefficients as well as similar models of physical systems. There is still much to understand at the level of basic research. The mathematics we have developed also offers a mathematical foundation for the design of numerical algorithms for computing the macroscopic properties of composite materials, which is of practical importance to engineers.

What does being a SIAM member mean to you?

SIAM plays an indispensable role in promoting applied mathematics; supporting mathematicians; and allowing us to communicate our work, keep up-to-date on the latest exciting research, and collaborate with each other.



Scott N. Armstrong, New York University



Charles K. Smart, University of Chicago

Reservoir Computing: Harnessing a Universal Dynamical System

By Daniel J. Gauthier

There is great current interest in developing artificial intelligence algorithms for processing massive data sets, often for classification tasks such as recognizing a face in a photograph. But what if our goal is to learn a deterministic dynamical system? Relevant applications include forecasting the weather, controlling complex dynamical systems, and fingerprinting radio-frequency transmitters to secure the internet of things.

Training a “universal” dynamical system to predict the dynamics of a desired system is one approach to this problem that is well-suited for a reservoir computer (RC): a recurrent artificial neural network for processing time-dependent information (see Figure 1). It can operate in many modes, including prediction mode, the task described above. While researchers have studied RCs for well over 20 years [1] and applied them successfully to a variety of tasks [2], there are still many open questions that the dynamical systems community may find interesting and be able to address.

An RC is distinguished from traditional feed-forward neural networks by the following qualities:

- The network nodes each have distinct dynamical behavior
- Time delays of signals may occur along the network links
- The network’s hidden part has recurrent connections
- The input and internal weights are fixed and chosen randomly
- Only the output weights are adjusted during training.

The last point drastically speeds up the training process.

Mathematically, an RC is described by the set of autonomous, time-delay differential equations given by

$$\begin{aligned} \frac{dx_i}{dt} &= -\gamma_i x_i + \gamma_i f_i \left[\sum_{j=1}^J W_{i,j}^{in} u_j(t) \right. \\ &\quad \left. + \sum_{n=1}^N W_{i,n}^{res} x_n(t - \tau_{i,n}) + b_i \right], \\ y_k(t) &= \sum_{m=1}^N W_{k,m}^{out} x_m, \\ i &= 1, \dots, N \quad k = 1, \dots, K, \end{aligned} \quad (1)$$

with J inputs u_j , N reservoir nodes x_i , and K outputs with values y_k . Here, γ_i are decay constants, $W_{i,j}^{in}$ ($W_{i,n}^{res}$) are fixed input (internal) weights, $\tau_{i,n}$ are link time delays, b_i are biases, and $W_{k,m}^{out}$ are the output weights whose values are optimized for a particular task. The nonlinear function f is typically sigmoidal, which we can take to the limit of an on-off thresholding (Boolean) function, as is done in traditional Hopfield networks. The reservoir maps the J input data streams to a higher dimensional phase space — dimension expansion.

For the prediction task, we adjust $W_{k,m}^{out}$ using a finite-duration “training” data sample so that the resulting output represents the input data in a least-square sense. After training, the input signals are disconnected and the outputs are wired to inputs to start the prediction phase.

In greater detail, $\mathbf{W}^{out}$ is determined by injecting an input training data set $\mathbf{U}$ over a time T_{train} and observing the network dynamics $\mathbf{X}$ over this interval. Based on these observations, we modify the weights

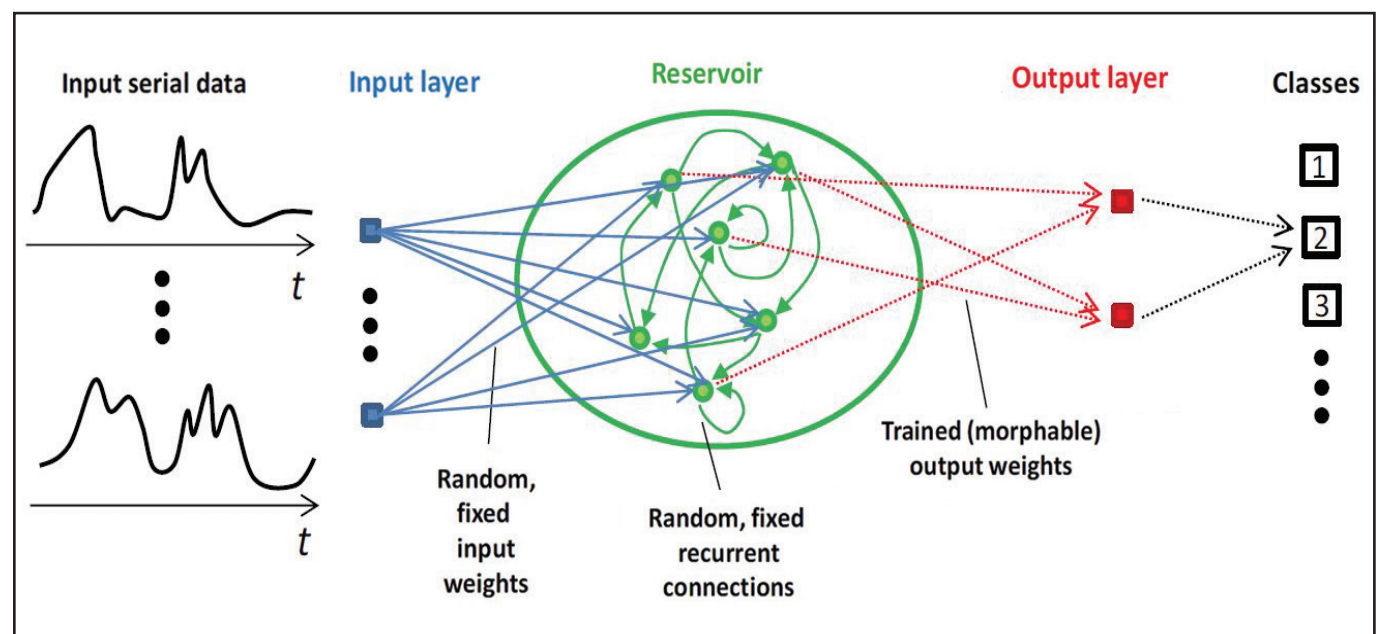


Figure 1. Illustration of the reservoir computer architecture. Figure credit: Daniel J. Gauthier.

to minimize the error of the output $\mathbf{Y}$ to the desired output $\mathbf{Y}^{des}$, resulting in

$$\mathbf{W}^{out} = \mathbf{Y}^{des} \mathbf{X}^T (\mathbf{X} \mathbf{X}^T + \alpha^2 \mathbf{I})^{-1}, \quad (2)$$

where α is a regularization parameter, $\mathbf{I}$ is the identity matrix, and T indicates the transpose.

We can solve (2) in a least-square sense using pseudo-inverse matrix routines that are often included in a variety of computer languages, some of which can take advantage of the matrices’ sparseness. A nonzero value of α ensures that the norm of $\mathbf{W}^{out}$ does not become large, which improves the generalizability of the system to different inputs and increases noise tolerance. We can also find a solution to (2) using gradient descent methods, which are helpful when the matrix dimensions are large, and leverage toolkits from the deep learning community that take advantage of graphical processing units. Use of recursive least-squares is another approach.

An RC can work very well in the prediction task. For example, it is possible to learn the full attractor of a dynamical system when the reservoir dynamics is projected to a lower-dimensional phase space before training [3]. We can also learn the attractor with standard training approaches and accurately find Lyapunov exponents from the time series produced by the RC, even for spatial-temporal dynamics [7]. Furthermore, we can utilize the predicted time series as an observer in a control system [4] or for data assimilation of large spatiotemporal systems without use of an underlying model [6]. These results suggest that an RC is a powerful tool for characterizing complex dynamical systems.

While these conclusions are compelling, designing an RC for a particular task is largely a trial-and-error undertaking, and authors tend to present results that work without dwelling on those that fail. The following is an open question: how can we optimize the parameters in (1) and (2) to obtain the most accurate prediction in either the prediction or classification tasks, while simultaneously allowing the RC to function well on data that is similar to the training data set? Early studies focused on the so-called echo state property of the network—where the output should eventually forget the input—and the consistency property, where outputs from identical trials should be similar over some period. These conditions were initially assumed to be guaranteed when the spectral radius of $\mathbf{W}^{res}$ is less than one (for the case when $b_i = 0$). However,

this scenario ignores the input dynamics and is mostly a statement of the stability of $\mathbf{X} = 0$. Recent work is beginning to address this shortcoming for the case of a single input channel, demonstrating that there must be a single entire output solution given the input [5].

While a base of past research exists, many questions that demand quantitative and rigorous answers remain. For example, how large must N be to achieve a desired error rate? How should we adjust γ_i relative to the timescales of the original dynamical system? Why do sparsely-connected reservoirs often perform best?

At the 2017 SIAM Conference on Applications of Dynamical Systems, held in Snowbird, Utah, last May, Edward Ott and I organized a minisymposium on RCs to discuss these and other problems. Ott showed that RCs can learn the “climate” of a dynamical system and accurately forecast spatiotemporal chaos in a scalable manner. Roger Brockett indicated that dense network connections might give rise to partial or full synchronization of the reservoir nodes, thus diminishing the diversity of waveforms that an RC can learn. Brian Hunt suggested that an RC must synchronize to the input data in a generalized sense when used for the prediction task. Finally, I discussed a hardware-based RC capable of predicting at a rate exceeding tens of MHz.

In summary, RCs can serve as a universal dynamical system capable of learning the dynamics of other systems. This may prove advantageous when obtaining data for the learned dynamical system is expensive or difficult, for example. While the field is progressing rapidly, there are still substantial openings for others to join the effort.

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Wrinkles and Folds

Continued from page 9

bound demonstrate the adequacy of the ansatz when they are close to agreement, and the underlying arguments help explain why certain configurations are preferred.

Wrinkling is observed in a diverse array of different situations. When a sheet is under tension, any wrinkles must be parallel to the tensile direction, and understanding the length scale of wrinkling is the main goal. The situation is more complicated when wrinkling serves to avoid biaxial compression. In such situations, even the orientation of the wrinkling is far from clear.

The 2018 SIAM Annual Meeting is co-located with the 2018 SIAM Conference on Mathematical Aspects of Materials Science. My invited talk, which is part of both meetings, will develop the aforementioned topics, focusing on recent examples in which the identification of energy scaling laws has produced some interesting surprises.

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— Robert V. Kohn, New York University