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Generalized Hypergraph Cut Algorithms and Their Applications

By Nate Veldt

In graph theory, "cuts" are sets of edges whose removal partitions a graph into disconnected clusters. One of the most fundamental cut problems is finding a minimum s-t cut, which separates two special nodes s and t into different clusters while minimizing the number of edges between these clusters. Polynomial-time solutions for this problem (and its dual, the maximum s-t flow problem) date back to the 1950s, and the search for increasingly faster algorithms still continues today. Researchers frequently use minimum s-t cut algorithms as subroutines for other graph problems and apply them to tasks like image segmentation, data clustering, and community detection in social networks.

2023 marks the 50th anniversary of Eugene Lawler's proof that a *hypergraph* minimum s-t cut problem is also polynomial-time solvable [2]. In hypergraphs, nodes are organized into *hyperedges* that contain an arbitrary number of nodes and are useful for modeling *multiway* relationships. The hypergraph minimum s-t cut problem aims to separate special nodes s and t while minimizing a hypergraph cut penalty. *But what constitutes a hypergraph cut penalty?* When it comes to graphs, the only way to cut an edge is to separate its two nodes into different clusters. However, there are many ways to partition a hyperedge's nodes across two clusters. Lawler's algorithm applies to the standard hypergraph cut penalty, which simply counts the number of hyperedges that are cut (i.e., that span both clusters).

The standard hypergraph cut penalty arises naturally in a variety of settings, but there are also multiple applications where certain ways of cutting a hyperedge are more desirable than others [3, 4]. My colleagues and I recently revisited the hypergraph s-t cut problem with a renewed interest in what it means—in both theory and practice—to cut a hyperedge [8]. We found that even a seemingly minor generalization of the standard hypergraph cut penalty yields a rich space of theoretical questions, complexity results, and algorithmic primitives for many applications in hypergraph-based data analysis.

See **Hypergraph** *on page 3*

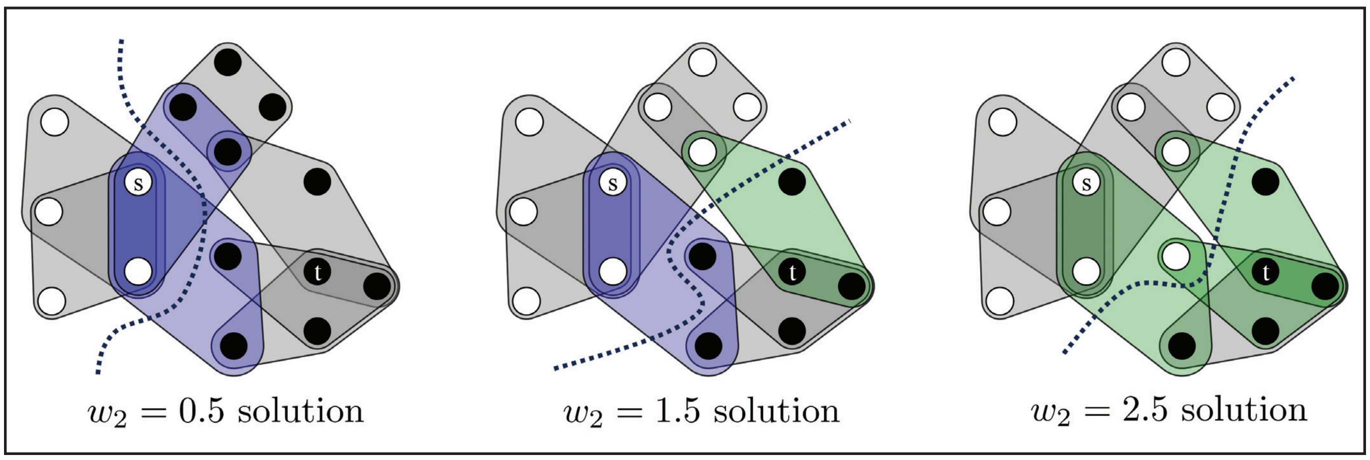

Figure 1. *The cardinality-based s-t cut problem aims to separate special nodes s and t into two different clusters (shown here with differently colored nodes) while minimizing a generalized hypergraph cut penalty. A hyperedge is cut if it spans both clusters. A four-node hyperedge has a cut penalty of $w_1 = 1$ if exactly one of its nodes is contained in one of the clusters (green hyperedges). It receives a cut penalty of w_2 if it has two nodes in each cluster (blue hyperedges). The optimal solution depends on the choice of w_2. Figure courtesy of the author.*

The Pancreatic Beta Cell: Biology and Mathematics Advance Together

By Arthur S. Sherman, Patrick A. Fletcher, Richard Bertram, and Leslie S. Satin

The human pancreas contains roughly one gram of beta cells, which secrete the hormone insulin when glucose levels rise after a meal; the insulin then returns glucose back to baseline over the course of several hours. Upon reaching baseline, insulin secretion ceases. This process is a classic example of a homeostatic negative feedback loop. In the absence of beta cells, blood glucose would fluctuate wildly with each meal and damage the body's tissues — as is the case with type 1 diabetes, wherein the immune system kills almost all beta cells. Type 2 diabetes is more common and results from a deficiency in insulin secretion relative to the necessary amount for glucose control; this deficiency generally comes with age and weight gain and can potentially cause heart disease, dementia, blindness, peripheral neuropathy, and kidney failure. For most people, the beta cells compensate for reduced insulin efficiency by increasing insulin secretion. But when such compensation is inadequate, blood glucose levels slowly increase over many years until they reach a critical threshold and rise dramatically.

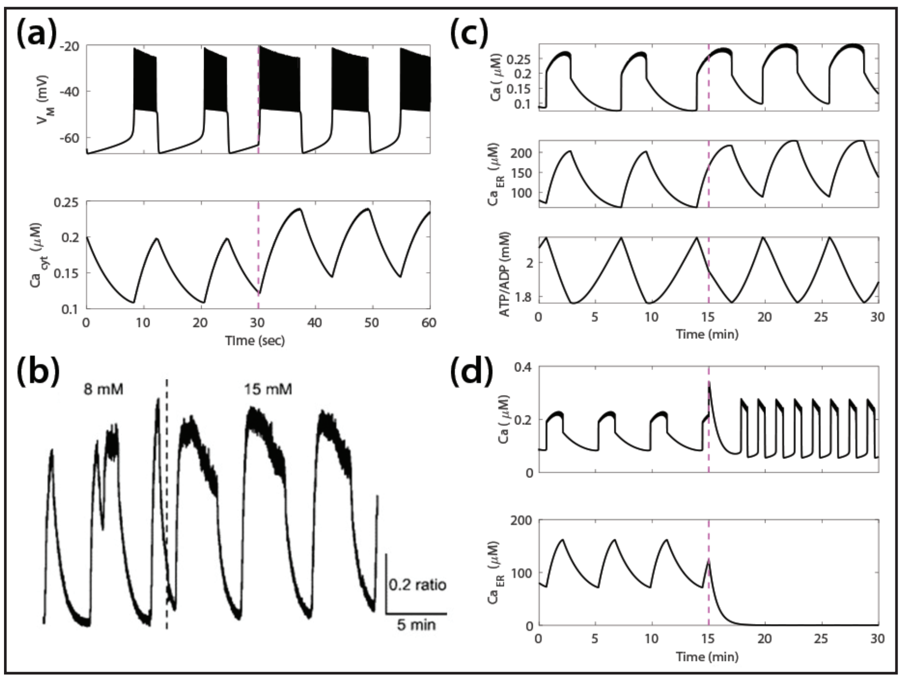

Figure 1. *Simulations with the original and augmented Chay-Keizer models compared to data.* **1a.** *In the original model, increasing glucose at $t = 30$ seconds (dashed line)—represented by reduced conductance of adenosine triphosphate (ATP)-sensitive K^+ (KATP) channels—increases plateau fraction and calcium.* **1b.** *Experimentally measured calcium is a square wave, not a sawtooth wave.* **1c.** *Augmented model where the endoplasmic reticulum (ER) and ATP/adenosine diphosphate (ADP) oscillate in phase with calcium. ATP/ADP does not increase when glucose increases at $t = 15$ minutes, in agreement with experiments [5].* **1d.** *In the augmented model, oscillations persist when ER calcium uptake is blocked at $t = 15$ minutes, in agreement with experiments. Figures 1a, 1c, and 1d courtesy of the authors, and 1b courtesy of [6].*

Understanding insulin secretion's dynamic response to meals, short-term cycles of feasting and fasting, and lifelong variations in body weight is therefore crucial for diabetes treatment. Mathematical modeling has addressed two key questions in this research space: How do beta cells secrete the appropriate amount of insulin to keep glucose in the healthy range? And how does the pancreas generate the observed five-minute pulses of insulin secretion?

Experimental studies in the 1970s and 1980s revealed that beta cells respond to elevated glucose levels with bursts of action potentials: periods of spiking that alternate with periods of silence. The action potentials bring in calcium, which triggers insulin secretion. As glucose increases, the bursts become longer and the silent periods become shorter (i.e., the *plateau fraction* increases). But how does glucose exert this effect, and how does the increased plateau fraction lead to the secretion of more insulin? Experiments demonstrated that the regulation of electrical activity depends on the rate of glucose metabolism in the beta cell, which acts as a surrogate for blood glucose concentration. However, the link from metabolism to electrical activity and secretion remained unknown.

In 1983, the Chay-Keizer model attempted to assemble the experimental observations into a coherent, quantitative framework [1]. The voltage spikes in this model bring in calcium that slowly builds up and binds to calcium-activated potassium (KCa) channels; after many spikes, this binding process turns off the burst. Calcium pumps then reduce the calcium level once again, paving the way for the next burst. Calcium thus acts like a slow variable in a relaxation oscillator, gradually rising and falling with each period of oscillation. Researchers also determined that an adenosine triphosphate

See **Pancreatic Beta Cell** *on page 4*

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5 From Sequences of Images to Trajectories: A Tracking Algorithm for Dynamical Systems
Generic image detection algorithms are often not optimally suited for dynamics problems. Aminur Rahman, Erdi Kara, and J. Nathan Kutz use a machine-learning-based approach to develop new object tracking algorithms, which they test against existing state-of-the-art algorithms for walking droplets and granular intruders.

7 Automating Conference Scheduling with Genetic Algorithms at CSE23 and Beyond
Alicia Klinvex recently made the inaugural effort to automate the scheduling process for a SIAM conference, designing the methodology and writing a set of C++ and Python codes for the 2023 SIAM Conference on Computational Science and Engineering. Klinvex and Tamara Kolda outline the processes and decisions that informed the code.

8 Describing the Universe with Breadth and Depth
Paul Nahin reviews Chris Budd's newest book, *Climate, Chaos and COVID: How Mathematical Models Describe the Universe*. He praises Budd's account of mathematical reasoning's contributions to insights about the physical world, ranging from the spread of diseases to chaos theory and even wind energy extraction.

8 Behind the Lab Coat: A Scientist's Journey to Influence Science Policy in Washington, D.C.
2023 Science Policy Fellowship recipient Bashir Mohammed discusses his longstanding passion for science policy; recounts his first experiences with policymaking in Washington, D.C.; and recaps key presentations and conversations from the spring meeting of the SIAM Committee on Science Policy.

11 A Hamiltonian Look at a Soap Film
Mark Levi considers a soap film that is stretched between two rings that share a common axis. He explores the Hamiltonian system for this scenario and presents several observations that pertain to the minimal surfaces that span the rings, the distance between the rings at which the soap film will snap, and other topics.

A Career She "Could Not Have Envisioned": Remembering Evelyn Boyd Granville, Mathematician and Programmer

By Laura E. Turner

Evelyn Boyd Granville, a renowned African American mathematician in the early Space Age, passed away on June 27, 2023, at the age of 99. This brief account of her remarkable career highlights some of her many achievements and provides further insight into her instrumental work as a programmer.

Granville[1] was born in Washington, D.C., in 1924. D.C. was largely segregated until the 1950s, so she attended racially segregated public schools but enjoyed visits to museums (such as those on the National Mall) and libraries that were open to everyone. Her outstanding Black teachers at Dunbar High School encouraged and prepared her for success [3].

A studious pupil, Granville matriculated at Smith College in 1941 and focused her efforts on mathematics. She excelled there, receiving scholarships and beginning independent study in her junior year [7]. As a senior, Granville was elected to Phi Beta Kappa and qualified for associate membership in Sigma Xi; she graduated *summa cum laude* in 1945 with a fellowship for graduate study [3].

Granville then pursued a master's degree and doctorate at Yale University, where she studied functional analysis under Einar Hille and wrote a thesis titled "On Laguerre Series in the Complex Domain" [2]. In 1949, she became the second Black woman to earn a Ph.D. in mathematics in the U.S.; she was one of 10 U.S. women to receive a doctorate degree in mathematics that year.

After graduating from Yale, Granville became a research assistant at New York University's Institute for Mathematics and Mechanics (now the Courant Institute of Mathematical Sciences). She then joined the faculty at Fisk University, where she taught students including Etta Zuber Falconer and Vivienne Malone Mayes from 1950 to 1952. Next, Granville returned to D.C. and accepted a position at the National Bureau of Standards (now the National Institute of Standards and Technology), where she met mathematicians who were working as programmers and began considering a career in the field [3].

In 1956, Granville arrived at International Business Machines (IBM) with no computer experience. After a two-week training session at the Watson Computing Center, she spent a year writing programs at IBM's D.C. office, then transferred to New York City as a research mathematician to consult in numerical analysis at an IBM subsidiary. She enjoyed the work but not the location, so when IBM opened its Vanguard Computing Center (VCC) in D.C., Granville jumped at the opportunity to relocate [3]. Doing so led to her involvement with Project Vanguard.

Project Vanguard

Project Vanguard aimed to launch a scientific satellite into orbit around Earth, prove that it had entered orbit, and use it to conduct scientific experiments. IBM won the contract for the digital satellite orbit computing facility. As a result, it supplied six weeks of use of the IBM 704 — a state-of-the-art, high-speed digital computer (see Figure 1, on page 6); orbital computations for the lifetime of the satellite; the services of mathematicians for programming tasks; 100 hours of computing time; and a D.C. computing center [5].

Confirming a satellite's orbit required tracking it through the Minitrack Network, computing its orbit, and predicting its path. Vanguard satellites contained 108-Mc signal sources. Each time a Minitrack station within the worldwide network received a transmission, it divided the transmission into phase-difference readings that were converted to direction cosines. This information was sent in triplicate to the control center, relayed by teletype to the VCC, and fed into a punch card machine. The cards were then transferred to the 704, where a master program calculated the satellite's predicted latitude and longitude every minute up to ten days in advance [8]. The IBM system was symbolic, highly automatic, and card controlled; programming for Project Vanguard consisted of macrooperations that linked collections of subroutines with specific aims.

Evelyn Boyd Granville (1924-2023) works on the IBM 704—a high-speed digital computer—at IBM's Vanguard Computing Center in Washington, D.C., in the late 1950s. Photo courtesy of the Smith College Special Collections, Evelyn Boyd Granville papers (SSC-MS-00747).

IBM mathematicians began programming the 704 in 1956. By the spring of 1957, IBM had used simulated observations to predict and determine a satellite's preliminary elliptic orbit. The launch of Sputnik I in the fall provided an unexpected dry run, and the 704 successfully determined its orbit based on three accurate satellite positions.

Granville began to contribute to this project after arriving at the VCC around 1958. "At that time, the satellite was the size of a grapefruit," she later said, referring to Vanguard I [7]. She also worked on Vanguard 2E, a weather satellite that contained photocells that produced images of Earth's cloud cover [11].

In spite of some delays and failures, Project Vanguard met its scientific objectives. It also provided information about Earth's shape, equator, and poles, and specified modifications of a satellite's orbital path and rotational movement due to the Sun, Moon, and magnetic drag [5].

Project Mercury

Granville was also involved with Project Mercury, the first phase of the U.S. manned satellite program. By that point, the VCC had become the IBM Space Computing Center (SCC), and the 704 was replaced by the 709 and then the 7090: a faster, transistorized system. When NASA founded the Goddard Space Flight Center in 1959, its Computing and Communications Center featured duplexed 7090s that provided real-time position and velocity information for capsules, from launch through reentry [6].

NASA and IBM maintained joint use of the SCC until November 1960, when the mainframes were installed at Goddard. Granville left IBM (where she had become a staff assistant for trajectory problems) that same month, married Reverend G. Mansfield Collins, and moved to Los Angeles. She later described her work on Project Mercury as "one of the highlights" of her IBM career [9].

New Opportunities

In California, Granville joined the technical staff of a private company called Space Technology Laboratories (STL) [7]. Its Systems Research and Analysis Division managed space and missile system studies and housed the Computation and Data Reduction Center, where Granville worked on methods of orbit computations [3]. STL was under contract with NASA at the time, and part of its *Final Report [on] Earth Satellite Orbit Computations*—to which Granville contributed—discussed the Diliberto general perturbation method: a novel approach to predict the long-term motion of a near-Earth satellite that was applied to a new coordinate system to simplify analysis and results [10].

Granville left STL in 1962 for a more lucrative position at North American Aviation (NAA), whose new Space and Information Systems Division won a 1961 NASA contract to design, develop, and construct the command and service modules for Project Apollo. She became a research specialist at NAA and offered technical support to engineering departments [3]. In 1963, Granville returned to IBM as a senior mathematician in the Systems Development West Department of the Federal Systems Center (FSC). Her work included trajectory analysis and orbit computation for the U.S. Air Force's Athena spacecraft reentry

See **Evelyn Boyd Granville** *on page 6*

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[1] This text will refer to Evelyn Boyd Granville as "Granville" throughout. She grew up as Evelyn Boyd and took the name Granville when she married her second husband.

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Hypergraph

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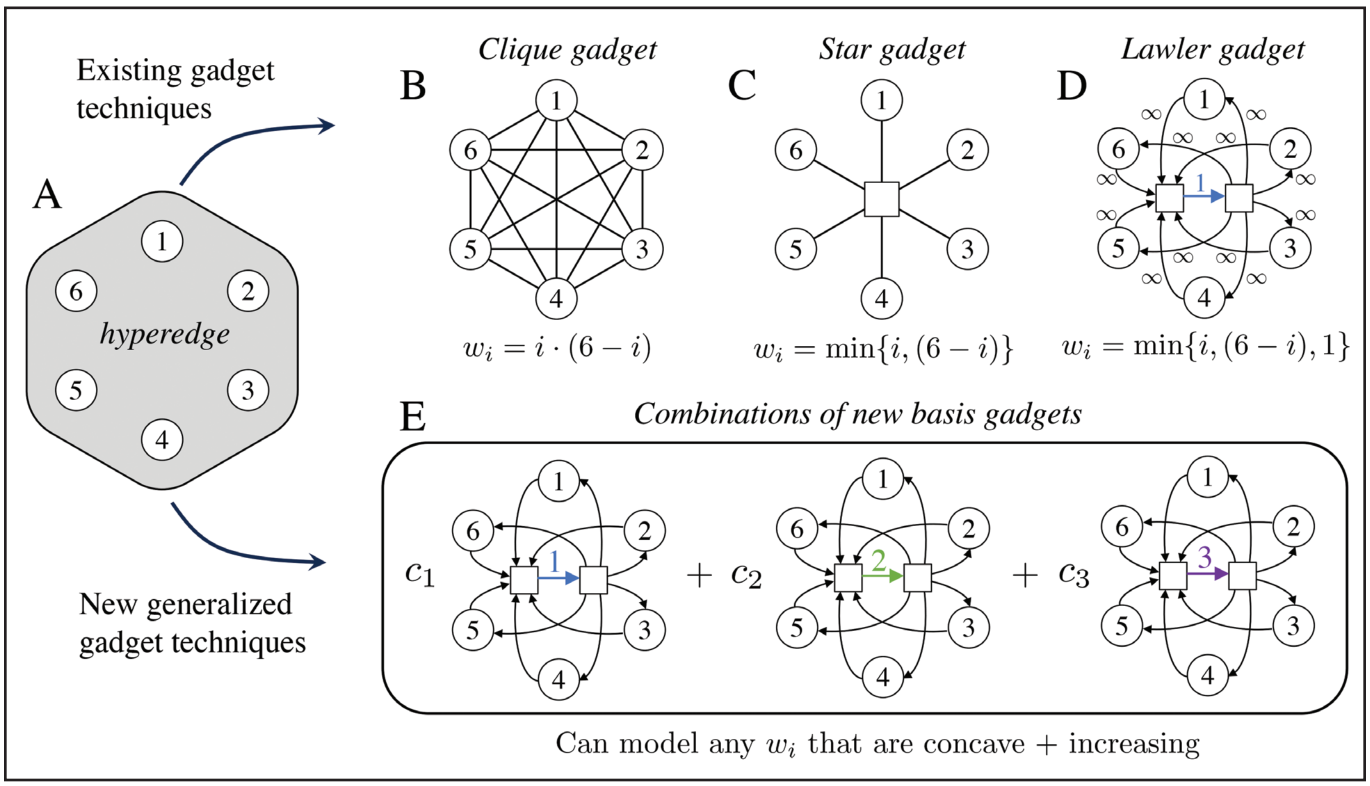

Figure 2. *Replacing each hyperedge* **(2a)** *with a graph gadget allows us to efficiently solve certain cardinality-based s-t cut problems. For all of the gadgets pictured here, edges without a label have a weight of 1. The clique* **(2b)**, *star* **(2c)**, *and Lawler* **(2d)** *gadgets model specific cardinality-based cut penalties $\{w_i\}$. We proved that positive linear combinations of new basis gadgets* **(2e)** *are sufficient to model all cut penalties $\{w_i\}$ that come from an increasing concave function. We also demonstrated that this is the largest class of cut penalties that can be modeled by graph gadgets. The three basis gadgets in* **2e** *are the exact gadgets that we use to model any such cut penalties for a six-node hyperedge by varying the nonnegative weights c_1, c_2, and c_3. Figure courtesy of the author.*

The Cardinality-based *s-t* Cut Problem

A natural generalization of Lawler's hypergraph s-t cut problem is to penalize hyperedges based on the number of nodes in each cluster. For the hypergraph in Figure 1 (on page 1), we can assign a penalty of $w_1 = 1$ for each hyperedge that places exactly one of its nodes in one of the clusters, and another penalty $w_2 \geq 0$ when exactly two of its nodes are in each cluster. The optimal partition then depends on w_2.

We formalized this idea as the *cardinality-based s-t cut problem* [8]. For a simplified exposition, let us assume that the input hypergraph $H = (V, E)$ is k-uniform—meaning that each hyperedge has exactly k nodes—and that the same type of generalized cut penalty is applied to every hyperedge. These assumptions simplify the explanation without fundamentally altering the results; the analysis easily extends to settings with hyperedges that vary in size and cut penalties. The cardinality-based s-t cut problem is

$$\min_{S \subseteq V} \quad \mathbf{cut}(S) = \sum_{i=1}^{\lfloor k/2 \rfloor} w_i \cdot |\partial_i(S)|,$$

subject to $s \in S$ and $t \notin S$. Here, $\partial_i(S) = \{e \in E : \min\{|e \cap S|, |e \cap V \setminus S|\} = i\}$ is the set of hyperedges with exactly i nodes in one of the clusters $S \subseteq V$ and $V \setminus S$, and $w_i \geq 0$ is the penalty for cutting a hyperedge in this manner. Without loss of generality, penalties are scaled so that $w_1 = 1$.

Lawler's work demonstrates that this problem is polynomial-time solvable if $w_i = 1$ for all $i \geq 1$ [2], but are other parameter settings amenable to efficient algorithms? Is the problem ever computationally intractable? Such questions are closely tied to motivating applications and practical considerations. Researchers have already employed many types of cardinality-based hypergraph cut penalties (even if they were not explicitly identified as such) in previous hypergraph partitioning applications [8]. Understanding the complexity of the cardinality-based s-t cut problem will help us establish rigorous theoretical foundations and algorithmic primitives for these and other downstream applications.

To explore these topics, we turned to a familiar strategy in hypergraph analysis: replace each hyperedge with a small graph *gadget*, which is defined by a new edge set and potentially new auxiliary nodes. This strategy produces a graph cut problem that is solvable with existing algorithms. Arguably the most common approach is to replace each hyperedge with a clique (see Figure 2b). Another common technique is to replace each hyperedge with a star that is centered at a new auxiliary node (see Figure 2c). Researchers often use clique and star gadgets as simple heuristics for hypergraph analysis or as a means of *approximating* the standard hypergraph cut penalty. However, we can also view them as a way to *exactly* model specific cardinality-based cut penalties. Applying clique gadgets to a k-uniform hypergraph and solving a graph s-t cut problem is equivalent to solving the cardinality-based s-t cut problem when $w_i = i \cdot (k - i)$. Meanwhile, the star gadget exactly models the penalty $w_i = \min\{i, k - i\}$. Lawler's hypergraph s-t cut algorithm relies on an alternative gadget that models the standard hyperedge cut penalty (see Figure 2d).

How do we know when we can model a set of cut penalties with such a gadget? We discovered a simple sufficient and necessary condition: a set of cardinality-based penalties can be modeled by a gadget *if and only if* they are represented by a *submodular* function. Formalizing this condition requires additional mathematical notation for encoding cut penalties as a set function; informally, the condition means that the sequence of values $\{w_1, w_2, w_3, \ldots\}$ follows an increasing concave curve. We can always represent cut penalties that satisfy this condition with a positive linear combination of newly-defined *basis* gadgets (see Figure 2e), where the coefficients are obtained by solving a small linear system.

What if this condition is not satisfied? In the case of four-uniform hypergraphs, we can model cut penalties with gadgets as long as $w_2 \in [1, 2]$. However, we proved that the problem is NP-hard when $w_2 \in [0, 1)$. When $w_2 > 2$, we know that gadget techniques fail, but the complexity of the problem remains unknown in this parameter regime. Figure 1 (on page 1) illustrates the problem's theoretical richness; although the three cut problems in this figure are fundamentally different in terms of algorithms and complexity, they are distinguished only by a (seemingly) minor change to one cut penalty. For hyperedges with more than four nodes, we proved NP-hardness results for several broader parameter regimes and highlighted broader regimes in which the complexity remains unknown.

Applications in Hypergraph-based Data Analysis

Our results contribute to broader research efforts on generalized hypergraph cut problems that are particularly motivated by recent data science applications. Just as graph s-t cut algorithms are often used as subroutines for other graph problems and applications, our hypergraph s-t cut algorithms can be directly incorporated into many frameworks for hypergraph clustering and partitioning.

We integrated our gadget techniques and s-t cut subroutines into new algorithms for finding localized clusters in large hypergraphs [5, 7]. In practice, cardinality-based cuts led to improvements in detecting clusters of posts on Stack Overflow[1] with the same topic tag (e.g., *Python* or *Verilog*) in a hypergraph whose hyperedges represent sets of questions that were answered by the same user. We also used our algorithms to detect clusters of same-category retail products (e.g., *fashion* or *software* merchandise) in a hypergraph whose hyperedges indicate sets of co-reviewed Amazon products.

We later used cardinality-based s-t cut subroutines to develop faster approximation algorithms for global *ratio cut* objectives, which seek to minimize the ratio between a generalized hypergraph cut penalty and the resulting cluster's size [6]. Earlier research revealed that incorporating generalized cut penalties into ratio cut objectives benefits downstream hypergraph-based classification tasks where hyperedges represent sets of data objects that share a categorical feature (e.g., a group of news articles that use the same rare word) [4]. In these settings, a hyperedge provides imperfect but useful evidence that a group of data objects should be classified similarly. We can choose cardinality-based cut penalties that favor clustering most of these data objects together, even if the hyperedge is cut.

We also developed faster approximate solvers for cardinality-based cut problems by replacing hyperedges with new *sparse* gadgets [9]. This technique led to faster approximate solutions for image segmentation tasks where a hyperedge represents a *superpixel*: a group of pixels in the same region of an image that share similar pixel intensities and often belong to the same object in the image. We can use cardinality-based cuts to encourage most nodes of a superpixel to cluster together, without placing an excessively high penalty on separating a few pixels from the rest.

Numerous questions remain open for the cardinality-based s-t cut problem, such as settling the problem's complexity in all parameter regimes and developing approximation techniques for NP-hard cases. The cardinality-based s-t cut problem is also just one direction within a broader research thrust on generalized hypergraph cut problems. Many recent advances in this area relate to other hypergraph cut objectives and generalized cut penalties that extend beyond cardinality-based cuts [1, 3, 4, 10]. There are a lot of exciting opportunities for further exploration, in terms of both open mathematical questions and new ways to leverage existing techniques for emerging applications where complex, multiway interactions play a central role.

Nate Veldt received the 2023 SIAM Activity Group on Applied and Computational Discrete Algorithms Early Career Prize.[2] He presented the corresponding prize lecture on his work with hypergraphs at the 2023 SIAM Conference on Applied and Computational Discrete Algorithms,[3] which took place earlier this year in Seattle, Wash.

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[2] https://www.siam.org/prizes-recognition/activity-group-prizes/detail/siag-acda-early-career-prize

[3] https://www.siam.org/conferences/cm/conference/acda23

Pancreatic Beta Cell

Continued from page 1

(ATP)-sensitive K$^+$ (KATP) channel—which is closed by ATP and opened by adenosine diphosphate (ADP)—serves as the link between beta cell metabolism and increased plateau fraction. As glucose increases, KATP channel activity decreases, thus requiring more KCa channel activation and hence more calcium to terminate the bursts (see Figure 1a, on page 1). The beta cell's metabolism, which acts as a measure of blood glucose concentration, therefore increases calcium and insulin secretion by way of increased plateau fraction.

In 1987, John Rinzel demonstrated that the pattern of spikes superimposed on a plateau arises from bistability between silent and spiking states in the fast subsystem; the slow variable (calcium) carries the system cyclically between the two states (see Figures 2a and 2b). This phenomenon is called *fold/homoclinic* bursting because each active phase begins at a saddle node (fold) and ends at a homoclinic bifurcation. Rinzel's work also laid the foundation for a general theory of the many types of bursting—characterized by various sets of bifurcations—that occur in different cells [9]. Eugene Izhikevich later identified over 100 distinct types of bursts, including some that had not yet been observed experimentally [4]. Additional work found that bursting in certain pituitary cells—which resembles beta cell bursting—is better fit by one of these predicted types, which is delineated by saddle node and subcritical Hopf bifurcations (see Figures 2c and 2d).

One can derive the bifurcations that are traversed during bursting—as well as their topological arrangement—by unfolding a higher codimension bifurcation [3]. Fold/homoclinic and fold/sub-Hopf bursting, along with almost all other known types, result from a codimension-four doubly-degenerate Bogdanov-Takens point [7].

Though the Chay-Keizer beta cell model is quite beautiful, it is wrong in several respects. When technology to measure calcium dynamics in cells became available, biologists learned that calcium acts like a fast variable (rather than a slow variable) in a relaxation oscillator (see Figure 1b, on page 1). The Chay-Keizer model also does not account for the wide range of periods—from seconds to minutes—that are present in beta cells. Cytosolic calcium is slow compared to spike generation, but not slow enough to account for the five-minute pulses of insulin secretion.

To address these issues, researchers added two new mechanisms to the Chay-Keizer model. The first is the endoplasmic reticulum (ER): an internal reservoir of calcium that has much slower kinetics than the cytosolic calcium, thus slowing calcium oscillations and giving them the correct shape. Second, KATP channel activity was assumed not only to set the plateau fraction, but also to oscillate slowly due to oscillations in the ATP/ADP ratio (see Figure 1c, on page 1). These metabolic oscillations provide another form of negative calcium feedback; when calcium levels are high, ATP is consumed to pump calcium out of the cell or into the ER, which reopens some KATP channels and subsequently terminates calcium entry.

Although glucose generally raises ATP/ADP, the mean ATP/ADP level paradoxically does not increase with glucose when the system is bursting [5]. This counterintuitive model property holds because the increased ATP production is balanced by the rise in ATP consumption to handle the larger calcium influx. The bifurcation diagram (like the one in Figure 2b but with ATP/ADP in place of calcium) reflects this effect, as the saddle-node and homoclinic bifurcations are invariant with respect to glucose. Further experimental advances eventually confirmed the predictions of the augmented Chay-Keizer model. This improved model can also accommodate the wide range of oscillation periods by varying the proportion of slow and very slow components. At last, the calcium exhibits very slow oscillations that account for the five-minute pulses of insulin secretion.

However, Sandra Postić and her colleagues recently challenged this hard-won synthesis of experimentation and modeling with new data and proposed an alternative mechanism in which beta cell oscillations are governed by the release of calcium from the ER — not by outside entry through plasma membrane ion channels [8]. In their study, the stimulation of calcium release triggered oscillations in basal glucose, while the inhibition of release suppressed oscillations when glucose was just above the threshold. The authors concluded that calcium release is both necessary and sufficient for oscillations, and relegated calcium entry to a subordinate role of refilling the ER.

Utilizing the long history of oscillation modeling based on calcium release, we rebutted this recent work and argued that the calcium release mechanism is at odds with existing data [2]. If the calcium that raises cytosolic calcium levels comes from the ER, then the two calcium pools would be out of phase (contrary to experiments). The canonical calcium entry model exhibits the correct behavior (see Figure 1c, on page 1). The release model in [8] also predicts that depletion of the ER will terminate oscillations, which does not occur experimentally. However, the canonical model again gets this right due to the redundancy of ER and ATP/ADP mechanisms (see Figure 1d, on page 1). We also confirmed that the canonical model can account for the new data.

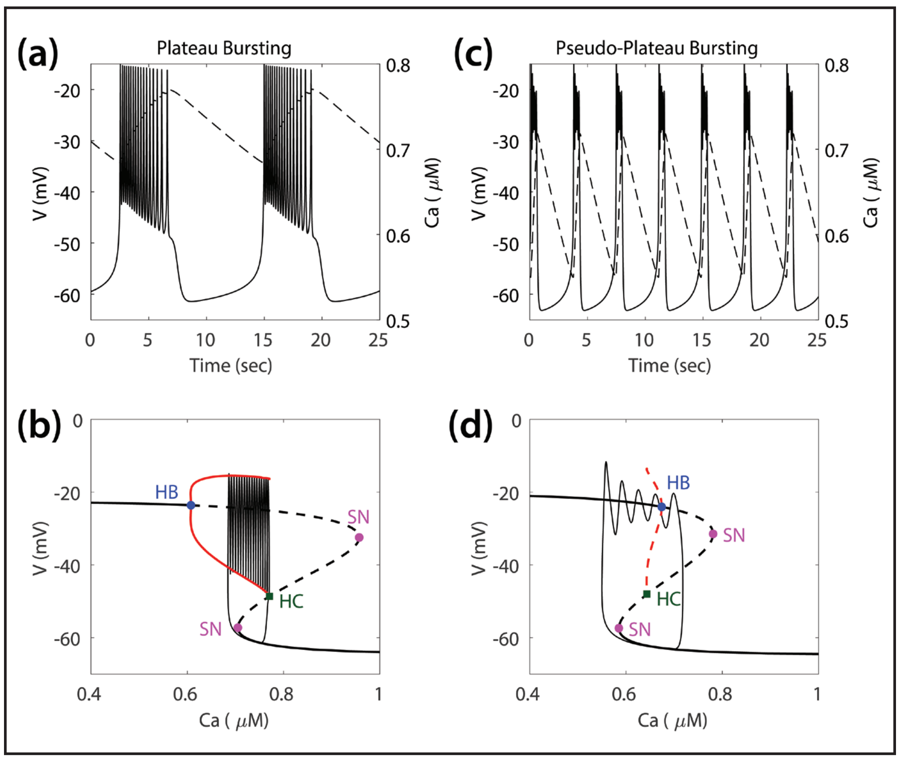

Figure 2. *In beta cell models, bursting with spikes that appear on the plateaus is generated by a family of stable limit cycles* **(2a)** *and classified as fold/homoclinic* **(2b)**. *Bursting in certain pituitary endocrine cells looks similar* **(2c)** *but is better described by bursting models of fold/subHopf type* **(2d)**, *in which decaying transients (a "pseudo plateau") generate the spikes. A predicted consequence is that it is very difficult to perturb the oscillations upward from silent phase to active phase [10]. Figure courtesy of the authors.*

To its credit, Postić's recent study drew attention to the range of glucose where most of life is spent: just below and above the threshold [8]. But as a corollary, small ionic currents cause major effects in that regime. Though such currents can shift the threshold for electrical activity, this threshold is primarily set by the KATP channels that act as gatekeepers for calcium entry. We hence concluded that calcium release is neither necessary nor sufficient for calcium oscillations (see Figure 3).

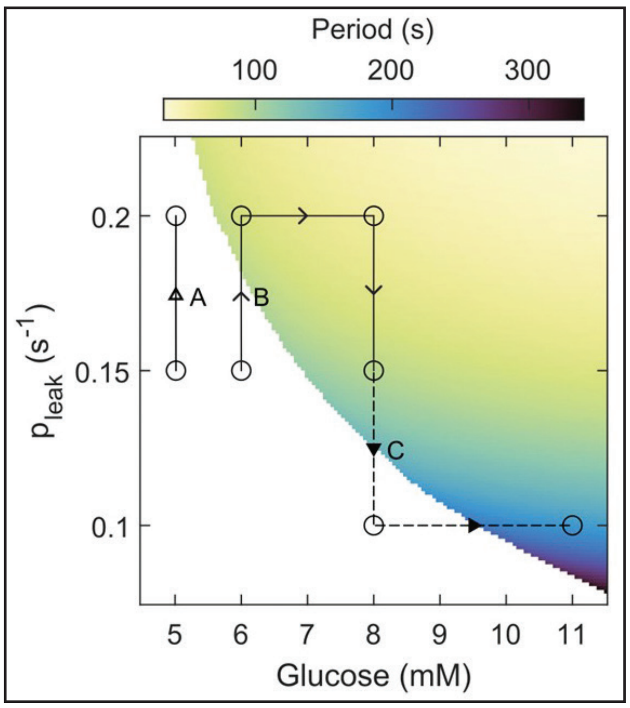

Figure 3. *In model simulations, small currents that are activated when the endoplasmic reticulum (ER) empties shift the threshold for oscillations (colored region) but are neither necessary nor sufficient. In five mM glucose, increasing ER leak fails to trigger oscillations (see line A). Increasing the leak triggers oscillations in six mM glucose, but increased leak is not necessary in eight mM glucose (see line B). Reducing the leak in eight mM glucose stops oscillations, but raising glucose to 11 mM restores them (see line C). Figure courtesy of the authors.*

A combination of mathematics and biological experimentation has successfully addressed a plethora of specific problems that pertain to beta cell oscillations. Moreover, the stunning diversity of oscillation patterns derives from a simple, unified framework in which a relatively small number of mechanisms quantitatively combine in different proportions. We believe that the pleasing concordance between the model and various phenomena arises because cells encounter the previously identified bifurcations as they randomly mutate, and the bifurcations that prove useful are fixed by natural selection.

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From Sequences of Images to Trajectories: A Tracking Algorithm for Dynamical Systems

By Aminur Rahman, Erdi Kara, and J. Nathan Kutz

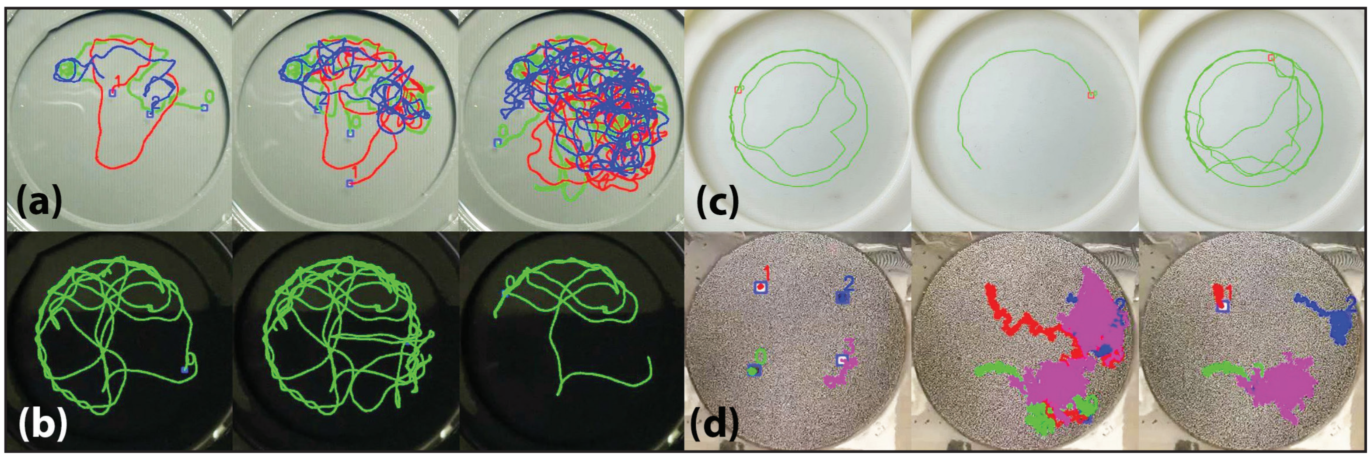

Figure 2. *Sample trajectories of multiple walkers and granular intruders.* **2a.** *Standard lighting for three droplets.* **2b.** *Single walker with the lights turned off.* **2c.** *Single walker with extreme light saturation.* **2d.** *Four granular intruders. Figure adapted from [8].*

In the context of dynamical systems, researchers are often interested in the trajectory of an object or agent under the influence of physical laws. To obtain accurate physical observations, humans can carefully measure the trajectory in question (often frame-by-frame in a video) [10]. Alternatively, one may use edge detection, background subtraction, or a host of other computer algorithms — including machine learning (ML) techniques. MATLAB and Python conveniently house software packages that identify images (such as `imfindcircles` and `OpenCV`), which users can employ to automatically track an object frame-by-frame via a simple *for loop*. Indeed, the success of modern ML and artificial intelligence algorithms in areas such as vision, speech, and language would suggest that object tracking should be a trivial algorithmic task when compared to achievements like ChatGPT. However, the computer vision community's generic image detection algorithms are often not optimally suited for dynamics problems.

Consider a ball that is rolling on a surface. At first glance, the contrast between the ball and surface makes this problem seem like a simple scenario for MATLAB's Image Processing Toolbox[1] (see Figure 1a). However, significant unexpected difficulties required months of debugging [6]. While computer algorithms aim to reduce human effort, assembling the automation can often require almost as much work as when a human inspects each frame. Moreover, blindly performing the automation without verifying the algorithm's validity for the specific experiment is even more troubling and can generate erroneous results.

Now consider a more difficult problem wherein the object and background are the same material. In Figure 1b, the object is a walking droplet (*walker*) and the background is a vibrating fluid bath on which the walker bounces [3]. Background subtraction does not work because it is difficult to determine the background's exact location, and edge detection also does not work because we do not know where the fluid bath ends and the droplet begins. In this case, an algorithm must identify the droplets and ignore the mirrored images on the bath. For this and many other real-world problems, no simple automation techniques significantly reduce human input.

Given these realizations, we developed new object tracking algorithms[2] and tested previous state-of-the-art (SOTA) algorithms for two dynamical problems: (i) Walking droplets and (ii) granular intruders [8]. Like many tracking algorithms, our ML-based approach follows the tracking-by-detection idea. First, we locate the objects of interest (i.e., walkers and intruders) in the frame; these *detections* are then associated with each other in subsequent frames to help track individual objects. For the detection phase, we utilize YOLOv8 (You Only Look Once version 8):[3] a popular deep-learning-based object detection program. At this stage, the critical observation is to match the number of detections with the actual number of objects in the experiment and impose a high confidence score on each detection. This method eliminates false-positive identifications that may corrupt the tracking efforts. For the sake of interpretability, we employ the simplest identification approach: we calculate the distances between objects in two frames and use the *Hungarian algorithm*—a combinatorial optimization algorithm that solves an assignment problem in polynomial time—to identify corresponding objects in two subsequent frames. Figure 2 displays some of our tracking algorithm's captured trajectories [8]. Figures 2a-2c depict several walking droplet experiments, while Figure 2d illustrates samples from the granular intruder experiment.

Our algorithm accurately tracks more than 98 percent of frames in a wide spectrum of experimental settings, which creates very high-fidelity data (see Figure 3). Tracking failure results in an *identity (ID) switch* and can manifest in different forms; for instance, trackers may lose an already tracked object, confuse the initial object identities with other class identities, or fail to track the objects altogether. To compare our algorithm's performance against other methods, we tested five SOTA models: `StrongSORT` [5], `Observation-Centric (OC)-SORT` [4], `Deep OC-SORT` [9], `BoT-SORT` [1], and `ByteTrack` [11]. Surprisingly, all of these methods fail for multiple droplet experiments and make ID switches (see Figure 4, on page 6).

General computer vision applications utilize a handful of standard performance metrics—such as multi-object tracking accuracy, multiple object tracking precision, and the number of ID switches—with some given tolerance. However, dynamicists typically seek to identify the trajectories of multiple objects with absolute accuracy; the tracker must therefore be completely free of ID switches, as even a single switch leads to false trajectories. As such, trajectories

See **Tracking Algorithm** *on page 6*

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[1] https://www.mathworks.com/products/image.html

[2] https://github.com/erkara/TrackingWalkers-YOLOv8

[3] https://docs.ultralytics.com

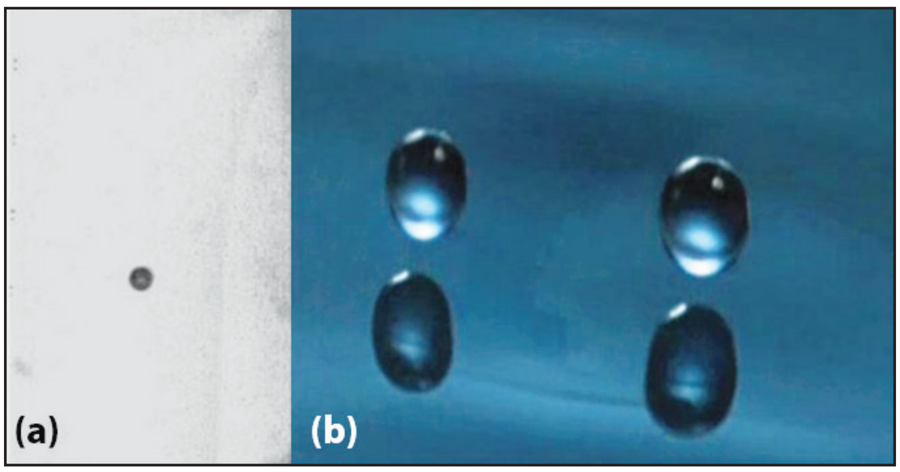

Figure 1. *A stark difference in contrast.* **1a.** *Black ball on a white surface.* **1b.** *Two droplets on a vibrating fluid bath, with visible reflections of the droplets on the bath. Figure 1a courtesy of [6] and 1b courtesy of [3].*

Experiment	Total Detections	Total Frames	Frame Detection Rate
Control	7491	7494	100.00
Lights Off	7859	7884	99.99
Lights Low	7956	7962	99.99
Lights High	7391	7426	99.99
Two Droplets	7824	8032	99.34
Three Droplets	8657	9034	98.63
Res Mid	9768	9798	99.98
Res Low	7752	7805	99.95
Faraday	7998	8118	99.40
Corral White	7542	7692	98.56
3white	12530	12720	98.81
2white2black-short	17893	18918	98.50
2white2black-long	36259	36663	99.57

Figure 3. *Frame detection rates for walking droplet and granular intruder experiments.*

Evelyn Boyd Granville

Continued from page 2

research and development program [1]. By 1966, she was a member of the Signal Analysis Department of IBM FSC-West Coast Operations, where she participated in a project for the Jet Propulsion Laboratory's space exploration program [9].

Return to Academia

Granville and Collins divorced in 1967. Due to a simultaneous downturn in IBM government contracts, Granville returned to academia. She joined the faculty at California State University, Los Angeles (CSULA); developed an interest in mathematics curriculum standards and teaching preparation at the elementary level [4]; and coauthored a textbook on the subject in 1975.

Granville remarried in 1970 and moved to East Texas in 1984 with her husband, Edward V. Granville [3]. She retired from CSULA that year but returned to the workforce to briefly teach computer literacy and mathematics in junior high and high school, then to teach at Texas College for three years in 1985, and finally to serve as a visiting professor of mathematics at the University of Texas at Tyler in 1990. She retired for good in 1997 [7].

Recognition and Legacy

Granville's name seldom appears in scientific publications (entire teams were credited instead), which makes it difficult to determine her individual contributions. Nevertheless, she received a number of prestigious awards and honorary degrees over the years, including the Wilbur Lucius Cross Medal from the Yale Graduate School Alumni Association as well as honors from the National Academy of Engineering and the National Academy of Sciences.

Perhaps surprisingly—given her pioneering status as a Black woman mathematician and programmer—Granville did not feel that her studies and career were marred by racism or sexism; instead, she indicated that her experiences were generally pleasant. In fact, she suggested that her success partly reflected both the dazzling rarity of women like her at the time and new opportunities for women and minorities in industry after World War II. However, Granville also acknowledged the lingering stigma that women in mathematics faced then and still face today.

In 2005, Granville reflected on her early career transition from Fisk University. "I left academia and started on a career in government and private industry that I could not have envisioned when I left Dunbar High School as a shy seventeen-year-old," she said [4]. Granville also contrasted the opportunities for women in her youth with those in a world with personnel requirements that were engendered by World War II, the Cold War, and the electronic computer industry. "I had seen professional women solely in the position of teachers," she said. "These were my role models. Now, I began to see women as mathematicians, engineers, chemists, biologists, [and] computer programmers" [4]. Given her trailblazing professional successes, Granville has undoubtedly served as a role model for those who have followed in her footsteps.

Figure 1. *The mainframe of an IBM 704: a state-of-the-art, high-speed digital computer in the late 1950s. Figure courtesy of Lawrence Livermore National Laboratory via Wikimedia Commons.*

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Tracking Algorithm

Continued from page 5

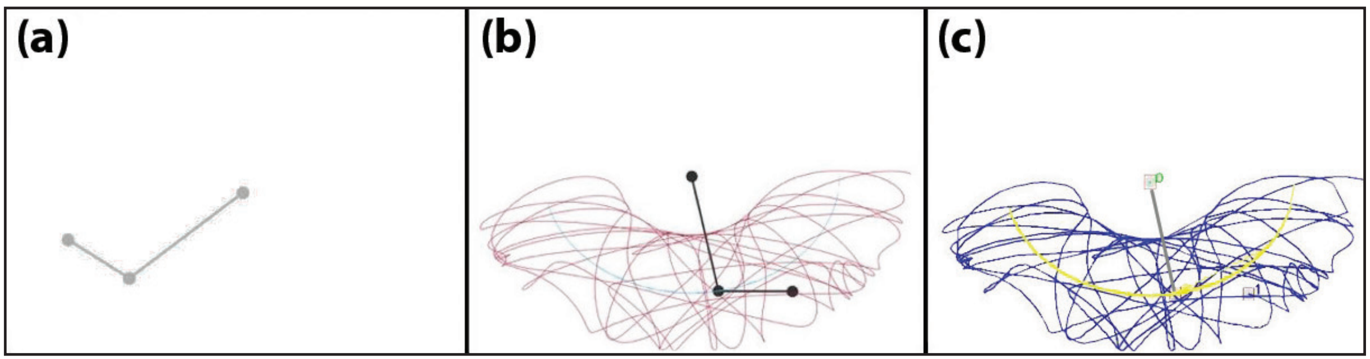

Figure 5. *Tracking a simulated double pendulum.* **5a.** *A single frame of the double pendulum, with the pivot at the center and two nodes of different arm lengths.* **5b.** *Ground truth for the pendulum's motion for a 20-second run.* **5c.** *Tracking results of the model that was trained with 10 frames from the original experiment video. Figure courtesy of the authors.*

from these SOTA models may not always be useful. Our model is free of ID switches and hence more robust for dynamicists — especially when attempting to infer the underlying dynamics.

As an illustrative sample, consider the double pendulum: a canonical example of a chaotic system. We use MATLAB's `ode45` to numerically simulate the pendulum, which yields a ground truth for the tracking algorithm (see Figure 5). We record the simulation as a 20-second video with a frame rate of 60 hertz, where all of the dynamical information is hidden. For an additional challenge, we give the nodes and arms of the pendulum a light gray color that is difficult to see — especially as a moving picture. We then train the algorithm with ten frames of the experiment video, which contains a total of 1,200 frames. Doing so reveals close agreement between the ground truth and the tracking algorithm. As a next step, users could potentially employ sparse identification methods like `SINDy` [2, 7] to discover the differential equations that govern the dynamics. Concurrent utilization of these methods could potentially automate a workflow that begins with empirical observations and ends with a dynamical systems model.

Our tracking algorithm reliably reduces the number of required human hours to gather tracking data in dynamics problems. Dynamicists can subsequently spend that time on more enjoyable tasks, such as developing predictive interpretable models, analyzing bifurcations, or proving the existence of interesting topological properties of phase space. Furthermore, students will have the chance to absorb far more dynamics training from research projects than they otherwise would by simply tracking objects on a frame-by-frame basis. Ultimately, this tracking framework has the potential to significantly improve the workflow of many projects and enable the accurate inference or characterization of the underlying dynamical system that generates the observations.

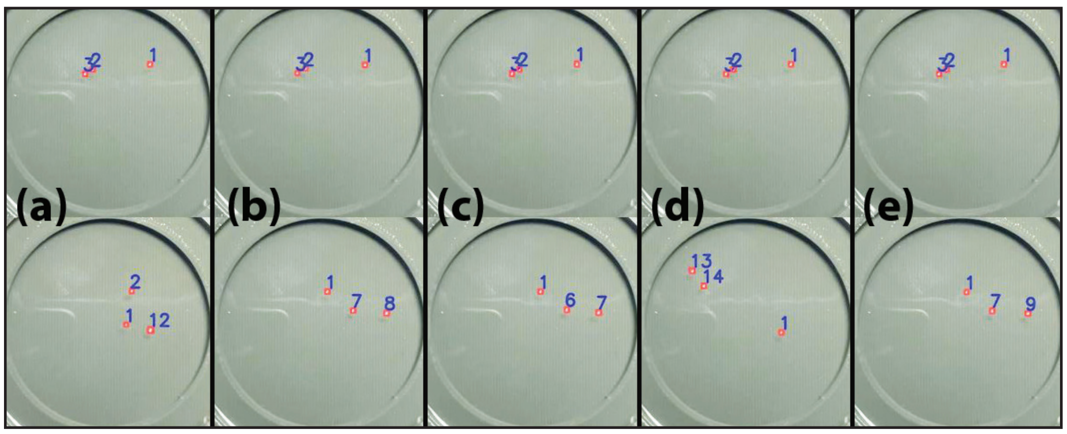

Figure 4. *Frame-by-frame identity (ID) switching and new false assignments in previous state-of-the-art models. The top row depicts initial ID assignments and the bottom row shows ID assignments in a later frame.* **4a.** `StrongSORT`. **4b.** `Observation-Centric (OC)-SORT`. **4c.** `Deep OC-SORT`. **4d.** `BoT-SORT`. **4e.** `ByteTrack`. *Figure adapted from [8].*

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Automating Conference Scheduling with Genetic Algorithms at CSE23 and Beyond

By Alicia Klinvex
and Tamara Kolda

Scheduling large conferences—such as the 2023 SIAM Conference on Computational Science and Engineering[1] (CSE23), which was held earlier this year in Amsterdam, the Netherlands—is quite difficult. CSE23 took place over the course of five days and consisted of roughly 2,000 presentations in 400 minisymposia across 12 timeslots and 40 rooms of dramatically varying capacity (from 20 to 1,746 people). In the past, conference organizers and SIAM staff have manually assigned presentations to minisymposia and mapped the minisymposia to timeslots and rooms by hand; this is naturally a tedious and error-prone undertaking. However, looking at the task as a mathematical problem makes it much more palatable. This year—and for the first time in SIAM history—the scheduling process for a SIAM conference was automated thanks to Alicia Klinvex (Naval Nuclear Laboratory), who designed the methodology and wrote a set of C++ and Python codes for CSE23. Interested readers can view this code online.[2] Here, we'll outline the processes and decisions that informed the code's design and hopefully encourage future conference organizers to adopt a similar methodology.

Scheduling Constraints

Our code had to account for a number of scheduling limitations:

1. **Speaker Conflict:** No speaker or minisymposium organizer can be in two rooms at the same time.
2. **Room Equipment:** Minitutorials and certain minisymposia—like a CSE23 session with live demonstrations on real pool tables[3]—require rooms with special setups.
3. **Timeslot Suitability:** Some speakers and minisymposium organizers are only available during specific timeslots. Because timeslots are not always the same length, longer minisymposia cannot be scheduled in short timeslots.
4. **Multipart Sequence:** Some minisymposia have multiple parts. Part I must come before part II, which must come before part III, and so forth.
5. **Room Size:** More popular minisymposia should take place in larger rooms, thus requiring an automated method to estimate attendance.
6. **Topic:** Minisymposia that address similar topics should be assigned to different timeslots, e.g., all machine learning minisymposia should not take place simultaneously. An automated method to estimate the similarity of two minisymposia is therefore necessary.
7. **Multipart Adjacency:** Multipart minisymposia should ideally occur in the same room during adjacent timeslots.

Metadata Collection

SOFTWARE AND PROGRAMMING

We used the citation counts of recent publications to estimate the prospective attendance (and hence the required room size) of a given lecture. Since some presenters had common/repeated names, we first checked for Google Scholar entries with their names and current affiliations. However, this method is very subjective to nicknames and other name changes; unless presenters explicitly added multiple names to their Google Scholar accounts or included papers that published under a different name, the data may be incorrect. We therefore welcome suggestions for better ways to estimate session attendance — readers can submit their ideas as issues on our GitHub repository.

We applied two different methods to evaluate the likeness between two minisymposia. When testing the code on abstracts from the 2019 SIAM Conference on Computational Science and Engineering,[4] we first utilized Python's Natural Language Toolkit[5] to measure the abstracts' similarity, then employed k-means++ to cluster the data into groups. We assumed that minisymposia in the same group were similar to each other. Later, when working with CSE23 data, each organizer had to pick three "topic codes" that we used to assess similarity.

Generating a "Good Enough" Schedule

Because scheduling is an NP-complete integer programming problem, we are unlikely to find the globally optimal result for our constraints. However, a simple genetic algorithm provides a remarkably good solution. Our approach is as follows:

1. Start with a randomly generated population of potential schedules.
2. Compute the penalty for each schedule based on the desired characteristics.
3. Breed the members of the current population—favoring those with the smallest penalties—to obtain a new population.
4. Introduce genetic mutations to the new population.
5. Go back to step 2 and repeat.

For our purposes, the first step is clear; we perform random permutations on the set of minisymposia to obtain an initial population of schedules.

To breed two schedules in step 3, we let k be a random number of timeslots (between 0 and the total number of timeslots), select the first k timeslots of the first parent schedule, and copy the data to the first k timeslots of the child schedule. We then generate the remaining data from the second parent while maintaining the property that each minisymposium appears in the schedule only once. We also make easy fixes to satisfy the adjacency criteria for multipart minisymposia and room assignments, which repositions various sessions.

For step 4, we implement genetic mutations by swapping two random minisymposia within a schedule.

Schedule Penalty Scheme

In order to rank a population, we must define a penalty for each schedule that it contains. Every scheduling consideration contributes to the score. The first four considerations are mandatory and have high penalties for violations of the requirements, while the remaining three considerations fall into the "would be nice" category and incur significantly smaller penalties. We calculate each penalty in a specific way:

1. **Speaker Conflict:** +1 for each pair of minisymposia in the same timeslot that share a common speaker or organizer.
2. **Room Equipment:** +1 for each time a specific room request is not honored.
3. **Timeslot Suitability:** +1 for each time a schedule constraint is not honored.
4. **Multipart Sequence:** +1 for each time a later part of a multipart minisymposium is scheduled before its predecessor.
5. **Room Size:** We sort the rooms based on size from $r-1$ (largest) to 0 (smallest), where r is the total number of rooms. Ties are broken arbitrarily. Suppose that there are n minisymposia; each minisymposium $i \in \{1,2,\ldots,n\}$ has an associated value $m_i \in \{0,1,\ldots,r-1\}$ that indicates the index of the smallest room to which it can be assigned and a value $a_i \in \{0,1,\ldots,r-1\}$ that specifies its actual assignment. The penalty is $\Sigma_{a_i<m_i}(m_i-a_i)^2/\Sigma_i m_i^2$, which is always less than 1.
6. **Topic:** We focus on the case with topic codes. Each pair of topics has a preassigned similarity of 0 (none), 1 (some), or 2 (identical). Every minisymposium has three topics, so we sum up the similarities across all nine possible pairings of keywords for a value between 0 and 18. The topic penalty is the sum of all similarities between pairs of minisymposia in the same timeslot, divided by the sum of the similarities for all minisymposia. This penalty is also always less than 1.
7. **Multipart Adjacency:** We consider two factors for multipart minisymposia. First, we sum up the number of times that a later part of a multipart minisymposium is not scheduled for the slot that immediately follows its predecessor. Second, we sum up the number of times that a later part of a multipart minisymposium is not scheduled in the same room as its predecessor. We divide this outcome by the number of minisymposia that have a predecessor, meaning that the maximum value of this penalty is 2.

See **Conference Scheduling** *on page 9*

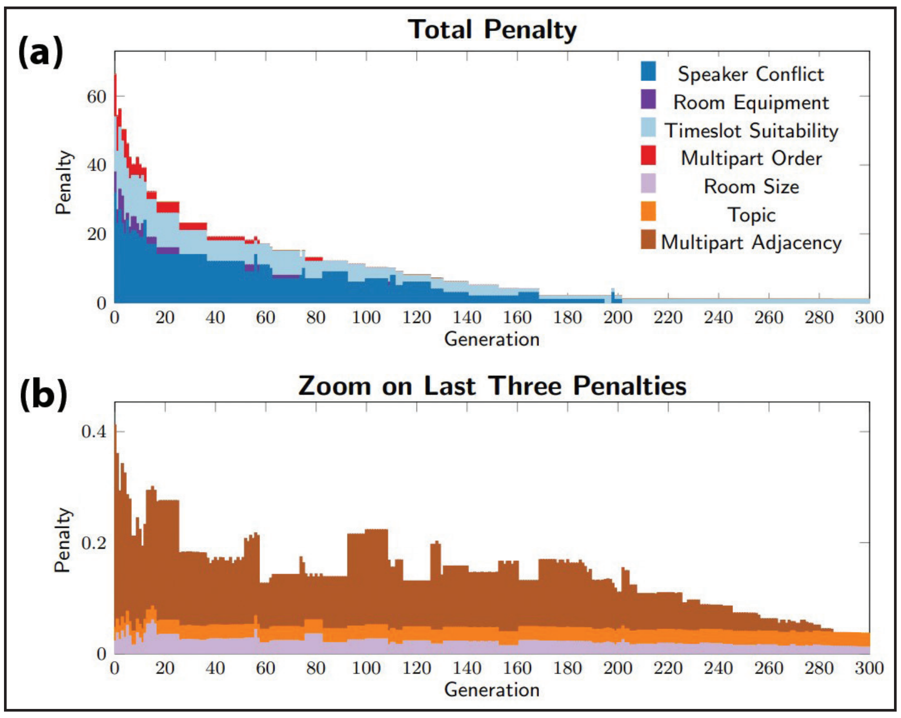

Figure 1. *Reduction of the penalty for the 2023 SIAM Conference on Computational Science and Engineering (which included 400 minisymposia, 12 timeslots, and 40 rooms) over 300 generations of the genetic algorithm with a population of 10,000 schedules.* **1a.** *The sum of all of the penalties.* **1b.** *The sum of the last three penalties, which are very small compared to the first four but are nonetheless minimized by the genetic algorithm. Some penalties do not go to zero. Figure courtesy of the authors.*

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[1] https://www.siam.org/conferences/cm/conference/cse23

[2] https://github.com/tgkolda/genetic_scheduling

[3] https://meetings.siam.org/sess/dsp_programsess.cfm?SESSIONCODE=75756

[4] https://www.siam.org/conferences/cm/conference/cse19

[5] https://www.nltk.org

SIAM Establishes the Life Sciences and Dynamical Systems Travel Fund

SIAM is pleased to announce the establishment of the new Life Sciences and Dynamical Systems Travel Fund, which is made possible with the backing of SIAM member Simone Bianco. SIAM is incredibly grateful for his generous gift, which will help students and early-career researchers who are historically underrepresented in science, technology, engineering, and mathematics (STEM) attend the SIAM Conference on the Life Sciences and SIAM Conference on Applications of Dynamical Systems. At these meetings, travel fund recipients will have an opportunity to present research, network and advance their careers, and grow as leaders.

Bianco is a principal investigator and Director of Computational Biology at the Altos Labs Bay Area Institute of Science. He has been a proud member of SIAM for 12 years, remains a vital participant of the SIAM Activity Group on Life Sciences and SIAM Activity Group on Dynamical Systems, and serves as a SIAM Visiting Lecturer.

Simone Bianco, Altos Labs Bay Area Institute of Science.

"I'm excited to join forces with SIAM to launch a travel fund for underrepresented minorities in STEM," Bianco said. "We value diversity and inclusion in mathematics and its applications, especially in dynamical systems and the life sciences. I owe a lot to the SIAM community for its support and encouragement, and I am thankful for the opportunity to pay it forward to the next generation of scholars."

The Life Sciences and Dynamical Systems Travel Fund will provide three student and/or early-career conference attendees who are historically underrepresented in the field with up to $3,000 towards their conference registration and reasonable costs of attendance, including travel, lodging, and meals.

Interested students and/or early-career researchers will be asked to submit a SIAM Travel Award application, an applicant statement, a copy of their CV, and a letter of recommendation from an advisor (this is optional for early-career applicants). Applications will be collected via the same portal as regular SIAM Travel Award applications; applicants for the 2024 SIAM Conference on the Life Sciences and 2025 SIAM Conference on Applications of Dynamical Systems will have to opt into consideration for the Life Sciences and Dynamical Systems Travel Fund.

Many thanks to Bianco for his philanthropic contribution to fund this new program!

Describing the Universe with Breadth and Depth

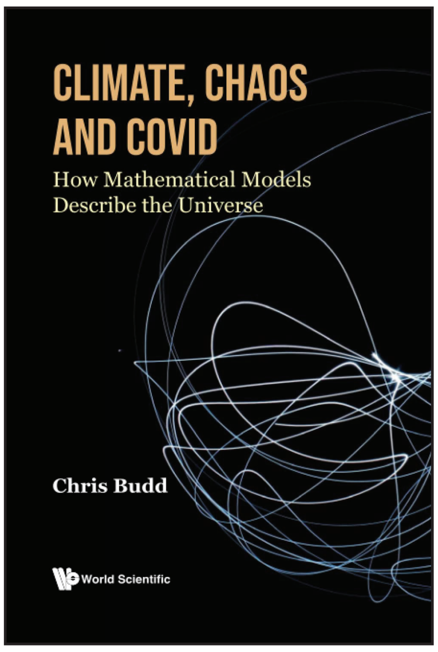
BOOK REVIEW
By Paul J. Nahin

Climate, Chaos and COVID: How Mathematical Models Describe the Universe. *By Chris Budd. World Scientific Publishing Europe Ltd., London, England, April 2023. 312 pages, $78.00.*

With *Climate, Chaos and COVID: How Mathematical Models Describe the Universe*, applied mathematician and SIAM member Chris Budd has crafted an exceptionally well-written account of mathematical reasoning's contributions to enormous insights about the physical world. A nuts-and-bolts experimental physicist could not have done a better job. Budd is currently a professor at the University of Bath in England, having previously served as the Gresham Professor of Geometry at Gresham College from 2016 to 2020. His book is an expansion of 24 public lectures on mathematical modeling that he presented during his four years at Gresham.

Both the breadth and depth of *Climate, Chaos and COVID* are highly impressive. I specifically mention *depth* because Budd is not shy about including equations; in fact, he makes a persuasive case for why they *should* be included, even in a book like this that is meant for a much wider audience than just professional mathematicians. And I mention *breadth* because the text covers a remarkably large number of topics.

Budd begins with Galileo's discovery of simple pendulum physics during an apparently less-than-exciting 16th-century religious service (the swaying of an overhead chandelier was far more interesting to Galileo than whatever the priest happened to be saying). And yes, differential equations do appear. Budd then goes on to write equally admirable essays about some of the following topics (though this is *not* an exhaustive list): the geometry of locating whales in the ocean; the spread of diseases (this is where COVID-19 comes into play); James Clerk Maxwell's theory of the electromagnetic field (including *partial* differential field equations) and its ramifications for radio; chaos theory (including the butterfly effect, long-range weather forecasting, and the Lorenz equations); mathematical models for the study of climate change; the math of electrical power distribution systems (he does not avoid the complex number algebra that is associated with electrical engineering); wind energy extraction; the heat equation (including Fourier series); the strength of materials; and Newton's theory of gravity, with applications to both long-term concerns (i.e., the stability of the solar system) and current issues (i.e., the physics of near-Earth satellites).



Climate, Chaos and COVID: How Mathematical Models Describe the Universe. By Chris Budd. Courtesy of World Scientific Publishing Europe Ltd.

In addition to the text's more serious discussions, Budd includes numerous personal observations and philosophical insights on "doing math" that I found both pertinent and informative. For better or worse, he also has a well-developed sense of humor that does periodically lead to corny jokes, such as *"Why did the mathematician cross the road? To prove that the other side exists."* Nevertheless, this easily forgiven "flaw" just demonstrates that Budd wrote the book with more than a purely academic audience in mind. And to be fair, I should add that this seemingly off-the-wall question quickly transforms into a nice example of mathematical modeling to find "the best way to cross a road" given the impact of pedestrian road crossings on the flow of automotive traffic.

I strongly recommend *Climate, Chaos and COVID* to anyone who both loves mathematics and disagrees with G.H. Hardy's well-known assertion that good math can only be math that has no applications. Budd's book is an elegant illustration that effectively refutes Hardy's claim.

Paul J. Nahin is a professor emeritus of electrical engineering at the University of New Hampshire. He is the author of more than 20 books on mathematics, physics, and electrical engineering; his latest book, The Mathematical Radio, is set to publish through Princeton University Press in early 2024.

Behind the Lab Coat: A Scientist's Journey to Influence Science Policy in Washington, D.C.

By Bashir Mohammed

I have always been fascinated by arithmetic and computers. As a child, I enjoyed taking things apart to visualize and understand their underlying mechanisms. I can still vividly recall the experience of building my first computer; observing what seemed like a silicon city, I was astounded by the elegant arrangement of chips, integrated circuits, and other components on the motherboard. Ever since college, I have wanted to not only contribute to science but also benefit humanity. This aspiration inspired me to pursue a master's degree and then a Ph.D., and eventually secure a postdoctoral research fellowship at Lawrence Berkeley National Laboratory (LBNL).

In 2019, I was honored to earn second place at the renowned Berkeley Lab Research SLAM[1] contest. This event challenges early-career scientists and postdocs to present their work to a non-specialist audience in a concise, appealing, and clear manner. I firmly believe in the importance of clarifying complex mathematics and computer science topics for nontechnical audiences, and my participation in this contest led to an invitation to represent LBNL at the International Year of the Periodic Table Elemental Slam on Capitol Hill.[2] Only six postdoctoral researchers from the U.S. Department of Energy (DOE) National Laboratories were chosen for this competition, during which I delivered a presentation about my work to U.S. legislators in Washington, D.C. The experience was a significant milestone in my career and offered a unique opportunity to engage with members of Congress and inquire about policy processes and scientific funding. As a result, I began to seek out further occasions to interact with federal officials and deepen my understanding of science policy decisions. When I came across the call for applications for the SIAM Science Policy Fellowship Program,[3] I was immediately drawn to the possibility of leveraging my passion for science communication to positively impact the SIAM community in the U.S. and beyond.

I applied for the SIAM Science Policy Fellowship Program to learn more about critical legislative issues that pertain to science, technology, mathematics, and engineering (STEM); gain insight into the U.S. federal budget and appropriations processes; explore my passion for science policy; and advocate for applied mathematics and computational science. My application to the Fellowship Program included a personal statement and detailed description of a policy issue that I'm passionate about; I chose the National Quantum Initiative.[4] I was awarded the Fellowship in January 2023, alongside four other early-career researchers.

As a Science Policy Fellowship recipient, I am required to attend the biannual spring and fall meetings of the SIAM Committee on Science Policy[5] (CSP), which works tirelessly to amplify the recognition of applied mathematics research among legislative decision-makers. By effectively communicating the value and significance of SIAM to Congress, the CSP ensures that the SIAM community's voice is heard in the heart of Washington, D.C. The committee actively liaises with vital stakeholders and advocates for science policy topics that are crucial to the SIAM community. Its members draft impactful white papers and position statements on diverse subjects, from the National Quantum Initiative and the CHIPS and Science Act[6] to efficient power grid strategies and urgent matters like climate change. The CSP also engages in direct dialogues with policymakers to address a variety of key concerns, such as funding for prominent institutions like the National Science Foundation (NSF), National Institutes of Health (NIH), Department of Defense (DOD), and the DOE Advanced Scientific Computing Research[7] (ASCR) program. To strengthen SIAM's influence in Washington, D.C., the CSP collaborates with Lewis-Burke Associates LLC[8] — a government relations firm that bridges the advocacy and communication gap between SIAM, federal agencies, and Congressional offices on issues at the forefront of applied mathematics and computational science.

During the spring CSP meeting in Washington, D.C., I conversed with senior members of SIAM from academia, industry, and the DOE National Laboratories. This meeting featured a half-day orientation that introduced Fellowship recipients to the foundational elements of SIAM's history with science policy and communicated essential information about the federal budget, legislative process, and science advocacy. With guidance from Lewis-Burke, we examined significant budget items that are related to mathematics research and reviewed effective strategies for engaging with policymakers and their teams. While in Washington, D.C., I also met with lawmakers, legislative staff, and officials from various federal agencies and participated in outstanding training webinars on pivotal budget and policy topics that were curated by Lewis-Burke. These collective experiences enriched my understanding of advocacy work and provided deeper insight into the policy processes that shape science funding decisions.

Throughout the course of the CSP meetings, leaders from scientific institutions with a focus on mathematical research—including NSF, NIH, and DOE—discuss their present and anticipated budgets and outline their scientific objectives for the coming year. In the spring of 2023, CSP representatives convened with Sean Jones, assistant director for the NSF Directorate for Mathematical and Physical Sciences (MPS), and David Manderscheid, division director for the MPS Division of Mathematical Sciences. Jones and Manderscheid emphasized the need for increased funding to support initiatives for artificial intelligence, climate science, and biotechnology. We also conversed with

See **Science Policy** *on page 10*

SIAM Science Policy Fellowship recipient Bashir Mohammed takes part in a Congressional visit to the office of the U.S. Senate Committee on Energy and Natural Resources in Washington, D.C. Photo courtesy of Griffin Reinecke.

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[1] https://slam.lbl.gov

[2] https://www.congressweb.com/events/index.cfm?action=Event_Page&eventcode=mAGykC&bypass=tr

[3] https://www.siam.org/students-education/programs-initiatives/siam-science-policy-fellowship-program

[4] https://www.quantum.gov

[5] https://www.siam.org/about-siam/committees/committee-on-science-policy-csp

[6] https://new.nsf.gov/chips

[7] https://www.energy.gov/science/ascr/advanced-scientific-computing-research

[8] https://lewis-burke.com

Conference Scheduling

Continued from page 7

The total penalty for the schedule is simply the sum of these listed components. The speaker conflict, room equipment, timeslot suitability, and sequence penalties are much larger than the room size, topic, and adjacency penalties. In reality, it may be impossible to generate a schedule with zero penalty. For instance, there will always be some overlap in the case of 24 linear algebra minisymposia and 12 available timeslots, and speaker constraints may prevent a multipart minisymposium from occurring in adjacent timeslots.

Many potential variations exist for the aforementioned scheduling structure, but this simple scheme performed well for CSE23.

Software

Our GitHub repository includes the following tools:

- A Python script for data mining the citation counts from Google Scholar's application programming interface
- A Python script that clusters minisymposia based on their abstracts and returns the most common words for each cluster, so that the user understands approximately what topic the cluster represents
- A C++ code that uses a genetic algorithm to assign contributed lectures to minisymposia
- A C++ code that uses a genetic algorithm to generate a conference schedule
- A Qt graphical user interface[6] that tweaks an existing schedule and alerts users if their changes have made the schedule unfeasible.

Results

To obtain the best possible schedule according to our penalty criteria, we ran our genetic scheduler code overnight on a standard workstation with a population size of 10,000 for 100,000 generations.

Our software minimizes the penalties for the first four constraints within the first 250 generations (see Figure 1, on page 7). We were able to generate a schedule without any speaker conflicts, where all minisymposia were assigned to rooms with appropriate equipment and all multipart minisymposia occurred in the correct order. However, the minimum penalty for timeslot suitability is 1 because the room equipment requirements ensure that one of the minitutorials will be assigned to a shorter timeslot than the others. The multipart adjacency penalty converges to 0 within the first 300 iterations, meaning that all multipart minisymposia take place in adjacent timeslots in the same room. The small penalties that are associated with the remaining constraints continue to decrease until roughly generation 5,000, after which they stagnate for the remainder of the 100,000 generations.

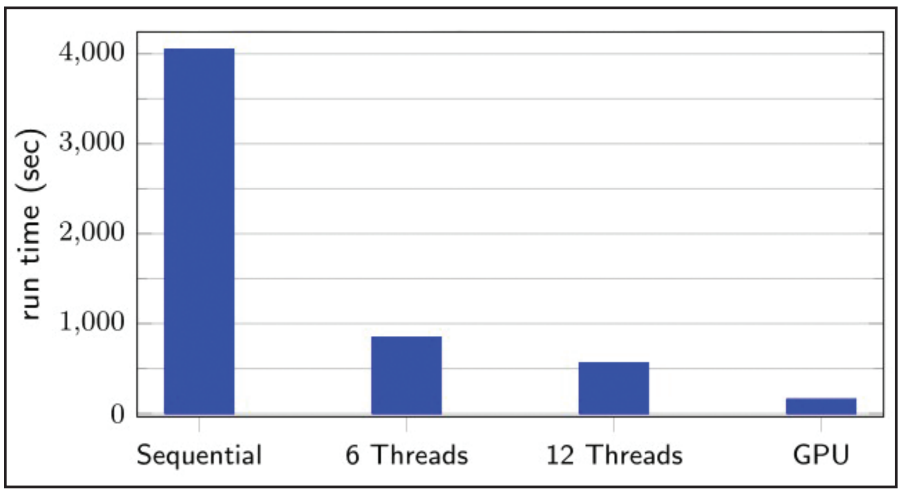

Figure 2. *Run time for 250 generations of the genetic algorithm for the 2023 SIAM Conference on Computational Science and Engineering (which included 400 minisymposia, 12 timeslots, and 40 rooms) with a population of 10,000 schedules on a laptop with a six-core i7 (ninth generation) central processing unit and an NVIDIA GeForce GTX graphics processing unit. Figure courtesy of the authors.*

Performance Portability

Many parts of this algorithm can be performed in parallel. For instance, computation of the penalties, breeding, and mutations are all independent tasks. Since we wrote our C++ code with the Kokkos performance portability library,[7] it can run on any hardware—from a cell phone to a graphics processing unit (GPU)—without modifications to the source code [1]. Using a population size of 10,000, we tested the performance of 250 generations on a laptop with a six-core i7 (ninth generation) central processing unit and an NVIDIA GeForce GTX GPU. Our code scales well and requires very little time to generate a reasonable schedule, even on a laptop (see Figure 2).

Future Enhancements

Though our algorithm had great success in scheduling CSE23, there is always room for improvement. In the future, we hope to explore several possible enhancements:

- Using natural language processing to determine the similarities between minisymposia based on abstracts
- Minimizing overlap for coauthors
- Using actual room sizes rather than a sized-based ranking of rooms
- Utilizing different metrics to estimate minisymposia attendance
- Collecting actual attendance data from meetings for use in future estimates
- Grouping similar topics in nearby rooms in the conference venue.

Ultimately, however, our genetic scheduler code performs quite well across diverse architectures and automatically optimizes conference schedules. We hope that organizers will use it to schedule other meetings in the future.

Acknowledgments: The authors would like to acknowledge Bob Frost (Naval Nuclear Laboratory) for helpful discussions about the penalty metrics and Karen Devine (Sandia National Laboratories) for constructive feedback about future enhancements.

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[1] Edwards, H.C., Trott, C.R., & Sunderland, D. (2014). Kokkos. *J. Parallel Distrib. Comput.*, *74*(12), 3202-3216.

Alicia Klinvex evaluates future technologies for the Naval Nuclear Laboratory and has a background in high-performance numerical linear algebra. She was a member of the Organizing Committee for the 2023 SIAM Conference on Computational Science and Engineering. Beginning in 2024, Klinvex will serve on the SIAM Membership Committee. Tamara Kolda is a consultant under the auspices of her California-based company, MathSci.ai. She previously worked at Sandia National Laboratories. Kolda specializes in mathematical algorithms and computational methods for data science, especially tensor decompositions and randomized algorithms. She co-founded the SIAM Journal on Mathematics of Data Science and serves as its editor-in-chief.

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[6] https://doc.qt.io/qt-5.15/qtgui-index.html

[7] https://github.com/kokkos/kokkos

Science Policy

Continued from page 8

Asmeret Asefaw Berhe, director of the DOE Office of Science, who oversees nearly eight billion dollars in funding for scientific research across the U.S. at national labs, universities, and private companies. Berhe was joined by staff from the DOE's ASCR program—a main funder of applied mathematics research—including Ben Brown, director of ASCR's Facilities Division, and Steve Lee, a program manager. The DOE officials discussed the success of the Exascale Computing Project[9] (ECP); current DOE priorities, such as diversifying and bolstering the computational science workforce; and plans for DOE offices (including ASCR) to transition research funds now that ECP has run its course. We likewise met with Alexandra Isern, assistant director of the NSF Directorate for Geosciences (GEO), who discussed how SIAM's recent "Report of the SIAM Convening on Climate Science, Sustainability, and Clean Energy"[10] is guiding GEO's thinking in the climate research space.

At the 2023 spring gathering, I was privileged to interact with policymakers who endorsed the DOE Science for the Future Act and the National Quantum Initiative. The latter was central to my research endeavors at the time, so I was able to articulate the ramifications of the DOE's fiscal decisions on quantum and computational science work. For example, an ongoing pivotal research initiative called the Quantum Application Network Testbed for Novel Entanglement Technology[11] (QUANT-NET)—a collaboration between LBNL, the University of California, Berkeley (UC Berkeley), and the California Institute of Technology—is an avant-garde, software-controlled quantum computing network that links LBNL and UC Berkeley. This revolutionary endeavor combines unparalleled expertise in quantum technologies, optics, materials, networks, and testbed operations. The idea for QUANT-NET originated at the 2020 DOE Quantum Internet Blueprint Workshop,[12] where distinguished representatives from DOE National Laboratories, universities, industry stakeholders, and other U.S. agencies outlined a vision for the country's first nationwide quantum internet.

Beyond my involvement with the CSP, I also completed an independent policy project during which I was honored to speak at the White House Office of Science and Technology Policy Open Science Listening Session[13] in May 2023. I focused my remarks on pressing priorities within the SIAM community and underscored the invaluable role that SIAM has played in shaping my career path and fostering my professional growth. While access to freely available information and publications is undoubtedly vital, open science policies must also recognize the significance of nurturing communities that support the development of early-career researchers. To advocate for this type of support, I highlighted the importance of conferences and other events that facilitate the exchange of ideas and offer networking opportunities for attendees. These gatherings encourage researchers to forge meaningful connections, collaborate on groundbreaking projects, and ultimately drive scientific progress.

My speech also emphasized the need for targeted publishing initiatives that reach relevant audiences to ensure that our work has a substantial impact. By disseminating our findings to the right readers, we maximize the potential for real-world applications and advancements. Finally, I expressed my gratitude for the instrumental role of the SIAM Science Policy Fellowship in my professional advancement. This and other similar opportunities provide mentorship, guidance, and unparalleled connections with experts in the field.

Firsthand insight into program initiatives is essential to understanding how public needs directly influence research trajectories. The ripple effects of these decisions on the SIAM community—from undergraduate fellowships to multiyear enterprises—accentuate the CSP's pivotal role. My involvement in the SIAM Science Policy Fellowship Program has deepened my recognition of the CSP's integral contributions to science policy decision-making and heightened my interest in the policy processes that shape funding decisions. With ongoing budget and policy deliberations, the SIAM community must maintain its presence and voice in Washington, D.C.; in fact, the trajectory of the scientific community depends upon these determinations. It's been wonderful to take part in the CSP meetings as a SIAM Science Policy Fellow, and I look forward to the upcoming CSP fall meeting on November 15th.

Bashir Mohammed is a Senior Staff AI Architect at Intel, where he conceptualizes and implements AI integration for the enhancement of Intel's Edge product. By utilizing the power of generative AI and large language models, he propels innovation and transformation within Intel's Network and Edge Group and Distributed Edge Infrastructure Platform Group.

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[9] https://www.exascaleproject.org

[10] https://www.siam.org/Portals/0/Programs/climate_convening/Report_SIAMClimateConvening.pdf

[11] https://quantnet.lbl.gov

[12] https://www.energy.gov/sites/prod/files/2020/07/f76/QuantumWkshpRpt20FINAL_Nav_0.pdf

[13] https://www.whitehouse.gov/ostp/news-updates/2023/07/11/readout-of-ostp-open-science-listening-sessions-with-early-career-researchers

SIAM Science Policy Fellowship recipients attended the SIAM Committee on Science Policy spring meeting in Washington, D.C., this March to connect with policymakers and learn about budget and legislative processes that affect applied mathematicians and computational scientists. From left to right: 2023 SIAM Science Policy Fellow Bashir Mohammed (Intel), 2023 SIAM Science Policy Fellow Jeffrey Larson (Argonne National Laboratory), SIAM President Sven Leyffer (Argonne National Laboratory), 2023 SIAM Science Policy Fellow Julie Bessac (National Renewal Energy Laboratory), and Lewis-Burke senior associate Griffin Reinecke. Photo courtesy of Bashir Mohammed.

A Hamiltonian Look at a Soap Film

MATHEMATICAL CURIOSITIES

By Mark Levi

A soap film stretched between two rings that share a common axis—as in Figure 1—has a surface of minimal area that, when divided by 2π, is

$$\int_{-a}^{a} \underbrace{y\sqrt{1+(y')^2}}_{L(y,y')}\,dx = \int_{x=-a}^{x=a} y\,ds \tag{1}$$

and subject to boundary conditions

$$y(\pm a) = r. \tag{2}$$

Alternatively, (1) is the potential energy of the film whose surface tension[1] is $1/2\pi$.

The Euler-Lagrange equation for the minimizer of (1) does not look appealing, and I relegate it to a footnote later on. But interestingly, the equivalent Hamiltonian system turns out to be very symmetric and simple. Indeed, the standard definition[2] of momentum p yields

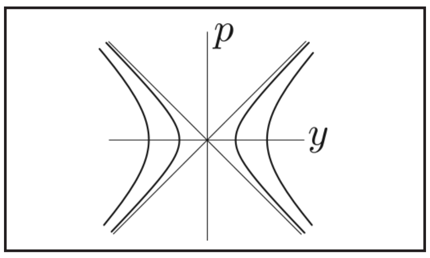

Figure 2. *Trajectories of the Hamiltonian system (5). Since $H=\text{const.}$ along each trajectory, every solution behaves like a solution to a linear system (although (5) is nonlinear).*

$$p \overset{def}{=} L_{y'}(y,y') = \frac{yy'}{\sqrt{1+(y')^2}} = y\sin\theta, \tag{3}$$

where θ is marked in Figure 1. And by a short computation, the Hamiltonian $H \overset{def}{=} py' - L$ comes out to be

$$H = -\sqrt{y^2-p^2} = -y\cos\theta. \tag{4}$$

Trajectories of the Hamiltonian system, i.e., the level curves of H, are hyperbolas $y^2-p^2=\text{const.}$ (see Figure 2). And Hamilton's equations $y'=H_p$, $p'=-H_y$ are pleasantly simple:[3]

$$y' = -p/H, \quad p' = -y/H. \tag{5}$$

Since $H=\text{const.}$ along solutions, we conclude that $y''=H^{-2}y$. By the symmetry of the boundary conditions (2), $y=y_0\cosh(x/H)$. Setting $x=0$ in the expression for H makes $y=y_0$ and $p\overset{(3)}{=}0$. Consequently, $|H|=y_0$ and thus

$$y = y_0\cosh(x/y_0). \tag{6}$$

Here, y_0 must be chosen so that (2) holds.

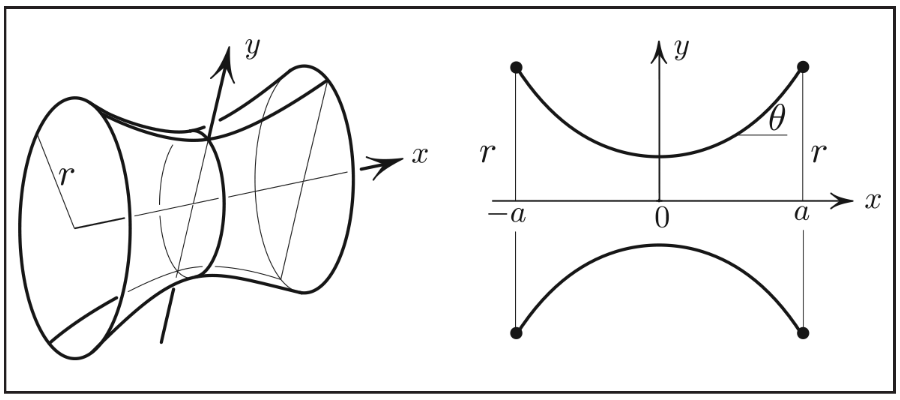

Figure 1. *Soap film — a minimal surface that spans two circular hoops.*

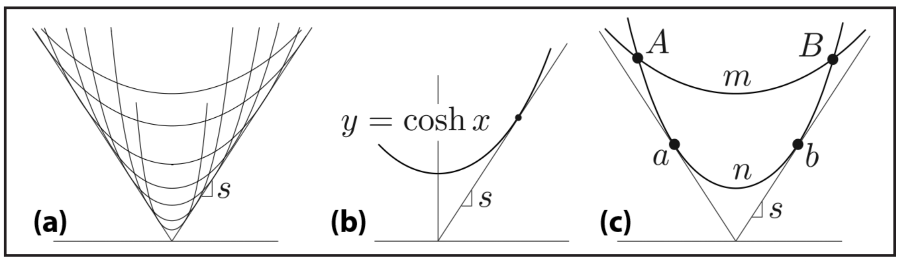

Figure 3. 3a. *Graphs of (6) fill the sector.* **3b.** *The definition of slope $s=\min_{x>0} x^{-1}\cosh x = 1.996\ldots$.* **3c.** *Points A and B satisfy $r/a>s$ and two possible shapes exist for the soap film, but only AmB is stable and physically observable. Both curves AnB and AmB are geodesics in the metric $y\,ds$, but only AnB has a conjugate pair of points a and b. As such, it cannot be minimal; in fact, its Morse index is 1 [1]. In contrast, AmB has no conjugate points and is thus a minimizer of the "length" $\int y\,ds$. The case of $r/a=s$ is critical and unstable, as the two solutions coalesce into a saddle node of potential energy.*

Some Observations

1. *All minimal surfaces spanning two rings are dilations of one another.* This is evident even without (6) from the fact that dilations preserve the property of area minimization.

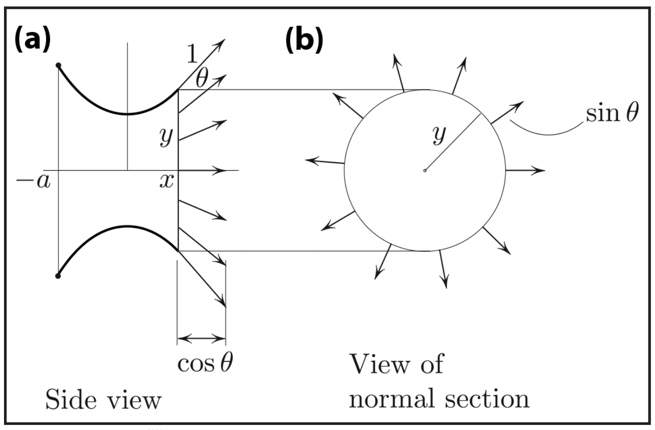

Figure 4. 4a. *H is the horizontal force that acts on any section of the soap "tube," up to a constant factor that depends on the surface tension. $H=\text{const.}$ as a function of x is the consequence of Newton's first law.* **4b.** *Here, $y\sin\theta=p$ is the cumulative force on a portion of the tube that acts in the plane of the section.*

2. *If the rings are spread too far apart for fixed r, the soap film will snap.* How far is too far? The graphs of (6) fill the sector $y\geq s|x|$, where $s=1.996\ldots$ is the slope of the line through the origin tangent to the graph of $y=\cosh x$ (see Figure 3b). A soap film can therefore span two rings iff $r/a\geq s\approx 2$. The maximal possible distance between the rings is almost equal to their diameter!

3. *Two critical functions of (1) exist if $r/a>s$ in Figure 3.* However, only one is physically realizable (the other is unstable). If we had somehow managed to give the film an initial shape that was close to AnB, it would either snap to AmB or pinch off.

4. Equilibrium shapes are geodesics in the metric $y\,ds$, and we can think of them as rays of light propagating through the medium with the speed of light $c=1/y$. Indeed, the travel time for the light is $\int dt = \int ds/c = \int y\,ds$ — the same expression as the area in (1). So the area can be interpreted as either the potential energy of the film or as the travel time in the artificial optical medium.

5. More generally, if (1) is replaced by $\int_a^b F(y)\,ds$, then the corresponding Hamiltonian becomes $H=F(y)\cos\theta$ and the momentum is $p=F(y)\sin\theta$.

Physical Meaning of *H* and *p*

In dynamics, H and p are the energy and momentum. But in our static problem where x is the static counterpart of time, the meanings of H and p are different; instead, they are the forces that are described in the caption of Figure 4.

A Geometrical Interpretation of *H* and *p*

Figure 5a depicts an alternative interpretation of H and p (here, $y(x)$ is any function). In Figure 5b, y is of the form (6); as F slides along the x-axis, the length $|FR|=\text{const.}$ and the velocity of R points at F (proving the latter is left as a challenge).

The figures in this article were provided by the author.

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[1] Levi, M. (2014). *Classical mechanics with calculus of variations and optimal control: An intuitive introduction*. In *Student mathematical library* (Vol. 69). Providence, RI: American Mathematical Society.

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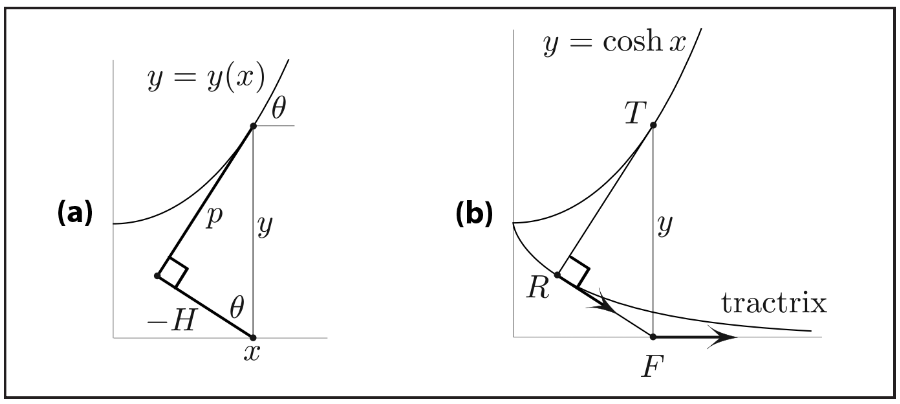

Figure 5. 5a. *Geometrical meaning of the momentum and the Hamiltonian.* **5b.** *The moving segment RF of constant length $|H|$ is a "bike" whose "front wheel" F follows the x-axis; the velocity of the "rear wheel" R is aligned with the segment RF and follows a tractrix, the involute of the catenary.*

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[1] Surface tension is the force that is applied to each side of an incision to hold the slit together per the incision's unit length.

[2] In almost all textbooks, the definitions of p and H are pulled out of thin air, although they do have a very natural and eye-opening motivation [1].

[3] In contrast to the messier Euler-Lagrange equation: $\frac{d}{dx}\frac{yy'}{\sqrt{1+(y')^2}} - \sqrt{1+(y')^2} = 0.$

Wildebeest Self-organization via Active Matter Theory

By Matthew R. Francis

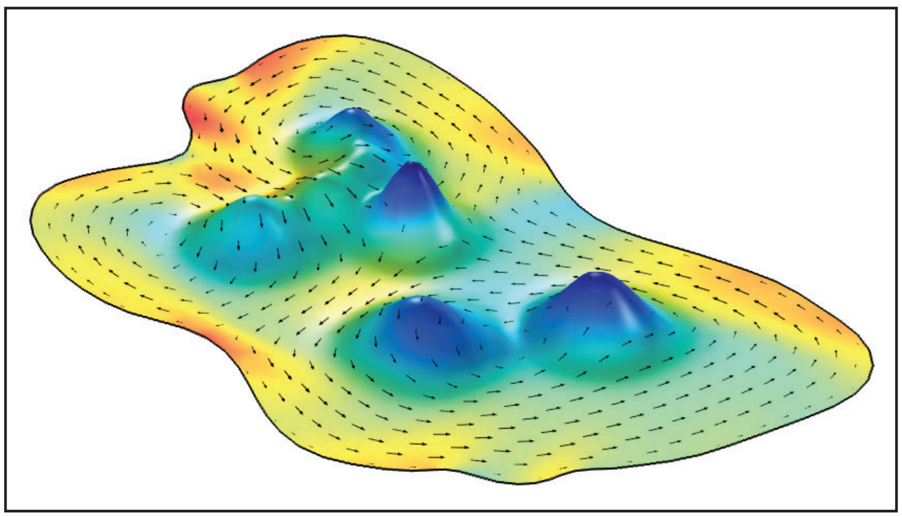

Figure 2. *A surface that was generated via the finite element method to provide topography for a simulated wildebeest herd. The small black arrows indicate the vector field of the wildebeest, illustrating their movement over and around obstacles. Figure courtesy of Christina Hueschen.*

From the motion of molecules over cell membranes to the movement of sheep during sheepdog trials, collective motion across a surface poses a fascinating and difficult set of problems. Unlike flocks of birds in three dimensions or herds on flat plains, groups that are confined to arbitrary, curved, two-dimensional surfaces bring a level of geometrical complexity to the mathematical simulation of flows. The orientation of an animal or molecule is also significant; sheep have heads and tails, for instance, and biological molecules have distinct physical and often electrical polarities.

For arbitrary surfaces, the topology and—more mundanely—the topography affect self-organization in subtle ways. A recent paper in *Physical Review E* approached this general problem in the context of wildebeest herding on various surfaces [1]. The authors had two different goals: (i) Understand the self-organization of actin molecules on the surface of the parasite *Toxoplasma gondii* and (ii) scientifically recreate a famous scene from Disney's *The Lion King*.

"We started with an analogous situation to pipe flow," said Christina Hueschen, a biologist at Stanford University who authored the study with Alexander Dunn and Rob Phillips. "The channel was flat, like the canyon where Scar, the evil uncle [in *The Lion King*], drives the wildebeest down. We put in an obstacle and were excited to see how behaviors differ between this active system compared to a Newtonian fluid, like pipe flow past an obstacle."

To explore this problem, Hueschen and her colleagues treated a single herd of wildebeest—also known as gnu (see Figure 1)—with a nonlinear continuum model for active matter. They drew upon a type of differential geometry and a common numerical method in engineering to extend the theory onto arbitrary curved surfaces for the first time. "We tried to make these different toolkits accessible across fields," Hueschen said. The use of wildebeest as the primary example made the methodology both concrete and eye-catching for other researchers who might not otherwise be inclined to read an article on either subspecialty.

A Gnu Approach to Active Matter

Flocking birds and herding animals have inspired artists and naturalists since antiquity; in fact, some cave paintings might even depict herding behaviors. The theory of active matter, however, is much more recent — in the 1990s, John Toner and Yuhai Tu adapted the widely-used XY model from condensed matter physics to understand flocking and other forms of self-organization [2]. Their approach, which treats polar matter as a nonequilibrium fluid that is dominated by friction and minimal self-interaction, turned out to be extremely applicable to a wide range of phenomena in physics and biology.

The Toner-Tu active matter equations—which govern the density $\rho(\mathbf{r},t)$ and velocity $\mathbf{v}(\mathbf{r},t)$ fields for the wildebeest—are written as

$$\frac{\partial \mathbf{v}}{\partial t} = \beta(v_{\text{pref}}^2 - v^2)\mathbf{v} - \sigma\nabla\rho + D\nabla^2\mathbf{v} - \lambda\mathbf{v}\cdot\nabla\mathbf{v},$$

with parameters $\{\beta,\rho,D,\lambda\}$. The first term ensures that the wildebeest velocities remain close to a preferred speed v_{pref}, which is set by the preferred density ρ_c and an additional parameter α:

$$v_{\text{pref}}^2 = \alpha(\rho - \rho_c)/\beta.$$

The σ term contains the density's gradient and is an effective pressure that prevents wildebeest clumping, while the Laplacian term with D controls diffusion. The last piece, which is parameterized with λ, is a Navier-Stokes advection term; it guarantees that the wildebeest carry the information about their orientation and velocity through the "fluid." Finally, this model assumes wildebeest conservation (i.e., no animals are born or die for the duration of the simulation):

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0.$$

Real-world data from wildlife tracking efforts or microscopy inform both the choice of parameters and the demands of the simulation.

However, analytical solutions of the active matter equations are only possible for certain systems, such as flocking in an empty, geometrically flat space or on highly symmetrical curved surfaces like spheres or cylinders. Real-world surfaces of *Toxoplasma* cells or the Serengeti ecosystem are neither flat nor symmetrical, which limits the application of the Toner-Tu model in its original form.

Hueschen and her colleagues decided to utilize extrinsic differential geometry[1] because their research involves surfaces that are embedded in three-dimensional (3D) space. This method allowed them to project the fully 3D Toner-Tu equations onto the surface of interest with a standard geometrical operator:

$$\hat{P} = I - \mathbf{n}\otimes\mathbf{n},$$

where I is the identity operator and $\mathbf{n}$ is the normal vector at each point on the surface. When the projection operator acts on the velocity vector, it only selects the components that are tangent to the surface:

$$\hat{P}(\mathbf{v}) = \mathbf{v} - \mathbf{n}(\mathbf{n}\cdot\mathbf{v}) = \mathbf{v}^{\parallel}.$$

Extrinsic differential geometry also defines the curved-surface versions of the Toner-Tu model's gradient, Laplacian, and advection terms in a standard way. The projected gradient of the density is relatively simple:

$$\nabla_\Gamma\rho = \hat{P}(\nabla\rho) = \nabla\rho - \mathbf{n}(\mathbf{n}\cdot\nabla\rho),$$

where ∇_Γ denotes the gradient operator that is projected onto the surface. The advection and Laplacian terms are more complicated because they require projection of the velocity vectors and differential operators. For instance, the advection term is most easily expressed in matrix form—using the Einstein summation convention over repeated indices—with Cartesian coordinates:

$$[\nabla_\Gamma\mathbf{v}^{\parallel}]_{ij} = [\hat{P}(\nabla\mathbf{v}^{\parallel})\hat{P}]_{ij} = (\delta_{ik} - n_i n_k)\frac{\partial v_k^{\parallel}}{\partial x_m}(\delta_{mj} - n_m n_j).$$

To further simplify the simulation, the authors employed the finite element method (FEM) to divide the surface into a set of (flat) triangles with a normal vector at each vertex — a common technique in a wide range of engineering and computer graphics applications. "We wanted to use commonly available numerical tools, and the finite element approach allows one to solve any [partial differential equation] at the nodes and then interpolate between," Hueschen said. In other words, formulating the Toner-Tu model with extrinsic differential geometry and FEM turns an analytically intractable problem into one that everyday commercial software can feasibly handle.

All This and Toner-Tu

Hueschen and her collaborators compared their FEM-based numerical algorithms with other scientists' analytical solutions to the Toner-Tu equations for specific geometries, including flat surfaces, cylinders, and spheres. For their *Lion King* simulation, the authors utilized a "racetrack": a flat, rectangular surface with rigid sides and periodic boundary conditions at the ends (analogous to a two-dimensional "pipe"), which matches known active matter solutions. They also demonstrated that their numerical simulations match the analytical results for symmetrical surfaces, including spheres.

With the comparison to established solutions in hand, the researchers then added a single hill to the racetrack to identify potential changes in wildebeest herding behavior. Real herds "scatter" off obstacles by increasing their density on either side of the obstruction and thinning out over hills, or avoiding overly steep inclines entirely (see Figure 2). Although the basic Toner-Tu model does not include gravity—since gravity is not relevant to microscopic examples like molecular self-organization on cell surfaces—the team created a modified version of the equations to represent the way in which herds might account for gravity when encountering hills in the terrain.

But the real power of the advanced Toner-Tu model lies in its versatility. "We reformulated these Toner-Tu flocking equations into a general curved surface form that is solvable as long as one has any surface where the normal vectors are defined," Hueschen said. "You don't need a parameterization or coordinate system. In two minutes, you can plug in a new geometry and resolve the equations on the hilly Serengeti or a weird banana shape."

The need to define normal vectors does somewhat limit the methodology, as it cannot handle especially complicated surfaces without some initial smoothing. Yet despite the current focus on the wildebeest example, the toolkit is still quite powerful and general. This flexibility is important because the researchers were primarily interested in actin molecules' ability to self-organize on the very complex surfaces of *Toxoplasma* cells — knowledge that is potentially useful when modeling the way in which these parasites infect mammal brains. Other examples of biological self-organization include cell motion on the surface of embryos and cytoskeleton patterns that give cells their shapes, neither of which exhibit strong geometrical symmetries.

Despite the complicated mathematics, Hueschen emphasized how much fun she and her colleagues had while working on this problem. "There was sort of an element of joy the whole time," she said. Delight is never a bad thing when exploring new (or *gnu*) methodologies.

Figure 1. *A blue wildebeest—a large African herbivore that lives in herds that might stretch for many kilometers—at the Ngorongoro Crater in Tanzania. Figure courtesy of Muhammad Mahdi Karim via Wikimedia Commons.*

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[1] As opposed to the intrinsic differential geometry of manifolds, which defines arbitrary curved surfaces or other spaces without embedding them in a higher-dimensional space.

References

[1] Hueschen, C.L., Dunn, A.R., & Phillips, R. (2023). Wildebeest herds on rolling hills: Flocking on arbitrary curved surfaces. *Phys. Rev. E*, *108*, 024610.

[2] Toner, J., & Tu, Y. (1995). Long-range order in a two-dimensional dynamical XY model: How birds fly together. *Phys. Rev. Lett.*, *75*(23), 4326.

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

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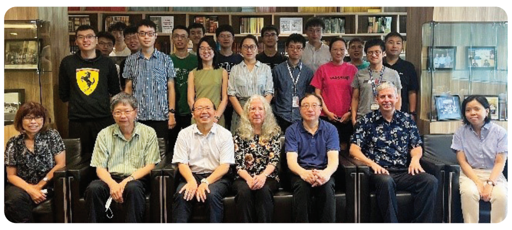

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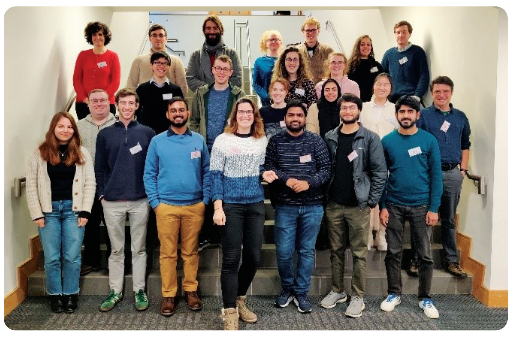

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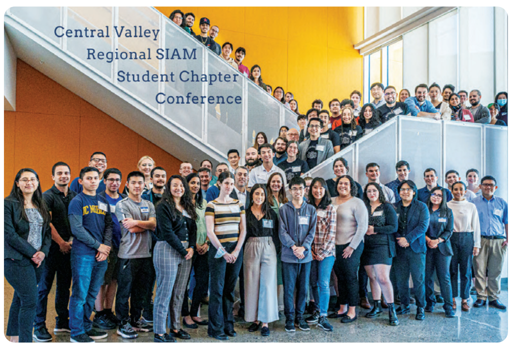

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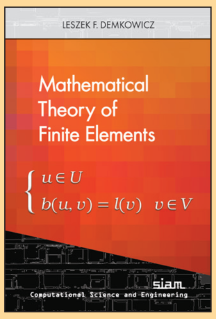

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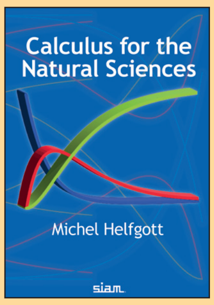

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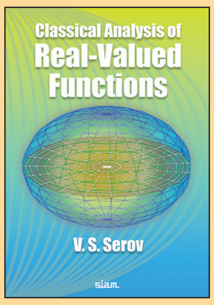

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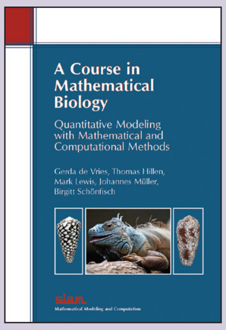

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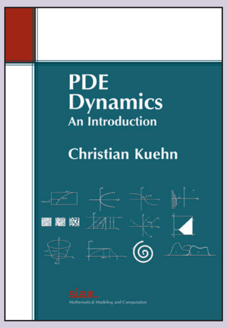

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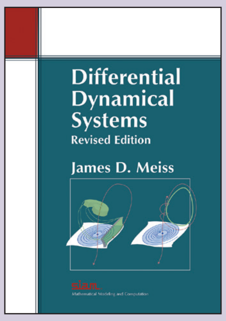

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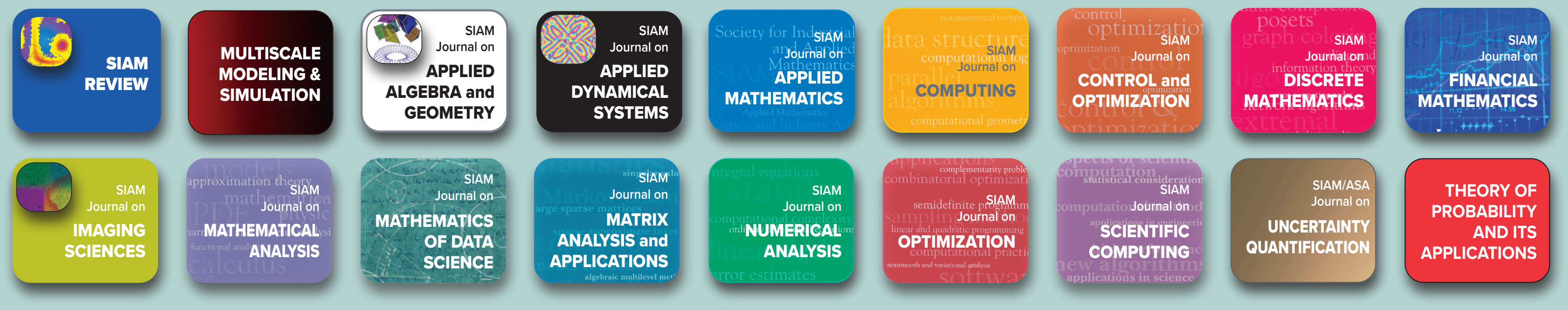

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