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Theory Guides the Frontiers of Large Generative Models

By Manuchehr Aminian

Modern generative machine learning (ML) and artificial intelligence (AI) models are large in every sense of the word. For example, OpenAI's Generative Pre-trained Transformer 3 (GPT-3) language model from 2020 contains 175 billion trainable parameters. The 2023 GPT-4 model cost at least \$100 million to train [3], with more opaque but similarly important energy costs. Although it is difficult to measure the scope of data that trains such models—as well as any associated ethical and legal issues—their collective significance is evident in multiple high-profile lawsuits that have followed the models' commercialization [1].

While these models are data hungry, they may no longer be data bottlenecked. In 2022, a Google DeepMind group observed that the "compute budget" (aggregate floating-point operations) yields a linear tradeoff between the selection of "more data" versus "more parameters" in frontier models [2]. The team harnessed this observation to train a smaller model named Chinchilla that was competitive with large language models (LLMs) like Gopher and GPT-3. And earlier this year, the language model DeepSeek-R1 caused waves in the AI community for being open weight and having a parameter count that is

several scales smaller than GPT-4 — making it less expensive to query and fine-tune while exhibiting a similar performance.

How do we begin to comprehend this paradigm? A guiding principle of scientific computing is that the incorporation of domain-specific knowledge can accelerate a model. Landmark algorithms of the 20th century, such as the fast Fourier transform and fast multipole method, follow this prin-

ciple by exploiting additional properties of the class of problems to accelerate naive computation in applications such as density functional theory or n-body problems. These accelerations are transformative in science and engineering and have facilitated the solvability of many intractable real-life scenarios. A persistent quest for applied mathematicians in ML is to understand the feasibility of similar breakthroughs.

Theory Versus Practice for Optimization in Machine Learning

Courtney Paquette of McGill University and Google Research explored this topic during her CAIMS/SCMAI-PIMS Early Career Award Lecture¹ at the Third Joint

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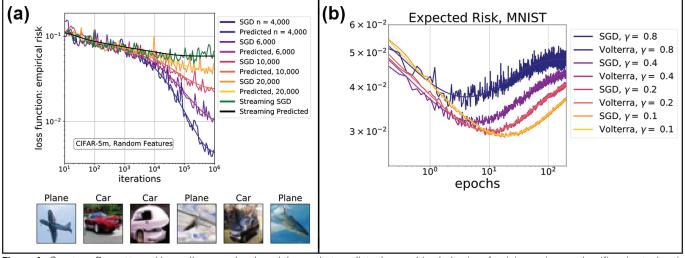


Figure 1. Courtney Paquette and her colleagues developed theory that predicts the resulting behavior of training an image classifier via stochastic gradient descent (SGD). The observed "risk"—a normed residual on unseen data—is tracked closely by an a priori calculation that pertains to the spectrum of Hessian matrix $H = X^T X$. 1a. Theoretical predictions match the loss on varying training data sizes n on the CIFAR-5m dataset. 1b. Similar agreement occurs for different learning rates γ when one conducts training on the Modified National Institute of Standards and Technology database (MNIST) dataset. Figure courtesy of Courtney Paquette; Figure 1b adapted from [5].

Active Hydraulics as Analog Computers to Solve Complex Problems

By Matthew R. Francis

M athematical models for complicated physical systems rarely have exact solutions. In turn, models that *do* have exact solutions often fail to quantitatively describe real-world phenomena, though they may sometimes provide qualitative insights that facilitate the construction of more realistic theories.

Now, a new set of active matter experiments have matched an exact solution for a particular system known as the *six-vertex* or *ice-type model*. Researchers previously used this model—which dates back to the 1930s and was solved in the 1960s—in a wide range of applications, none of which explicitly matched the precise solution to the equations. However, physicists Camille Jorge and Denis Bartolo of the University of Lyon in France recently found that tiny beads in a square grid of tubes behave spe-

cifically and quantitatively as predicted by the six-vertex model's solution [3].

Unlike typical physics models where particles only act under external forces, an active matter framework allows the basic agents to move on their own. For this reason, active matter research has found applications in flocking animals [2], tangling proteins, and nonequilibrium systems for which Newtonian physics descriptions are too unwieldy.

Bartolo and his collaborators developed a form of active matter that they call *active hydraulics*: plastic particles that move at a constant velocity without being driven by fluid pressure. The direction of motion is entirely determined by local conditions, which are themselves set by surrounding particles in the fluid. The particles collectively and spontaneously form currents inside tubes based on the tubes' configurations, which prompts the active hydraulic

system to "solve" the six-vertex model within tubes that form a square lattice.

This finding has important implications for the description and control of other active matter systems, including organisms like bacteria, artificial particles for drug delivery, and microrobotics. It also serves as a strong demonstration of active matter's usefulness as a kind of analog computer. The creation of different lattice configurations or introduction of biases in particle motion could potentially simulate many types of systems in statistical physics, materials science, and mathematical biology — ultimately providing a set of tools beyond computer models for complex systems.

"We didn't intend to look at the sixvertex model," Jorge said, noting that the experiment offers hints about how to reverse engineer solutions for more sophisticated models. "Maybe it's a new, easier way to do physics — not starting from the very fundamental basics of physics, but just trying to have a broad description that captures the essence of the phenomenon."

The Six-vertex Model

The six-vertex model is based on Nobel Prize-winning chemist Linus Pauling's attempts to understand the structure of water ice [5]. By the 1930s, experiments revealed that the oxygen atoms in ice form a variety of tetrahedral structures, with hexagonal rings of molecules in two of the dimensions. However, the crystallographic methods of the time were unable to determine the positioning of the hydrogen atoms. Pauling realized that he could model the structure by linking each

See Active Hydraulics on page 4

1 This is technically known as a "wurtz-ite" (vurt-zite) configuration, though so much space is present inside the crystal structure of ice that the solid form of water is less dense than the liquid form. Most other materials are denser when solid

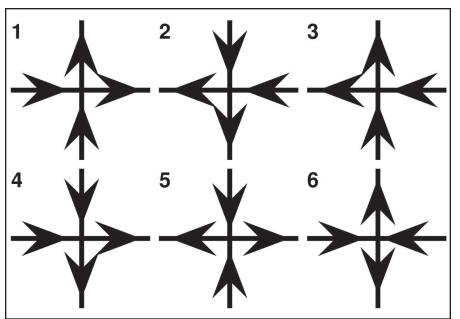


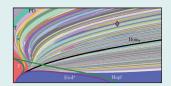
Figure 1. Possible vertices in the six-vertex or ice-type model; arrows indicate the direction of a hydrogen bond between molecules or the flow of plastic particles. Each pair of vertices in sequence is symmetrical under a mirror reversal along a diagonal and thus energetically equivalent in the absence of external influence. Figure courtesy of Matthew Francis.

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- Group Science: The Open Source Study of Higherorder Networks With XGI In recent years, new software packages have materialized to handle the demands of higher-order network science. Nicholas Landry and Laurent Hébert-Dufresne introduce the CompleX Group Interactions (XGI) package, which offers a suite of analytical tools, seamless integration with large-scale datasets, and extensive tutorials and documentation for higher-
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and corresponding eigenfunc-

tions highlight these macro-

phenomena, including their

appearance and disappearance.

11 OpenAI: Extraordinary Accomplishments, but at What Cost?

Investigative reporter Karen Hao has spent the last five years examining the inner workings of OpenAI, its competition, and its impact on the outside world. Her new book, Empire of AI: Dreams and Nightmares in Sam Altman's OpenAI, provides a detailed account of OpenAI's explosive growth and questionable office politics. Ernest Davis reviews the exhaustive text.

Amplifying Researchers' Voices in U.S. Science Policymaking

By Jillian Kunze

7 025 has seen sweeping changes to the funding and priority landscape for U.S. science. Executive orders have fueled uncertainty across a variety of research disciplines, and ongoing court challenges leave many questions unresolved. Policy shifts, reductions in force, and funding issues continue to impact federal scientific agencies. Furthermore, as some research areas are facing disruptions, others are experiencing newfound levels of attention. Amidst all of this chaos, many members of the research community are struggling to determine where they stand and how they can make meaningful contributions to policy dialogues.

During the Third Joint SIAM/CAIMS Annual Meetings¹ (AN25), which took place this summer in Montréal, Québec, Canada, a special session² offered an overview of current and anticipated changes in U.S. science policy and outlined opportunities for researchers to get involved. SIAM Vice President for Science Policy Alejandro Aceves of Southern Methodist University and SIAM Chief Executive Officer Suzanne Weekes organized the event, alongside several of the speakers. The session commenced with presentations about the current federal situation from Miriam Quintal and Kiana Newman of Lewis-Burke Associates LLC,³ SIAM's government relations partner in Washington, D.C. Sharon Crook of Arizona State University then chaired a panel that featured three applied mathematicians with science policy experience: Jonas Actor of Sandia National Laboratories, Emily Evans of Brigham Young University, and Rachel Levy of North Carolina State University.

SIAM has contracted with Lewis-Burke since 2001 as the Society's first point of advocacy to advance the applied mathematics community's interests in terms of funding, policymaking, and emerging programs and initiatives. Lewis-Burke coordinates with the SIAM Committee on Science Policy⁴ (CSP) and the SIAM Science Policy Fellowship Program,⁵ the latter of which provides an opportunity for postdoctoral fellows and early-career researchers to gain hands-on experience with U.S.-based advocacy and policymaking. Twice a year, Lewis-Burke representatives, CSP members, and SIAM Science Policy Fellows gather in Washington, D.C., to interact with congressional representa-

- https://www.siam.org/conferences-events/ past-event-archive/an25
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A special session at the Third Joint SIAM/CAIMS Annual Meetings—which were held in Montréal, Québec, Canada, this summer-addressed the current climate for science policy and detailed opportunities for community involvement. From left to right: presenters and organizers Jonas Actor of Sandia National Laboratories, Miriam Quintal and Kiana Newman of Lewis-Burke Associates LLC, Rachel Levy of North Carolina State University, Sharon Crook of Arizona State University, SIAM Chief Executive Officer Suzanne Weekes, and Emily Evans of Brigham Young University. SIAM photo.

tives and federal agency officers. These biannual meetings allow members of the SIAM community to advocate for important funding, learn about agency priorities, and provide feedback to lawmakers.

Current Federal Priorities That Affect the SIAM Community

Quintal kicked off the AN25 session with a primer on recent updates in federal science policy that may impact researchers in applied mathematics, computational science, and data science. Despite the current turbulence, she affirmed that there are still ways to advocate for the SIAM community's priorities. "It really does matter to make your voices heard and talk to your lawmakers," Quintal said.

One can understand the present federal science policy situation based on several categories: executive orders and court challenges; changes to federal agency policies and personnel; and the reconciliation, budget, and appropriations processes [2, 4]. While the Trump administration has deemphasized certain scientific interestslike climate change, infectious diseases, and social justice—other research areas have gained additional enthusiasm, such as artificial intelligence (AI), quantum computing, and nuclear energy. All of these research priorities are now generally situated in the context of global competitiveness and national security; of course, they are not spared from the reality of reduced federal funding as a whole.

The current administration's interest in AI is particularly strong, with the recent publication of an AI Action Plan⁶ that outlines priorities for innovation and infrastructure development. "There is a real interest in partnerships between academia and industry," Quintal said, noting the existence of opportunity spaces for the use

6 https://www.ai.gov/action-plan

K. Burke, University of California, Davis, USA Financial Mathematics and Engineering L. Veraart, London School of Economics, UK Geometric Design

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of AI and computational tools in education and government settings. Concurrent to ongoing challenges for higher education institutions, the federal administration is promoting apprenticeships, internships, and accreditation programs — particularly those that pertain to AI.

In terms of federal agencies, the U.S. National Science Foundation along with health agencies like the U.S. National Institutes of Health and the Centers for Disease Control and Prevention have experienced a deluge of freezes, award cuts, staff reductions, reorganizations, and priority changes, with more uncertainty likely to come. The Department of Energy (DOE) seems to be faring comparatively well, with approximately flat funding set aside for the Advanced Scientific Computing Research⁷ program and ample support for AI and quantum research, though it has faced its own version of challenges such as staff departures. And while the research arm of the Department of Defense is currently in a somewhat steady state, it could undergo more scrutiny in the future.

What Does Science Advocacy Involve?

In the next segment of the AN25 session, Newman discussed effective ways to advocate for scientific priorities. She detailed Lewis-Burke's engagement in the discourse around scientific funding and other relevant policy areas-such as immigration and taxation—to uplift certain priorities, promote higher toplines for specific programs, and enable the exchange of knowledge and expertise. "It is important for our community to be at that table and express areas that we are in line with or disagreement with," Newman said.

At the individual level, advocacy does not necessarily have to involve a trip to Capitol Hill. Any form of engagement is valuable, including participating in local town halls and community groups or coordinating with university government relations personnel. Even calling or sending a personal email to a local, state, or federal representative can be effectual. These messages allow policymakers to understand the impacts of their decisions within their own community and react appropriately. Politicians do have a responsibility to the needs of their districts (and often a goal of re-election), so there is certainly an impetus for them to listen to and address their constituents' concerns.

Researchers can offer lawmakers a unique value proposition by providing a technical basis for the soundness of potential policy decisions. Furthermore, delivering positive feedback on beneficial programs and

See Science Policymaking on page 5

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Large Generative Models

Continued from page 1

SIAM-CAIMS Annual Meetings² (AN25), which took place this summer in Montréal, Québec, Canada. Paquette's talk focused on her efforts to predict the behavior of large models that are trained via stochastic gradient descent (SGD). While her work may be classified as optimization theory, there are important distinctions. Paquette argues that mathematicians in this area of research need to understand the way in which traditional optimization theory contrasts with practical ML. In practice, noise is everywhere; training data have sources of noise or measurement error, initialization for iterative schemes that optimize parameter sets θ usually start with randomly initialized weights θ_0 , and the iterations often involve random sampling of the training data (as with SGD).

The *stochasticity* in SGD refers to this random sampling to evaluate the gradient of the objective function that updates θ_k :

$$\theta_{k+1} = \theta_k - \gamma \frac{\sum_{i \in \mathcal{B}_k} \nabla f_i(\theta_k)}{\beta}. \quad (1)$$

Here, $\gamma>0$ is the chosen stepsize (i.e., learning rate) and \mathcal{B}_k is the subset of the training data that is selected at each step. Choosing the sample size $\beta \!=\! |\mathcal{B}_k| \!=\! 1$ is called *streaming SGD*; if one opts to use all data at each step, then $\beta \!=\! n$ reduces to traditional gradient descent of a loss that is summed over the losses of each datum: $f(\theta) \!=\! \frac{1}{m} \sum_{i=1}^m f_i(\theta)$. To develop theory, Paquette and her

To develop theory, Paquette and her collaborators focus on the following loss function that corresponds to linear regression: given data $x_i \in \mathbb{R}^n$ (arranged as rows in matrix $X \in \mathbb{R}^{m \times n}$) and associated scalar output $b_i \in \mathbb{R}$, find parameter vector $\theta \in \mathbb{R}^n$ for which the loss $\frac{1}{2m}||X\theta-b||^2=\frac{1}{2m}\sum_{i=1}^m(x_i^T\theta-b_i)^2$ is minimized. While readers may recognize that the exact solution is $\theta^*=(X^TX)^{-1}X^Tb$ with mild assumptions on X, the purpose of Paquette's work is not to find a closed-form expression, but to understand the behavior of iterates θ_k in a way that can be generalized to predict SGD behavior in more complicated settings.

Often, researchers conduct this analysis by taking a limit of $\gamma \rightarrow 0$, which reduces (1) to a gradient flow. One of the novelties of Paquette's work [4] follows the infinite data paradigm, which keeps γ finite and instead studies a stochastic process over a long training sequence. This process occurs by taking a joint limit $n \to \infty$ and $d \to \infty$, with $d/n \rightarrow r$: a ratio of model parameters d to training data n. Paquette and her collaborators achieve this by embedding the discrete process of $k \in \{0,1,...\}$ into a continuous-time stochastic process with $t \in \mathbb{R}^+$; they can then analyze the stochastic process through its low-order moments via the so-called "universality" properties of random matrix theory. The chief result is that in this setting and with some additional

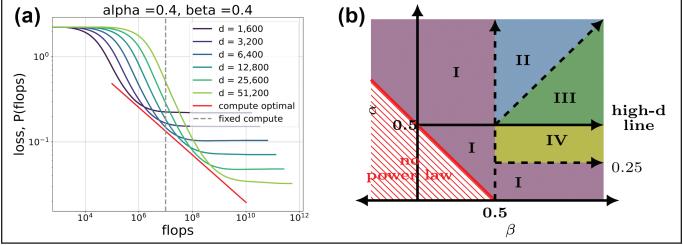


Figure 3. Given a mathematical model of a training process with controllable parameters α and β and model size d, a linear power law frontier exists between the loss and flops (compute) that enables the analysis of several "phases" of behavior. 3a. Varying loss curves under model capacity determine the compute-optimal curve. 3b. Phase diagram of different asymptotic behaviors. Figure adapted from [6] and courtesy of Courtney Paquette.

assumptions, the SGD iterates converge to a scalar function P(t):

$$\mathcal{P}(t) = \mathcal{P}(\Theta_{\gamma t}^{\mathrm{gf}}) + \int_0^t \gamma^2 h_2(t, s) \mathcal{P}(s) ds,$$

$$h_2(t, s) = \int_0^\infty x^2 e^{-2\gamma t x} d\mu(x).$$

Paquette describes $\mathscr{F}(\Theta^{\mathrm{gf}}_{\gamma t})$ as the $gradient\ flow\ process$. The measure $d\mu(x)$ is the spectrum of H, the Hessian of the objective and the data-generating process — which could be an exotic object in general. But when dealing with finite data, this spectrum is a sum of point masses at eigenvalues: $d\mu(x) = \frac{1}{d} \sum_{i=1}^d \delta(x-\lambda_i)$. Additionally, the integral reduces to a sum over the eigenvalues of H. In the case of a linear least squares problem, this Hessian is $H = X^T X$, or the squared singular values of the data matrix X.

To summarize, Paquette's recipe for an a priori prediction of the loss curve is to first estimate the eigenvalues of X^TX , then solve the scalar integral equation (2) in any fashion. Curves such as those in Figure 1 (on page 1) result. While computing the spectrum of X^TX can be challenging, approaches for (i) updating the spectrum with streaming data or (ii) using the spectrum's asymptotic behavior when X is the result of a known data generating process may improve the outlook. For example, the Marchenko-Pastur distribution is the limiting measure for data that is sampled independently from a process with fixed, finite variance, which yields useful analytical results.

Paquette confirmed that this theory matches well in practical settings, as evidenced in Figure 1 (on page 1) for varying dataset sizes and learning rates γ . She sees good agreement in theoretical loss curves with realized results over a wide range of finite data sizes.

Compute Efficiency and Compute Optimality

Predicting the loss curves of an SGD-trained model may seem like a cute parlor trick, but this approach to theory can provide useful guidance before the start of the training process. By embedding the training process into a stochastic process, Paquette's work assists with an intelligent choice of stepsize:

$$\gamma_* = \left(\frac{r}{2} \int_0^\infty \frac{x^2}{x - \lambda_{\min}} d\mu(x)\right)^{-1},$$

which depends on the minimal Hessian eigenvalue λ^- . Figure 2 illustrates this outcome for the so-called *isotropic features model* by sampling various values of r and learning rate γ . For a range of values r, the convergence rate for prescribed γ^* (gray solid line) is reasonably close to a choice that provides an optimal convergence rate; stepsizes that are far from optimal may result in no convergence at all. The overparameterized regime where r > 1 exhibits increasingly narrow bands of stepsizes that predict any type of convergence; here, γ^* is particularly useful.

What about the notion of training optimization on a fixed compute budget? During her AN25 lecture, Paquette explained some key points of her work to analyze a minimal mathematical training model that incorporates data complexity α , target complexity β , and parameter count d to analyze a one-pass SGD training process [6]. She and her colleagues represent compute cost as a simple product flops = kd—where k is the number of iterations of the optimization algorithm and d is the number of model parameters and perform an experiment that runs SGD for k iterations with varying d. Plotting loss as a function of flops rather than iterations generates a family of parameterized curves (see Figure 3). With fixed d, the use of compute (flops) past a certain turning point yields diminishing returns. This result occurs at various compute levels, as smaller models utilize fewer flops per iteration. If a practitioner has a sense of α and β for their training data, they can decide on the model size d that is appropriate for their compute budget. And if one can adaptively expand their model size d, they may schedule a growing d—i.e., a dynamically expanding model—such that a minimal number of flops can achieve a given loss by targeting and remaining near the training frontier. Figure 3b illustrates the complexity and research opportunities of even a simple model when capturing different types of behavior.

Many scientists feel that we are at a critical juncture of math, science, and society when it comes to the development of LLMs and other generative tools. The continued improvement of large models is reach-

ing a point of diminishing returns, where the thoughtless approach of "more data, more parameters, more compute" will soon become prohibitively expensive. Regardless of the prospective impact of AI, mathematical theory will retain its important role in this space to help us understand the data and energy efficiency of such models. While theory largely pertains to least squares problems—a far cry from the highly nonlinear models in practice—Paquette affirms that this area of research is surprisingly applicable. Despite the remaining mysteries that surround the success of large generative models, this kind of theory provides a solid ground as the field continues to advance.

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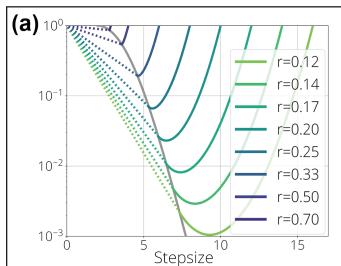
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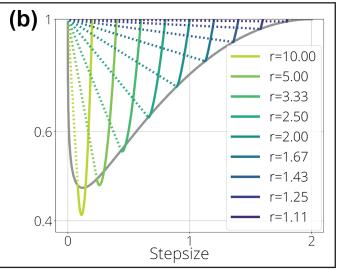


Figure 2. Average-case convergence rates as a function of stochastic gradient descent with stepsize γ in two regimes of r = d/n. 2a. Given underparameterized models when 0 < r < 1, a broad range of stepsizes result in fast convergence during training. 2b. In the overparameterized regime, the intervals of stepsize for which convergence is achieved are progressively narrow with increasing r. Figure adapted from [4] and courtesy of Courtney Paquette.

² https://www.siam.org/conferences-events/past-event-archive/an25

Career Opportunities Panel at AN25 Compares Employment Experiences Within and Beyond Academia

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By Lina Sorg

As graduate students and junior researchers prepare to enter the workforce, they face numerous decisions about the direction of their future employment. Some may wish to embark on tenure-track academic careers, while others might be drawn to opportunities in industry, government, or the U.S. Department of Energy's 17 National Laboratories. Given the versatility of a science, technology, engineering, and mathematics (STEM) education, there is no single path to success.

During the Third Joint SIAM/CAIMS Annual Meetings,² which took place this summer in Montréal, Québec, Canada, a comprehensive panel discussion³ explored the myriad career options that are available to applied mathematicians, computational scientists, and data scientists. The

- 1 https://www.energy.gov/national-lab
- ² https://www.siam.org/conferences-events/past-event-archive/an25
- https://meetings.siam.org/sess/dsp_programsess.cfm?SESSIONCODE=85664

panel, which was sponsored by SIAM's Career Opportunities Committee⁴ and chaired by Jason Torchinsky of Sandia National Laboratories,⁵ featured Jonas Actor of Sandia, Dhavide Aruliah of MKDA Consulting, Heather Zinn Brooks of Harvey Mudd College, Sigal Gottlieb of the University of Massachusetts (UMass) Dartmouth, and Anders Petersson of

Lawrence Livermore National Laboratory.⁶ Throughout the session, the speakers reflected on their individual trajectories, shared personal observations, and fielded questions from the audience.

As the conversation commenced, each speaker summarized the experiences that led to their current roles. Aruliah earned a B.Sc. and M.Sc. in mathematics and a Ph.D. in computer science, then completed two postdoctoral placements before join-

- 4 https://www.siam.org/get-involved/ connect-with-a-community/committees/careeropportunities-committee
 - https://www.sandia.gov
 - 6 https://www.llnl.gov

ing the faculty at the University of Ontario Institute of Technology. Although he went on to receive tenure and was eligible for full professorship, he chose to leave academia in favor of industry because he did not feel comfortable counseling students about industry-based careers without having experienced one himself. Aruliah worked remotely for several different companies

before ultimately founding MKDA Consulting.

Next, Petersson overviewed the path that led him to the national labs. He obtained a master's degree and Ph.D. in his home

country of Sweden, then moved to the U.S. to conduct postdoctoral research at Los Alamos National Laboratory⁷ and the University of California, Los Angeles. Petersson briefly returned to Sweden as a faculty member at Chalmers University of Technology, where he studied fluid mechanics applications for a few years before switching to industry. When he

7 https://www.lanl.gov

eventually received a call from a colleague about a job opening at Lawrence Livermore back in the U.S., he accepted the position and has been at the lab for the past 26 years.

Gottlieb earned her Ph.D. from Brown University, after which she remained at Brown for a year as a postdoctoral researcher and then joined UMass Dartmouth as an assistant professor. More than 25 years later, she is now the university's Chancellor Professor of Mathematics. "In many senses, I'm not working in the same place because it's changed so much," she said, explaining that she has helped establish new graduate programs and launch the Center for Scientific Computing and Data Science Research.⁸

Actor, who is currently a Senior Member of Technical Staff at Sandia, holds an M.A. and Ph.D. in computational and applied mathematics. Much of his graduate work focused on the interdisciplinary side of bioinformatics and data science, and he was ultimately drawn to the national laboratories by the prospect of building machine

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8 https://www.cscdr.umassd.edu

Active Hydraulics

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oxygen atom with four hydrogen atoms: two with tight molecular bonds to create H_2O , and two with looser hydrogen bonds to assemble the entire crystal structure. He speculated that doing so would explain some of ice's stranger properties.

Although this six-vertex model did not actually explain ice particularly well on a quantitative level, flattening the three-dimensional lattice to form a system of square cells (like graph paper) yielded a mathematical description with an exact solution. In this model, each intersection in the lattice has two arrows that point towards the intersection and two that point outwards — leading to six possible configurations (see Figure 1, on page 1). As an aside, the arrows in Pauling's original version pointed from the oxygen atom towards the hydrogen atom in a neighboring H₂O molecule.

The system is described by its partition function

$$Z = \sum_{k} \exp(-E_k/k_B T),$$

where $k_{\!\scriptscriptstyle B}$ is the Boltzmann constant, T is temperature, and

$$E_k = \sum_{i=1}^6 n_{i,k} \epsilon_i$$

is the energy for each possible configuration. Here, $n_{i,k}$ is the number of vertices in the lattice and ϵ_i is the energy of each vertex type. One can set the energy of each state for ice itself equal to zero, so Z simply tallies all of the possible configurations in the lattice. The antiferroelectric state—which exhibits a local electric field even in the absence of an external field, with electric polarization alternating between adjacent sites in a lattice—is denoted by

$$\epsilon_1\!=\!\epsilon_2\!=\!\epsilon_3\!=\!\epsilon_4\!>\!0 \ \ \text{and} \ \ \epsilon_5\!=\!\epsilon_6\!=\!0,$$

such that vertex types 5 and 6 are preferred energetically. The six-vertex model can thus describe the phase transition between a disordered state and an antiferroelectric state, among other systems.

Spinning Fluids Got to Go 'Round

On the experimental side, Bartolo's laboratory previously developed a type of active matter that was meant to resolve a common problem in these systems. For most varieties of active matter, self-organization often arises via collisions or other local interac-

tions that are difficult to model, leaving only macroscopic heuristic descriptions. The researchers surmounted this difficulty by exploiting an obscure electromagnetic effect that was originally described by Georg Hermann Quincke in the 19th century.

Quincke discovered that nonconducting spheres (e.g., made of glass or plastic) rotate at a fixed rate in a uniform electric field. As such, Bartolo and his colleagues placed tiny Plexiglas beads—which they dubbed "Quincke rollers"—between horizontal glass plates and applied a vertical electric field, which caused the beads to roll along the bottom plate at a constant velocity but in a random direction [1]. "In a straight pipe, the liquid has to flow because of the activity," Jorge said. "It's a spontaneous symmetry breaking. The liquid can flow from the left to the right or the right to the left without applying any pressure."

With these initial results in hand, Jorge and Bartolo built a square lattice of pipes. For ordinary fluids, it would be impossible to maintain a steady velocity through any part of this configuration. However, the spontaneous motion of the Quincke rollers allowed the researchers to execute an entirely new class of experiments with several profound results.

"When we [performed] the experiment, we had a constant magnitude of the current," Jorge said. The current maintained the same magnitude of $J_0 \approx 1,300$ particles/second in each segment of the lattice — an effective quantization of the fluid motion that can be represented mathematically as a spin. "When we put all these spins on a map, we had two arrows in and two out at each node of the network," Jorge continued. "We immediately recognized the six-vertex model from our physics background."

The flow of the active hydraulic particles was steady but did not have a defined order. However, the team found that the six vertex types are not equally likely to appear, even though they are all energetically equivalent; types 5 and 6 (where currents flow head-to-head into a junction) were roughly half as likely to occur as the configurations where currents flow through the junction in a straight line. Placing cylindrical posts in the centers of the junctions enabled the experimenters to change the system's effective energy configuration. They induced a phase transition as a function of the post radius; at larger radii, the 5th and 6th junc-

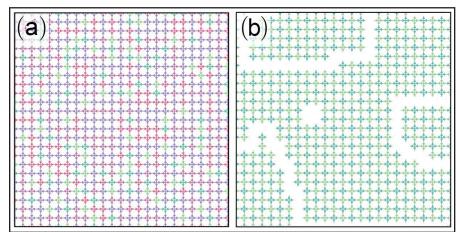


Figure 2. Placing posts in the middle of each junction changes the flow of the active hydraulic particles from random (2a) to something that is analogous to an antiferroelectric system, with clearly defined domains (2b). Figure adapted from [3].

tion types came to dominate the others, simulating a phase transition that is evident in six-junction models for antiferroelectric materials (see Figure 2).

In this completely ordered phase, the current only flows in closed loops, forming a self-similar pattern across scales — that is, a fractal. All of these results exactly match the six-vertex model's predictions, which no other experiments have replicated as precisely. The implications are noteworthy.

Four Rules for Active Hydraulics

Because the square lattice is a simple configuration, the six-vertex model and related models are able to exhibit exact solutions. Jorge, Bartolo, and their colleagues have already investigated the use of active hydraulics on more complex two-dimensional geometries [4], but the main value of these experiments stems from the resulting general principles.

For instance, a hexagonal (honeycomb) lattice consists of three—rather than four—pipes that are attached to each vertex. To satisfy mass conservation under a steady flow, some segments have no net current (any local motion averages to zero across the whole segment), thus creating more complicated configurations than in the square lattice instance. Even more elaborate behavior arises in triangular lattices, for instance, where six pipes enter each vertex.

Jorge and Bartolo identified four rules to help scientists understand active hydraulics in more complicated geometries.

- 1. Mass is conserved so that all of the current that flows into a junction will flow out again: $\sum J_{h} = 0$.
- 2. The current is quantized, which means that it can be represented as $0, +J_0$, or $-J_0$ depending on the direction at which it flows into a junction.

- 3. The system's phase is defined by the relative weight of each junction diagram, as in the six-vertex model.
- 4. If more than four pipes meet at a vertex, the geometry of the junction shapes the possible current configurations. For instance, a 32-vertex model—which offers many possible ways for the active fluid to enter and leave each junction, as well as zero-current segments—describes the triangular lattice.

In principle, these rules should apply to any lattice system. Since only a few models of this type have exact mathematical solutions, similar experiments could potentially provide a new technique for "calculating" solutions that would otherwise require approximate or numerical methods.

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² In other words, each of the first four junction types occur about 20 percent of the time, while the remaining two occur only 10 percent of the time.



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Science Policymaking

Continued from page 2

initiatives can keep the research community's priorities top of mind. "Advocacy puts applied mathematics and computational science on the map," Newman said. "If they see that there is demand and people advocate for this, it puts more awareness on our issues."

It can be difficult to perceive the immediate impacts of advocacy, especially given the busy schedules of staffers and representatives. But beyond the inherent worth of sharing one's voice and providing critical feedback are advantageous possibilities to slowly grow connections and become a resource for a political office. "Advocacy is an ongoing thing as you keep building relationships," Newman said. "You can do this over time; it's going to be a long-term achievement."

Workshops and special events are important occasions for scientists to influence the direction of future policy. For instance, the 2024 SIAM Quantum Intersections Convening⁸ resulted in a report⁹ with recommendations to U.S. federal agencies of strategies to bridge the gap between mathematics and quantum science [3]; a minisymposium session¹⁰ at AN25 overviewed some of the workshop's key outcomes. As an upcoming opportunity, the 2026 Joint Mathematics Meetings¹¹—to be held this January in Washington, D.C.—will feature a day for Mathematical Sciences on Capitol Hill¹² that is open to all conference attendees who sign up by November 10. After undergoing training and receiving briefing materials, participants will spend a full day engaging with congressional offices to convey the importance of the mathematical sciences.

Mathematical Experiences With Advocacy

The AN25 session concluded with a panel of three applied mathematicians who spoke about their respective experiences with science policy. Evans, who participated in the first cohort of SIAM Science Policy Fellows from 2018-2019, was motivated to gain knowledge about the functioning of the federal government that is not necessarily obvious for scientists. "I was always curious about the government, especially since funding seemed like a huge black box that I didn't understand at first," she said. "It was very exciting to learn how different pieces of the government work and how to advocate better."

Actor, who is a 2024-2025 SIAM Science Policy Fellow, affirmed his interest in the communication of scientific ideas and stories in policy contexts, where narrative and research can come together to shape future directions. For her part, Levy found that her involvement with the American Association for the Advancement of Science's Science & Technology Policy Fellowship¹³ program—a yearlong, full-time opportunity for researchers to serve in the federal government-helped her view politics and even professional relationships in a new light. "I really was able to be more effective in my own organization because of the skills and perspective that I developed," she said.

The panelists then offered some specific anecdotes of their own impacts in policy-driven environments. Evans reminisced about her attendance at the 24th Annual Coalition for National Science Funding on Capitol Hill as a SIAM Science Policy Fellow in 2018 [1]. This event was akin to a science fair that allowed congressional representatives and staffers to learn about the importance of scientific funding for

research and education. "I felt like I could really talk to them and show them that the money is really helping people," she said.

Actor recounted his experiences with DOE's Frontiers in AI for Science, Security, and Technology¹⁴ initiative, which determined how DOE would invest in AI at scale. He participated in workshops and helped to develop white papers that would ultimately facilitate the formation of priorities for future funding calls — all of which furthered his understanding of the feedback mechanisms between researchers and policymakers that determine the prospective directions of entire fields. "Language at conferences like this one gets assimilated and picked up in workshops and white papers," Actor said.

During her time in a senatorial office, Levy made a variety of contributions: collaborating with colleagues to create a primer on quantum science for policymakers, answering phone calls from constituents, working with an external policy group on financial modeling, and forging relationships to promote new legislation. These activities underscored the value of networking, making comprises, and remaining open to tangential connections that may unexpectedly become essential. "I learned so much about relationships," Levy said. "How do you talk to people you disagree with? That's the most important question right now."

As the session drew to a close, the panelists shared concrete recommendations for SIAM members who are interested in contributing to advocacy efforts. Despite the overwhelming stream of news and information, Actor encouraged the audience to stay aware of policy happenings and communicate regularly with friends and colleagues to help make sense of the deluge. He also noted the importance of tailoring advocacy messages to the appropriate audience. "Learn how to tell a story that they'll be receptive to," Actor said. "Not every story is going to be received the same way, depending on how it's told."

Similarly, Levy advised attendees to ask thoughtful questions about different people's priorities and tease out the intersections between their personal lives and their policy leanings. "Be relatable and focus on what people care about and how they spend their time," she said. Evans agreed about the merit of building connections. "The one thing I would recommend you do is talk to people," she said, referencing not only local and federal political representatives but also friends, neighbors, and even new acquaintances. "The more you advocate and talk to people, the more you can talk about the importance of funding science and math, and the more that message is going to get out."

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¹³ https://www.aaas.org/programs/science-technology-policy-fellowships

¹⁴ https://www.energy.gov/fasst

Group Science: The Open Source Study of Higher-order Networks With XGI

By Nicholas W. Landry and Laurent Hébert-Dufresne

The concept of group effects is not always intuitive. In the natural sciences, multibody interactions often involve a sum of pairwise interactions, but the natural laws that govern these interactions remain unchanged. When calculating gravitational fields, for example, Leonhard Euler's threebody problem can yield dramatically richer behavior than the two-body problem, but the underlying physical laws are the same. However, some interactions do change in groups; opinion dynamics may work differently as social networks expand, predation preference in ecosystems shifts with community composition, and many chemical reactions require multiple reactants. It is also combinatorially challenging to model groups, as a system of 1,000 parts can contain up to $\binom{1,000}{2} = \mathcal{O}(10^5)$ pair interactions but as many as $2^{1,000} = \mathcal{O}(10^{301})$ groups! Researchers need new software to efficiently store group interactions, analyze their structures, simulate their dynamics, and ultimately examine their impacts on nature and society.

Social scientists have long debated the reality of groups distinctly from their individual members, as well as groups' prospective impacts on individual behavior. Groups can develop specific norms, cultures, and sometimes seemingly minds of their own, which means that new phenomena and mechanisms can emerge at the group level. Experts have studied group ontology in

sociology [10], philosophy [8], and other disciplines, but they continue to deliber- **SOFTWARE AND** ate about groups' irreducibility when compared to their members [5, 9]. These ongoing queries resonate

with the philosophy of complex systems and network science, whose researchers typically embrace the fact that "the whole is more than the sum of its parts" [1]. As a result, a community has emerged in recent years that focuses on higher-order networks, contributing mathematical modeling tools, software, and large-scale datasets to solve computational challenges and improve our collective understanding of the differences between multibody interactions and mere sums of pairwise interactions.

Mathematically, higher-order networks often take the form of hypergraphs (i.e., a set of nodes and a set of arbitrarilysized interactions, or hyperedges) or simplicial complexes (i.e., hypergraphs with an added constraint of downward closure so that every sub-interaction exists within a given hyperedge) [7]. Unlike pairwise networks, where groups are simply implied

as dense subgraphs within a network's structure, higherorder networks explicitly model groups and thus facilitate the modeling of grouplevel dynamics.

Barriers to Working With Higher-order Networks

PROGRAMMING

However, higher-order networks pose several challenges. First, they can be extremely computationally expensive; exhaustive computation quickly becomes infeasible at the scale of practical applications. For instance, coauthorship networks can easily include millions of authors and publications. In contrast, empirical higher-order networks are often quite sparse, and large groups are much less common than smaller ones.

Network analysis algorithms leverage these properties to sidestep such combinatorial limitations and enable the study of empirical higher-order systems at scale. But higherorder datasets themselves pose difficulties as well, as a lack of standardized formats promotes ad hoc methods for data processing.

Overcoming these challenges requires efficient, user-friendly software that is integrated with large-scale datasets. Just as NetworkX,¹ igraph,² and graph-tool³ have become the lingua franca of network science software, newer software packages⁴ have materialized to handle the demands of higher-order network science: an analogue of pairwise network science in the age of big data. These packages provide a common language through which higher-order network scientists across diverse disciplines can collaborate via network data structures, efficient algorithms, and integration with large-scale network datasets.

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- https://networkx.org
- https://igraph.org
- https://graph-tool.skewed.de
- https://github.com/xgi-org/xgi/blob/ main/OTHER_RESOURCES.md

Career Opportunities

Continued from page 4

learning models with guarantees. Actor noted that the labs tend to value candidates with a traditional background in applied math, a thorough understanding of data science and data pipelines, and a demonstrated ability to leverage their skills within a changing landscape.

Brooks discovered her love of math in college and switched her area of study accordingly. "I didn't plan to go to grad school, but I had a wonderful mentor at the University of Utah who suggested that I apply to the graduate program," she said, adding that she was particularly interested in teaching. "It was in graduate school that I realized how wonderful a career in mathematics would be, and what a good fit it was for me." Brooks is now in her sixth year as an assistant professor at Harvey Mudd—a small, STEMfocused liberal arts college—and is coming up for tenure. "A liberal arts career path is an excellent option if you want a lot of flexibility in how you're allocating your time," she said. "I have an environment with supportive colleagues where I can choose—to some extent—how much time I allocate to research, teaching, and other service or professional development opportunities."

After these introductions, panelists shared pieces of advice that have shaped their perspectives. Actor recalled valuable guidance from a graduate school faculty member that has stuck with him over the years. "You don't have to know all of the answers when you start out," he said. "That's true at the beginning of your career, and it's also true as you go through your career." Gottlieb agreed, disclosing that she would have likely felt more confident in her early days as an assistant professor had she accepted this maxim. "I wish I knew earlier that the way we learn and develop competence is by trial and error," she said. "Doing things without knowing how to do them is exactly how you learn; you figure it out on the fly."

Brooks urged attendees to ask questions at every stage of their professional journeys and remain open to new experiences — even ones that do not necessarily align with their imagined future visions. "It's good to plan ahead, think about opportunities, and prepare for them, but you can't predict where the world will be in five or 10 years," Brooks said. "You really just have to be open to following things that you're excited about. Trust your curiosity and your instincts."

When an audience member inquired about the realities of the present job market, Aruliah acknowledged the difficulties that are associated with funding cuts in the U.S. but reminded listeners that economic downturns tend to correct themselves with time. "It's a bit of a brutal job market right now, I don't want to lie to you about that," he said, admitting that his own consulting business is feeling the effects of continued uncertainty. Gottlieb concurred that the academic job scene is similarly unpredictable, given questions about funding, grants, and institutions' capacities to support postdoctoral researchers. Aruliah hence advised job seekers to use this time to hone their skillsets in anticipation of future openings. "One thing that I've come to embrace is that fortune favors the ready," he said. "Think about the skills and experiences that you hope to have when things improve a little."

Conversation then turned to optimal funding strategies. Gottlieb, who spent six months as interim Vice Chancellor for Research at UMass Dartmouth, remarked that universities typically have some incentive to assist with grant writing. Even so, most academics who wish to run a project from start to finish will need to secure multiple simultaneous grants. A wide professional network is valuable under these circumstances, as existing connections can lead to collaborations with other researchers who may have accessible funding and a real interest in the study. "It's not what you know, it's who you know," Petersson said. "If you build your network of contacts, that can help your situation."

Brooks clarified that while grants and other sources of federal funding are certainly critical within academia, private sponsorship can serve as an additional resource for university researchers. She mentioned that most colleges have designated fundraising teams and/or departments that can promote scientists' projects, get donors excited about potential matchmaking, and generate opportunities for private funds.

Petersson then addressed funding within the national laboratories, which have internal sources of revenue for startup ideas though this money is quite competitive. "If you have a good story, you can get funding that may last for three years," he said. "But at the end of those years, you're encouraged to find additional funding." Therefore, the goal is to amass enough results to motivate external funders to support the ongoing venture. Actor thus recommended that lab employees build compelling portfolioscomprised of multiple smaller projects that serve as proofs of concept—that contribute to a unified yet versatile theme within the larger research landscape.

Next, the discussion shifted to networking. When an attendee expressed trepi-

dation about their ability to engage in intellectual dialogue with more senior researchers, Brooks reminded them that all established professionals were once junior scientists themselves. "It's really helpful to remember that the people you're talking to are just people," she said. "Networking doesn't have to be all research, all business, all the time. Human connections are never a waste of time."

Aruliah likewise encouraged early-career researchers to try to connect personally with their conversation partners at conferences and elsewhere, as exhibiting genuine interest in one's peers typically elicits a positive response. Actor agreed and suggested that attendees initiate conversations with researchers whose projects they admire, as such interactions can serendipitously lead to internships, postdoctoral placements, academic collaborations, and so forth. He also noted that scientists typically like to talk about their own work. "Try to get other people talking about what interests them," Actor said. "People think you're a great conversationalist if you listen."

When considering a job offer, Actor prompted job seekers to evaluate both the workplace culture and any prospective collaborators within the company, department, or group to ensure that the position is a good fit. Positive relationships with colleagues are especially important in academia, as people tend to remain in academic positions for a long time; in contrast, industry sees a much greater level of turnover. Gottlieb stated that applicants may want to talk to former employees to find out why they left the organization in question. "The people you work with are the most important," she said. "When things at an institution change but the colleagues don't, that makes it a good place to be."

As the session drew to a close, the panelists advised the audience to stay positive about their futures, remain flexible in the face of ongoing uncertainty, and hone their unique skillsets however possible. "Demonstrate excellence and have something in reserve where you know you can be the best at what you're doing," Actor said. "Know what's open and available, line yourself up to apply, and leverage your connections to get there. If you make sure that you stand out, you'll position yourself in a better place."

Lina Sorg is the managing editor of



During a panel session about career opportunities in academia, industry, and the national laboratories at the Third Joint SIAM/CAIMS Annual Meetings—which took place this summer in Montréal, Québec, Canada—a group of professionals at various stages of their careers reflected on their own trajectories and shared advice with the audience. From left to right: Anders Petersson of Lawrence Livermore National Laboratory, Sigal Gottlieb of the University of Massachusetts Dartmouth, moderator Jason Torchinsky of Sandia National Laboratories, Dhavide Aruliah of MKDA Consulting, Jonas Actor of Sandia National Laboratories, and Heather Zinn Brooks of Harvey Mudd College. SIAM photo.

Group Science

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The XGI Research Ecosystem

The CompleX Group Interactions⁵ (XGI) software package is an open source Python library for the analysis of higher-order networks [6]. XGI addresses the aforementioned challenges by offering a comprehensive ecosystem for higher-order network science research through a suite of analytical tools, seamless integration with a corpus of large-scale datasets, and extensive tutorials and documentation. The library can represent undirected and directed hypergraphs and simplicial complexes; read and write networks that are stored in common file formats; convert between different data structures; clean up common data artifacts; generate synthetic networks from random and classic models; analyze network properties such as clustering, assortativity, path lengths, node and group centrality, and connectedness; simulate dynamics; and visualize these networks.

XGI represents higher-order networks as a data structure, storing all node-group relationships for efficient computation. However, this depiction is not always suitable for all applications; for example, spectral measures of hypergraph structure rely on matrix representations. To account for this limitation, XGI can convert to and from more than 10 different higher-order data structures, including representative matrices, lists of groups, and node-group relationships. In particular, the field has especially advanced in the efficient measurement of higher-order statistics and generation of synthetic hypergraphs. In several cases, XGI's state-of-the-art algorithms have improved performance by several orders of magnitude when compared to exhaustive computation.

XGI is integrated with the XGI-DATA repository: 6 an open data repository on Zenodo⁷ that hosts 44 datasets of diverse domains, systems, and sizes. Each dataset is accompanied by computed statistics and information, such as how and when the set was collected, who created it, what the nodes and edges represent, and how to cite it. A single command loads the datasets via an HTTP request, streamlining scientific workflows. In parallel, the Hypergraph Interchange Format exists as a data sharing standard [3] to facilitate the sharing of higher-order network data between different scientific software packages and research teams.

As an example of XGI's potential, Figure 1 depicts the arxiv-kaggle dataset from XGI-DATA. This dataset comprises 1.8 million nodes (authors) and 2.8 million hyperedges (publications) that are loaded into XGI with the load_xgi_data method. XGI's cleanup method enables data cleaning, which removes single-author

- 5 https://xgi.readthedocs.io
- https://xgi.readthedocs.io/en/stable/xgi-data.html
- https://zenodo.org/communities/xgi

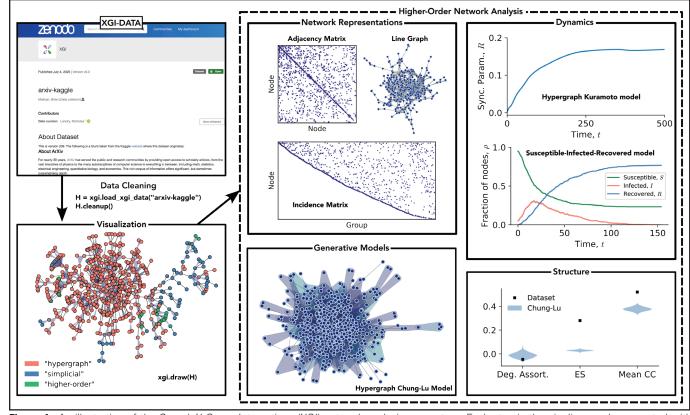


Figure 1. An illustration of the CompleX Group Interactions (XGI) network analysis ecosystem. Each step in the pipeline can be executed with just a few lines of code. In the lower right panel, "ES" stands for edit simpliciality and "CC" stands for clustering coefficient. Figure courtesy of Nicholas Landry; the XGI code that was used to create the figure is available at https://github.com/nwlandry/group-science-siam-news.

papers and papers that fall outside of the largest connected component — a technique that is useful to many data science pipelines. The H.edges.filterby() method then filters the dataset with a custom filtering function, which extracts papers that have two or three authors and "hypergraph," "higher-order," or "simplicial" in the title ultimately yielding a hypergraph with 593 nodes and 518 hyperedges. The filterby method is an example of XGI's statistics interface for node and edge properties, allowing users to easily convert between data formats, compute statistics on these properties, and even define one's own statistics. We can visualize the dataset with xgi.draw(H), where the node colors signify the average occurrence of higher-order keywords in the papers with which they are affiliated.

We can analyze this hypergraph in a variety of ways. First, we can leverage different data representations to unlock various measures from linear algebra or pairwise network analysis. Second, we can simulate multiple dynamics—such as the Kuramoto model or hypergraph susceptible-infectedrecovered model—on the hypergraph to analyze the resulting behavior. We are also able to generate synthetic higher-order networks with tunable structure, which may serve as null models or the theoretical foundation for analytical measures of structure or dynamics. And finally, we can measure the structure of a higher-order dataset to quantify degree assortativity, simpliciality, clustering coefficients, and so forth. A great place to start is the XGI project website,8 which contains a comprehensive collection of documentation and tutorials.

Looking to the Future

Toy models have already demonstrated the importance of group effects. Simple mathematical models of contagion that are mediated through group dynamics naturally exhibit phenomena that exist in the real world—e.g., polarization, collective action, and tipping points [2, 4]—and are often generated by a critical mass of influential *groups*, rather than individual agents.

Researchers are now advancing the frontiers of group science on two separate fronts. First, theoretical models require validation with more observational data, necessitating new experiments and model systems. And second, certain hypothesized dimensions of group dynamics, such as group states and the alignment of rationality between groups and their members, are still somewhat unexplored [9]. The way in which groups shape our world-by mediating the flow of information, influencing the formation of ideologies, driving the spread of infectious disease, etc.—is an exciting area of study. Higherorder networks will always be more computationally expensive than their pairwise alternatives, but open source software packages that leverage efficient algorithms, large-scale datasets, and compelling visualizations are unlocking this exciting field for practitioners across a diverse range of disciplines.

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⁸ https://xgi.readthedocs.io

Red Sock Award at DS25 Recognizes Outstanding Student Research in Dynamical Systems

By Twinkle Jaswal, Juan Patiño-Echeverría, Laura Pinkney, and Anna K. Thomas

S IAM's Red Sock Award¹ acknowledges the best poster presentations by students and/or postdoctoral researchers at the biennial SIAM Conference on Applications of Dynamical Systems. As per tradition, each awardee receives a monetary prize of \$100.00 and a pair of red socks in honor of James A. Yorke (University of Maryland, College Park), an influential figure in the dynamical systems community who is further distinguished by his signature crimson footwear.

The Red Sock Award became an official SIAM prize in 2013.² At each dynamical systems conference, an *ad hoc* prize committee of judges anonymously visits all of the posters during the Poster Session and Dessert Reception, assigning individual scores to each presenter for their display and overall delivery. The judges use these scores to select the winners, who are then recognized publicly during the conference.

At the 2025 SIAM Conference on Applications of Dynamical Systems³ (DS25)—which took place in Denver, Colo., this past May—the DS25 *ad hoc* committee awarded the coveted prize to Twinkle Jaswal of Illinois State University, Juan Patiño-Echeverría of the University of Auckland, Laura Pinkney of the University of Leeds, and Anna Thomas of the University of Pittsburgh. Here, the 2025 recipients of the Red Sock Award provide brief overviews of their prizewinning work.

Photosensitivity and Neuronal Synchronization

Twinkle Jaswal, graduate student, Illinois State University

My DS25 poster⁴ focused on the use of computational modeling to study photosensitive seizures. I explored the possible effect of external stimuli—specifically, flashing lights in combination with elevated temperatures—on neuronal synchronization. Excessive neuron synchronization is present during epileptic seizures [5], and temperature might be an aggravating factor for individuals who are predisposed to photosensitive seizures. Elevated core body temperature can also impair cognition and increase seizure risk, negatively impacting brain function.

(A)

200

150

My collaborators and I developed a temperature-dependent neuronal network that consists of a 15×15 lattice of Hodgkin-Huxley-type model neurons [3], each of which is governed by a set of temperature-dependent differential equations. Bidirectional gap junctions connect the neurons, and synaptic coupling strength is modulated by an Arrhenius temperature scaling factor: $\gamma(T) = 4.0^{(T-T_0)/10}$. We used $I_{\text{stim}} = A \sin(2\pi f t)$ to model visual stimulation, where A represents the stimulus amplitude, f denotes the frequency in hertz, and t is time in seconds. The uniform application of this stimulus to all neurons simulates the effect of rhythmic visual input that is transduced through the retina, influencing the entire network. We employed the Kuramoto order parameter R to measure synchronization across the network; a value of 0 indicates no synchronization, a value of 1 signifies complete synchronization, and values between 0 and 1 reflect partial synchronization.

At the brain's baseline temperature of 38° Celsius (C), our network reveals that flashing light alone can cause partial synchronization among neurons, even without synaptic connections (see Figure 1). This effect is especially noticeable in networks that are composed of neurons with similar firing properties. With the introduction of synaptic coupling, synchronization grows stronger and occurs across a wider range of visual stimulus amplitudes and frequencies.

To understand temperature's influence on synchronization when combined with visual stimulation, we simulated the network at 36°C, 38°C, and 41°C. Results show that as temperature increases, the neurons become more synchronized — even at lower visual stimulus intensities. At higher temperatures, a wider range of visual stimulus amplitudes and frequencies can lead to synchronization. These findings suggest that elevated temperatures make the network more sensitive to external rhythmic input, amplify the effects of visual stimulation, and heighten the brain's likelihood of entering a synchronized state.

Into the Wild: A Journey to Chaos in Four Dimensions

Juan Patiño-Echeverría, graduate student, University of Auckland

My DS25 poster⁵ shared new results on *wild chaos*, a higher-dimensional form of chaotic dynamics that only arises in vector fields with a dimension of four or higher. It is characterized by the persistent presence of tangencies between the stable and unstable manifolds of an invariant set [1]. My Ph.D. research focuses on a four-dimensional (4D) extension of the classic Lorenz system that is given by

5 https://meetings.siam.org/sess/dsp_talk. cfm?p=145179

(C)

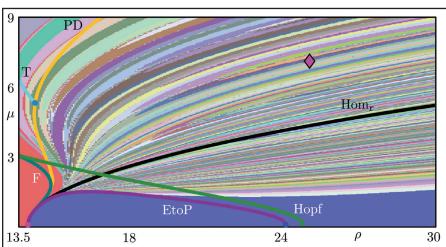


Figure 2. Dense homoclinic bifurcations in the (ρ,μ) -plane that are identified by the kneading invariant of $W^u_+(\mathbf{0})$ and distinguished by different colors. The magenta diamond indicates the point of the known wild attractor. Figure courtesy of Juan Patiño-Echeverría.

$$\begin{cases} \dot{x} = \sigma(y - x), \\ \dot{y} = x(\rho - z) - y, \\ \dot{z} = xy - \beta z + \mu w, \\ \dot{w} = -\mu z - \beta w, \end{cases}$$
(1)

with fixed parameters $\sigma = 10$ and $\beta = 8/3$. This system features the new parameter μ and exhibits a wild pseudohyperbolic attractor for a specific choice of ρ and μ [4].

Pseudohyperbolicity ensures that all trajectories in the attractor have a positive maximal Lyapunov exponent, and that this behavior is robust under perturbations. Our work seeks to understand the emergence of such a wild attractor when parameters change [8]. To that end, my colleagues and I explore the global bifurcation structure in the (ρ,μ) -parameter plane of system (1). The crucial novel aspect is the existence of rotational dynamics near the origin in the (z,w)-plane when μ is "switched on."

Our starting point is a bifurcation diagram with curves of homoclinic bifurcations and local bifurcations of equilibria and periodic orbits that are inherited from the Lorenz system when $\mu = 0$. We then found and continued new global bifurcations that are intrinsic to the 4D system (1). To identify the corresponding curves, we cataloged the "fate" of the one-dimensional unstable manifold of origin $W^{u}(\mathbf{0})$ (i.e., the set of points that converge to the origin in backward time) via kneading diagrams and Lin's method (see Figure 2) [8]. These bifurcation curves accumulate densely in a parameter region that contains the point with the known wild attractor [4]. We also analyzed the system's attractors by computing the Lyapunov spectrum that is associated with the branch $W_{\perp}^{u}(\mathbf{0})$. Doing so allowed us to identify additional regions that satisfy the required conditions, ultimately suggesting that a wild pseudohyperbolic attractor may arise in other parts of the (ρ, μ) -plane.

These results contribute to our overall understanding of the global organization of chaotic dynamics in 4D systems and may

time (ms)

inform future studies about the mechanisms through which wild chaos emerges.

Pattern Formation Driven by Three-wave Interactions With Two Critical Wavenumbers

Laura Pinkney, graduate student, University of Leeds

Patterns in nature arise in a variety of scenarios, such as stripes on a zebra or hexagons in a honeycomb. These examples both comprise patterns on a single length scale; stripes are composed of a single wave and hexagons arise from the interactions of three waves with the same wavenumber that are 60 degrees apart. In this simple instance of a three-wave interaction (3WI)—or resonant triad—the sum of two wavevectors equals the third. Given the existence of other pattern-forming systems with multiple length scales, we investigate problems that have two critical wavenumbers.

3WIs can explain pattern-forming behavior that is associated with the Faraday wave experiment, which periodically forces a container of fluid up and down and observes the patterns that appear on the surface. When the forcing exceeds a certain threshold, the flat state becomes unstable and yields to a variety of patterns. If the forcing contains a single frequency component, simple patterns like stripes, squares, and hexagons develop. But in the case of multiple-frequency forcing, 3WIs can arise with two critical wavenumbers and generate more complex structures such as superlattices, quasipatterns, and spatiotemporal chaos.

We consider problems with two critical wavenumbers, where resonant triads materialize between two waves of a larger wavenumber and a third wave of a smaller wavenumber (see Figure 3a, on page 9). The inclusion of a second wavenumber facilitates the formation of patterns on both a rhombic and hexagonal lattice (see Figures 3b and 3c, on page 9). We can represent the dynamics of these 3WIs via a set of nine complex ordinary differential equations (ODEs), with one equation for each amplitude of the wavevectors in Figure 3. This system's generalizability means that any pattern-forming scheme that exhibits 3WIs with two wavelengths can be reduced to the same system of equations.

At DS25,⁶ I presented an analysis of a partial differential equation (PDE) that adapted the Lifshitz-Petrich equation [6] to include independent linear growth rates [9] and additional cubic nonlinearities. My collaborators and I utilized weakly nonlinear theory to reduce the PDE to the 3WI ODE system. By analyzing the stability of patterns within the ODE system, we predicted the patterns in the PDE's solutions and used these predictions to identify regions of parameter space where we expected to find

See Red Sock Award on page 9

Figure 1. Simulation results at normal brain temperature with synaptic connectivity ($\eta = 1.0$). 1a. Raster plot without visual stimulus. 1b. Raster plot with visual stimulus where A = 5 and f = 20 hertz. 1c. Colormap that depicts the synchronization index R for different combinations of amplitude and frequency. Figure courtesy of Twinkle Jaswal.

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³ https://www.siam.org/conferences-events/past-event-archive/ds25

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4 https://meetings.siam.org/sess/dsp_talk
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⁶ https://meetings.siam.org/sess/dsp_talk cfm?p=145213

Red Sock Award

Continued from page 8

spatiotemporal chaos. We discovered significant regions of spatiotemporal chaos within our PDE, with multiple types of chaotic solutions (see Figure 3d). In the future, we hope to more deeply analyze the occurrence of different examples of chaotic dynamics.

Cellular and Parkinsonian Network **Dynamics in a Conductance-based** Model of the Pedunculopontine **Nucleus in Rodents**

Anna K. Thomas, graduate student, University of Pittsburgh

My colleagues and I develop conductance-based models of neurons in the pedunculopontine nucleus (PPN) within the brainstem to uncover the mechanisms that shape neuronal activity along motor pathways.⁷ According to recent studies, therapies that target specific deep subcortical brain areas can promote long-term motor recovery in dopamine-depleted rodents [7], but only when the PPN is intact [2]. Despite the PPN's recognized importance, computational models of the dynamics of Parkinson's disease rarely incorporate its contributions. Furthermore, there is no bio-

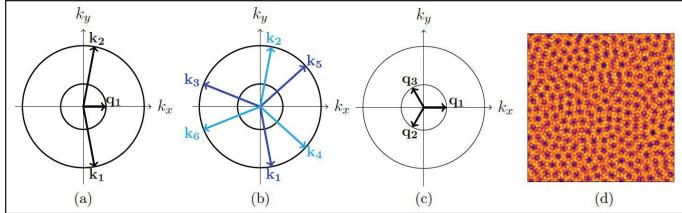


Figure 3. Three-wave interactions (3WIs) between wavevectors on two critical circles with radius 1 and q < 1/2 (outer and inner circles, respectively). **3a.** The wavevectors satisfy $k_1 + k_2 = q_1$, which means that triad interactions only occur between waves with one shorter and two longer wavelengths. 3b. Vectors that form hexagonal 3WIs on the outer circle. 3c. Vectors that form hexagonal 3WIs on the inner circle. 3d. The resulting complexity may lead to spatiotemporal chaos that exemplifies the solution amplitude on the physical domain at an arbitrary time. Figure courtesy of Laura Pinkney.

physically representative model of these neurons that captures the distinctive singlecell behaviors that are observed in electrophysiology experiments.

We propose a model that comprises a system of ODEs that describe the time evolution of a neuron's membrane voltage, associated ion channel variables, and intracellular calcium concentration. The neuronal model reliably encapsulates a variety of these characteristic activity patterns, including diverse post-stimulus rebound responses, gamma-band oscillations, and

presence of multiple timescales within the system-specifically for dynamical variables that represent the ionic gates of the T-type calcium channels—allows for the application of geometric singular perturbation theory, which analyzes transient model activity during post-stimulus responses. To observe and model single-cell activity on longer timescales-including highvoltage oscillations that subject the cell to slowly depolarizing ramps—we employed bifurcation analysis and demonstrated the neuronal activity's dependence on the mag-

Our approach offers both mathematical and biologically mechanistic explanations of the cellular processes that underly each of these activity patterns, laying the foundation for future investigations of PPN function within motor circuits that pertain to Parkinson's disease.

Congratulations to this year's recipients of the Red Sock Award!

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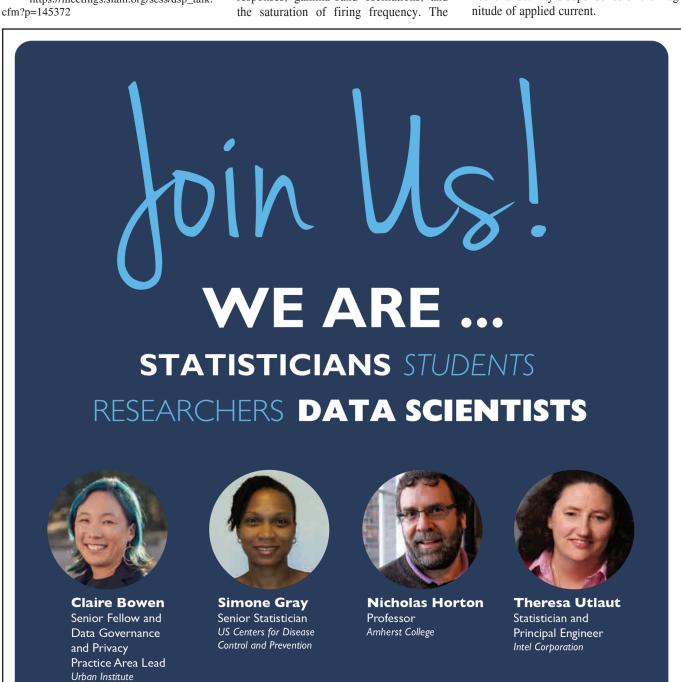
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Twinkle Jaswal is an M.S. student in computer science at Illinois State University. Her research focuses on computational neuroscience, particularly the influence of temperature and external stimuli on neuron synchronization. Juan Patiño-Echeverría is a Ph.D. student in mathematics at the University of Auckland. His research focuses on dynamical systems—particularly higher-dimensional forms of chaos-and combines both theoretical and computational approaches. Laura Pinkney is a Ph.D. student in the Department of Applied Mathematics at the University of Leeds. Her research focuses on the analysis of pattern-forming systems, and she uses tools from numerical analysis, dynamical systems, and asymptotic methods to investigate the significance of three-wave interactions. Anna K. Thomas is a Ph.D. student in the Department of Mathematics at the University of Pittsburgh. Her research interests include mathematical neuroscience and dynamical systems.



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Spectral Geometry for Dynamical Systems and Time-evolving Networks

By Gary Froyland

omplex dynamics can display emergence, whereby simple (e.g., physics-based) microrules describe the interactions and evolutions of individual states. Collectively, however—and at the level of many states—complicated and observable macrophenomena may appear. We often characterize macrophenomena as large collections of individual states that evolve as a group for a substantial duration of time. For example, a sizeable cohort of individuals might hold a collective opinion for several years, or a mass of hot air parcels in the atmosphere may remain over a fixed geographic location and cause a heatwave.

Here, we show that the modification of classical ideas from spectral geometry can produce linear operators that are induced by nonlinear microdynamics whose leading eigenspectra and corresponding eigenfunctions highlight these macrophenomena, including their appearance and disappearance. We consider situations where the domain of microstates is a continuum (e.g.,

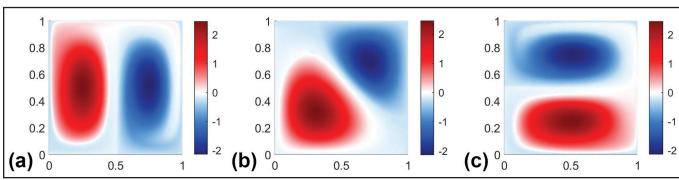


Figure 2. Evolution of two coherent sets in a highly nonlinear flow of the unit square. The deep red and deep blue colors indicate the two sets. 2a. Leading nontrivial eigenfunction f_2^D for the dynamic Laplacian. 2b. Pushforward of f_2^D by 1/2 of a time unit to t=1/2, namely $f_2^D \circ (\Phi^{1/2})^{-1}$. **2c.** Pushforward of f_2^D by one time unit to t=1, namely $f_2^D \circ (\Phi^1)^{-1}$. Figure courtesy of [4].

a manifold) and explore the same principles' application to discrete domains such as complex, time-evolving networks.

Spectral Geometry

Well-known connections exist between manifold geometry and the spectrum and eigenfunctions of the Laplace-Beltrami operator Δ on M [2, 9]. By classical theory, the eigenproblem $\Delta f = \lambda f$ on M with zero Neumann boundary conditions has count-

ably many eigenvalues $0 = \lambda_1 > \lambda_2 > \cdots$ with eigenfunctions $\{f_i\}_{i=1}^{\infty}$. Globally distant regions on M are encoded in the leading nontrivial eigenfunction f_2 via extreme positive and negative values. For instance, the deep red and blue regions in Figure 1 are globally far away from one another.

The Dynamic Laplace Operator

We can generalize the above observations to a setting where the Riemannian

manifold is subjected to general timedependent dynamics. For such a generalization, the Laplace operator must also be extended to incorporate dynamics. We use $\Phi^t: M \to \Phi^t(M)$ to denote a smooth transformation that describes the timedependent evolution over time $t \in [0, \tau]$; recall the natural pushforward operator $(\Phi^t)_* f = f \circ (\Phi^t)^{-1}$ and pullback operator $(\Phi^t)^* f = f \circ \Phi^t$ on functions $f: M \to \mathbb{R}$.

The dynamic extension of the classical Laplace operator is called the *dynamic* Laplacian Δ^D on the time interval $[0, \tau]$ [3]. We define it as

$$\Delta^D := rac{1}{ au} \int_0^ au \left(\Phi^t\right)^* \circ \Delta \circ (\Phi^t)_* \ dt = rac{1}{ au} \int_0^ au \Delta_{g_t} \ dt,$$

where $g_t = (\Phi^t)^* e$ is the pullback of the Euclidean metric e. The local coordinate

See Spectral Geometry on page 12

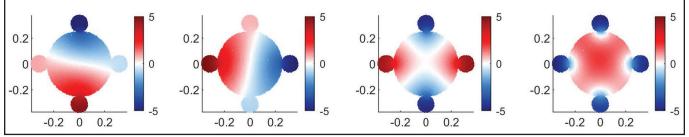


Figure 1. Laplace eigenfunctions f_2, \dots, f_5 of a two-dimensional manifold M. Note that the deep red and deep blue regions of f_2 (and by symmetry, f_3) are globally far from one another. Additional eigenfunctions f_4 , f_5 , and so forth further decompose M according to geometric structure. Figure courtesy of [4].

The Mechanics of the Powerball

The Powerball is a gyroscopic handheld wrist exerciser that was patented in 1973 by Archie L. Mishler. It is a gyroscope mounted inside of a plastic ball the size of an orange, with an opening that allows the user to give the gyro an initial spin. Surprisingly, by precessing the ball, one can cause the gyro to gain spin — and a remarkably fast one, capable of exceeding 250 revolutions per second. The resulting gyroscopic effect is so strong that a significant effort is required to precess the ball hence the exercise value of the device.

How is one's muscular effort converted into the gyro's spin? In this article, I describe the idea behind Mishler's admirable invention.

Construction of the Device

The ends of the gyro's axle extend into an equatorial groove on the sphere's inside surface, which constrains the axle to lie in the ball's equatorial plane (see Figure 1). Importantly, the axle is fused with the gyro; there are no bearings. When the gyro spins, so does the axle, rubbing against the wall of the groove that it touches. The axle is a tiny

¹ Precise details of construction—which I discovered by breaking apart my toy once it stopped working-are not important for the purpose of this discussion.

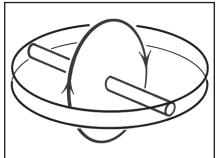
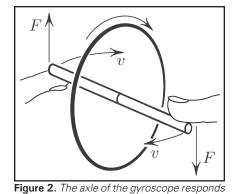


Figure 1. Schematic construction of the Powerball. The axle's ends can slide in a channel groove on the inside of the sphere (not shown).



orthogonally to a steady push.

bit narrower than the groove, so it can only have contact with one wall.

The Spin-up Mechanism

To understand how the MATHEMATICAL Powerball works, let us recall the gyroscope's key property (see Figure 2). The ends of a spinning gyro's axle respond to the steady forces F that are applied by

moving in a perpendicular direction.²

With the gyro having been given its initial spin, we tilt the ball to apply force F to the axle (see Figure 3). As in Figure 2, the axle responds by moving as shown. If the speed $v > \omega r$ (where ω is the spin angular velocity and r is the axle's radius), then

friction facilitates the gyro's rotation. This

explains the workings of the Powerball. Is it luck, or is there a deeper reason that the axle in Figure 3 responds by moving to the left? Had it moved right, the friction would have acted against the spin and we would be holding a dud! In that case, I believe that we could still salvage the idea by adding a differential mechanism

² This reaction occurs because changing the orientation of the axle causes paths of the wheel's particles of the sphere (to which they are confined) to acquire nonzero geodesic curvature. The resulting centrifugal force creates gyroscopic torque [2].

(though doing so would probably make the idea impractical).

In conclusion, here are two gyroscoperelated remarks.

Gyro as a Charged Particle on the Sphere

A gyroscope with perfect bearings is mathematically equivalent to an electrically charged point mass that is constrained to the sphere and subject to a magnetic field that is perpendicular to the sphere. The charge is proportional to the gyro's axial angular momentum. The Lagrange top (an axisymmetric top) is also equivalent to the particle on the sphere with a magnetic field, but

with additional gravitational force [1]. This observation makes the treatment of the Lagrange top much more transparent than in standard textbooks on the subject.

Sperry's Gyrocompass

CURIOSITIES

By Mark Levi

The behavior of the gyro in Figure 2 amounts to Newton's second law for rota-

tional motion: applied torque equals the rate of change of angular momentum. Loosely speaking, the gyroscope tries to align its axis with the axis of applied torque. Sperry's gyrocompass (still used in ships) works on this principle: a spinning gyro floating in a dish with its axis in a horizontal position orients itself in a north-south direction due to the Earth's rotation. The gyroscope tries to align itself with the Earth's rotational axis while keeping its own axis horizontal.

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The figures in this article were provided

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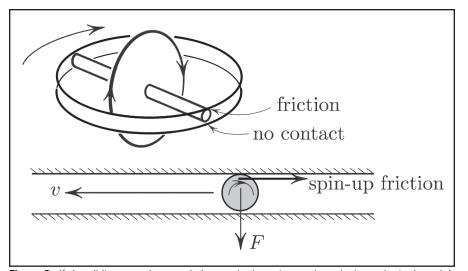


Figure 3. If the sliding speed $v > \omega r$ (where ω is the spin angular velocity and r is the axle's radius), then friction helps the gyro's rotation.

OpenAI: Extraordinary Accomplishments, but at What Cost?

BOOK REVIEW

By Ernest Davis

Empire of AI: Dreams and Nightmares in Sam Altman's OpenAI. By Karen Hao. Penguin Press, New York, NY: May 2025. 496 pages, \$32.00.

▼ n February 2020, *MIT Technology* ■ Review published an article by investigative reporter Karen Hao titled "The Messy, Secretive Reality Behind OpenAI's Bid to Save the World" [1]. The subhead was "The AI moonshot was founded in the spirit of transparency. This is the inside story of how competitive pressure eroded that idealism."

When OpenAI¹ was founded in December 2015, many people considered it a bright new hope for artificial intelligence (AI) research. The company was a nonprofit whose "primary fiduciary duty" was to humanity as a whole. Above all, as the name indicated, OpenAI would be open. The initial announcement² overflowed with idealistic promises, noting that "It'll be important to have a leading research institution which can prioritize a good outcome for all over its own self-interest... Researchers will be strongly encouraged to publish their work, whether as papers, blog posts, or code, and our patents (if any) will be shared with the world."

OpenAI began with \$1 billion, which seemed like a lot of money at the time. It was founded by Elon Musk, who was still widely admired 10 years ago, and Sam Altman, a relatively unfamiliar figure outside the world of high-tech venture capitalists. Ilya Sutskever—a rising young star who had successfully used deep learning for visual recognition (in collaboration with Alex Krizhevsky and Geoffrey Hinton)—was serving as research director. Peter Thiel, known for his right-wing pronouncements and involvement with the high-tech surveillance company Palantir,³ was a major initial investor.

OpenAI delivered surprisingly powerful AI products with astonishing speed. With equally astonishing speed, it abandoned its initial idealism. It quickly became clear that the initial \$1 billion was not enough; OpenAI would need a large regular income to compete with Google DeepMind.⁴ The charter,⁵ released in March 2018, differed in subtle but important ways from the initial announcement. In particular, it substantially reneged on its earlier promises of openness, ostensibly for safety reasons. In March 2019, OpenAI created a "capped profit" organizational arm and entered into a murky arrangement with Microsoft.

- https://openai.com
- ² https://openai.com/index/introducingopenai
- https://www.palantir.com
- https://deepmind.google 5 https://openai.com/charter

By the time Hao's article published in 2020, the initial hype and optimism surrounding OpenAI's public image had faded. Nonetheless, the article was disturbing — particularly Hao's description of her own experience. She was treated with suspicion as an unwelcome outsider; her interactions with employees were tightly controlled by the communications team, and many of the people with whom she spoke insisted on anonymity for fear of

retribution. Different scientific teams worked on projects that were kept secret even within the company. The overall picture was of

an organization that was achieving extraordinary successes at the cost of a working environment that was simultaneously messianic, frantic, and paranoid.

Hao has spent the last five years inves-

tigating the inner workings of OpenAI, its competition, and its subsequent impact on the outside world. During that time, OpenAI-and its flagship product, ChatGPT—have reached extraordinary heights even as the company's ethical degradation has sunk to extraordinary depths.

In particular, Altman has grown from a minor player in Hao's MIT Technology Review article to the chief executive officer and chief spokesman for OpenAI — and one of the most visible

and notorious figures in Silicon Valley. In her new book, Empire of AI: Dreams and Nightmares in Sam Altman's OpenAI, Hao notes that Altman presents as strategically brilliant, charismatic, and profoundly admired by many OpenAI employees, who threatened to resign when Sutskever and three board members attempted to fire him in November 2023. By all reports, Altman comes across as charming and sincere in person. However, Hao finds him to be megalomaniacal, entirely unscrupulous, manipulative, untrustworthy, and a pathological liar. She notes that he tells people— OpenAI employees, investors, and U.S. Senate subcommittees—what they want to hear with no regard for consistency or truth,

then later criticizes them, betrays them, and sets them against one another.

The secrecy surrounding OpenAI has deepened to the point that the organization no longer publishes any information about the internal workings of their products. For instance, the entire technical description of GPT-4 in the "GPT-4 Technical Report" [2] consisted of the following three-sentence affront to anyone who is impudent enough to ask questions:

> GPT-4 is a Transformer-style model pre-trained to predict the next token in a document, using both publicly available data (such as internet data) and data licensed

from third-party providers. The model was then fine-tuned using Reinforcement Learning from Human Feedback (RLHF). Given both the competitive landscape and the safety implications of large-scale models like GPT-4, this report con-

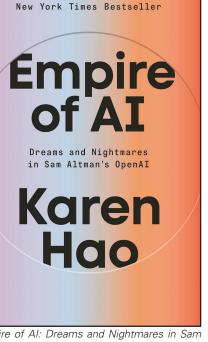
tains no further details about the architecture (including model size), hardware, training compute, dataset construction, training method, or similar [2].

Hao's account of OpenAI's explosive growth and tortuous office politics in Empire of AI is deeply researched, caustic, and exhaustive. At particularly dramatic moments-such as the attempted removal of Altman, now known at OpenAI as "the Blip"—it becomes a day-byday and even hourby-hour narrative of conspiracies, plots, and backstabbing in the fevered

Hao also sought out and became acquainted with some of Silicon Valley's victims around the world (in this part of the book, Google is as much of a villain as OpenAI). Oskarina Veronica Fuentes Anaya—a Venezuelan refugee living in Colombia and Mophat Okinyi, a poor Kenyan, were hired to annotate dregs of internet content for GPT training data — a job that paid a pittance, came with horrible working conditions, and caused severe psychological problems (OpenAI used middleman companies so that it could deny responsibility). The copper and lithium mines in Chile's Atacama Desert feed Silicon Valley's ravenous hunger for computer hardware but Immense data centers in drought-stricken Uruguay and elsewhere require vast quantities of potable water for cooling, hugely exacerbating the already severe water shortages in these areas. Local activists with shoestring budgets who oppose these injustices face immensely well-endowed company publicists who convince government officials that all will work out for the best. Meanwhile, the organizations in question assure the world at large that powerful AI will soon solve the problems of climate change, poverty, and the environment.

The empire metaphor that Hao uses in the title of her book is very apt. Powerful tech companies and their leaders do indeed resemble historical empires and empirebuilders in many respects, including their insatiable greed for wealth and power, alleged dishonesty and unscrupulousness, conviction that they are ultimately bettering the world, and blindness and lack of concern with any resulting damage.

Empire of AI ends on a more hopeful note. Hao acknowledges that there are better ways to build and use AI, describing a project by linguists Peter-Lucas Jones and Keoni Mahelona—in collaboration with the Maori community—that seeks to preserve the Maori language while maintaining deep respect for and sensitivity to the culture and its norms. Additionally, Hao applauds the global activities of environmental groups and social activists who oppose the destruction that high tech is creating. Personally, I am not sure that her optimism is warranted. While the AI industry could have initially taken other paths, those doors may have shut behind us. Sutskever and Dario Amodei have since left OpenAI to found companies that supposedly focus more heavily on AI safety, but we have yet to see concrete evidence that these corporations will be any better than OpenAI in practice. The corporate and political forces that drive AI in its current form are formidable. Now that the genie is out of the bottle, it will not be easy to put it back.



Empire of Al: Dreams and Nightmares in Sam Altman's OpenAl. By Karen Hao. Courtesy of Penauin Press.

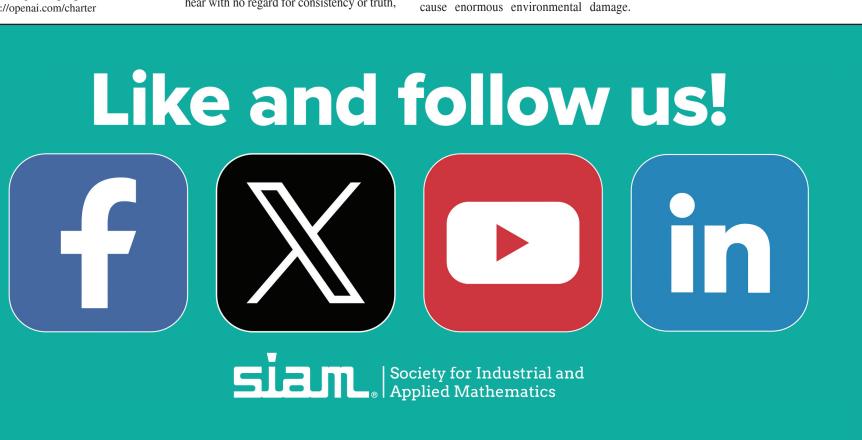
world of sociopathic billionaire technocrats.

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Spectral Geometry

Continued from page 10

representation of $g_t(x)$ is the matrix $D\Phi^t(x)^\top D\Phi^t(x)$ —i.e., the Cauchy-Green tensor for the flow of length t, initialized at x. Therefore, Δ^D is an average of Laplace-Beltrami operators for the Riemannian manifolds $(M,g_t),\ t\in [0,T]$. The leading nontrivial eigenvalue λ_2^D of Δ^D quantifies the global mixing that occurs over [0,T], while the dynamic Laplace operator provides a dynamic spectral geometry on manifolds that are subjected to general time-dependent nonlinear dynamics.

Dynamic Laplacian Eigenfunctions

To illustrate the way in which eigenfunctions of the dynamic Laplacian identify coherent features, we use a flow [10] to evolve the unit square $M\!=\![0,1]^2$ with time-dependent nonlinear dynamics Φ^t , $t\!\in\![0,1]$. Figure 2a (on page 10) depicts the leading nontrivial eigenfunction f_2^D and highlights two elliptical regions: one red and one blue. Each of these regions is a coherent set, with future evolutions in Figure 2b and 2c (on page 10). While the red and blue regions evolve, they do not mix; this is the essence of coherence.

Identification of Distinct Macrostructures

Multiple leading eigenfunctions of the dynamic Laplacian encode multiple coherent features, and spectral geometric theory utilizes additional eigenfunctions to underpin their use. Sometimes individual coherent features are not clearly represented in the eigenfunctions, necessitating a separation procedure. Sparse eigenbasis approximation (SEBA) [8] is a method that processes spectral clustering outputs to automatically disentangle distinct features; Figure 3 illustrates an example of SEBA in action. First, we use roughly 8,000 individual deepsea Argo float¹ trajectories to estimate the dynamic Laplacian; approximately 3,000 of these floats provide location signals in any given month [1]. In this dataset, only 10 percent of floats continue to transmit over the six years from 2011 to 2017. We then apply SEBA to the leading eight eigenfunctions of the dynamic Laplacian to separate the eight dominant coherent regions in the global ocean at a depth of 1,000 meters.

Emergence and Disappearance of Macrostructures

In many complex systems, multiple coexisting emergent features are ephemeral in

that they emerge and exist for some time before dissipating. Through a time expansion of the domain, we can "inflate" the dynamic Laplacian to create a spectral theory that also captures this emergence and disappearance [6]. In the resulting time expansion of the phase space, each Riemannian manifold (M,g_t) has its own t-fiber. Topologically, this time-expanded domain is simply

$$\mathbb{M} \coloneqq \bigcup_{t \in [0,T]} \{t\} \times M = [0,T] \times M.$$

The Inflated Dynamic Laplace Operator

To extend Δ^D from an operator on M to an operator on \mathbb{M}_0 , we apply Δ_{g_t} to the tth copy of M—i.e., to $\{t\} \times M \subset \mathbb{M}$ —for each t = [0,T]. We then employ diffusion in the temporal direction to dynamically connect the distinct t-fibers. In summary, we define a Laplace-Beltrami operator (the inflated dynamic Laplace operator) $\Delta_{G_a} \colon L^2(\mathbb{M}, G_a) \to L^2(\mathbb{M}, G_a)$, where the metric G_a is Euclidean in the time direction and g_t on each t-fiber:

$$\Delta_G F(t,x) = a^2 \partial_{tt} F(\cdot,x) + \Delta_{a} F(t,\cdot).$$

Researchers have used the associated spectral methodology to detect the breakup and reformation of atmospheric features, among other applications.

Emergent Structures in Complex Networks and Supra-Laplacians

In discrete settings, a graph or network replaces the manifold. Evolution on the network consists of temporal variation of edge weights, including their removal and insertion, as well as the addition or deletion of nodes. Instead of coherent sets, we search for time-evolving communities within the network where members of a single community are well connected by edges between community members; in contrast, members of distinct communities share relatively few connections. Scientists have utilized the dynamic Laplace matrix for graphs to spectrally study *persistent* time-varying communities [7].

Recent work [5] has adapted underlying theory and algorithms for the inflated dynamic Laplacian to supra-Laplacians on time-evolving graphs [11], leading to a greater theoretical understanding of these objects and the ability to detect changes via spectral methods in several communities over time. As a simple example, Figure 4a shows the leading nontrivial spacetime eigenvector of the supra-Laplacian [5] that was built from similarities [12] of U.S.

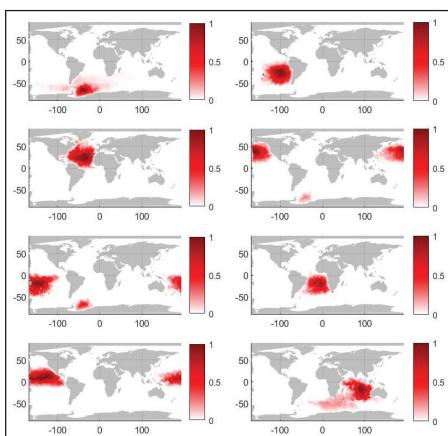


Figure 3. The application of sparse eigenbasis approximation (SEBA) to the leading eight eigenfunctions of the dynamic Laplacian in order to construct eight sparse SEBA vectors. Beginning in January 2011, each SEBA vector is supported in an individual coherent region of the deep ocean and remains coherent under ocean currents at a depth of 1,000 meters over a six-year duration (from 2011 to 2017). Figure courtesy of [1].

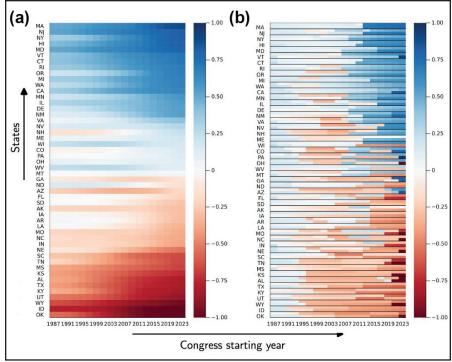


Figure 4. Quantification of political polarization in the U.S. Senate. **4a.** Leading nontrivial spatial eigenvector of a supra-Laplacian based on state voting similarities in the U.S. Senate. Deep red indicates strong membership in a Republican political bloc and deep blue indicates strong membership in a Democratic bloc. The evolution of membership in such groupings for each individual state is depicted horizontally. **4b.** The supra-Laplacian is built from the voting similarities of individual senators (two per state), which yield a larger eigenvector and more granular detail. A similar polarization in time is evident. Figure adapted from [5].

state voting patterns from 1987 to 2023. The deeper colors in recent years indicate the increasing polarization of U.S. politics over the last four decades. Similar calculations are possible at the level of individual U.S. senators during the same time period, where senators continually enter and leave a state's legislature (see Figure 4b). When mapped onto states, the leading nontrivial spacetime eigenvector of the supra-Laplacian for individual senators produces a more granular but consistent overall picture.

The advantages of spectral methods lie in their domain-global nature and computational accessibility. The aforementioned techniques—relevant to dynamics on both continuous and discrete domains—enable the application of spectral methods in time-varying dynamic settings and for the detection of multiple regime changes, such as the emergence of communities, coherent regions, and other macrostructures.

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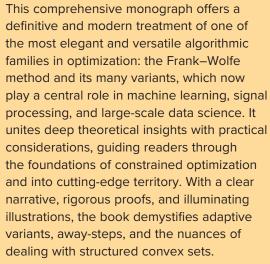
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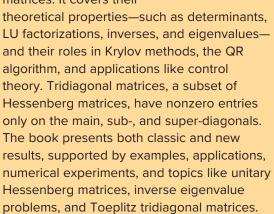
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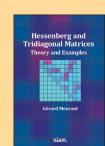
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