

## Bioinspired Nonlinear Flow Networks and Their Emerging Phenomena

By Miguel Ruiz-García and Eleni Katifori

Flow networks comprise a set of connections that carry and transport fluid. In linear networks, the current that circulates through each “duct” increases proportionally with the pressure difference between the inlet and outlet. But in animal and plant circulatory systems, each element’s resistance can be highly nonlinear. Due to the active nature of animal vessels [1, 6] or the presence of passive valves in plant vasculature [4], certain situations may manifest wherein the current *falls* as the pressure difference increases; such behavior is known as *negative differential resistance*.

Blood vessels are more like active organs than rigid ducts. Specifically, vascular musculature covers the arteries and allows them to contract or expand in response to different stimuli. For example, when a blood vessel that feeds an organ detects an increase in pressure at its inlet, it can respond by contracting (compressing its muscles) to reduce flow and protect the organ. This effect is called the *myogenic mechanism* [1], and similar circumstances

can cause a negative differential resistance in the flow through a blood vessel [6]. In plant vasculature, the xylem transports water from the roots to the leaves, ultimately forming a network of channels and valves (pit pores) that control the flow. These valves also present a highly nonlinear conductance with negative differential resistance [4]. Figures 1a and 1b depict schematics of both systems.

Inspired by the behavior of animal and plant vasculature, we recently proposed a model that accounts for these nonlinearities as well as volume accumulation/depletion in flow networks of any topology [5]. A set of nodes that are interconnected by edges form the network. Pressure is defined at each node ( $P_i$ ), and the flow through every edge depends on the pressure difference between the nodes that it connects:

$$I_{ij} \propto \Gamma(P_i - P_j).$$

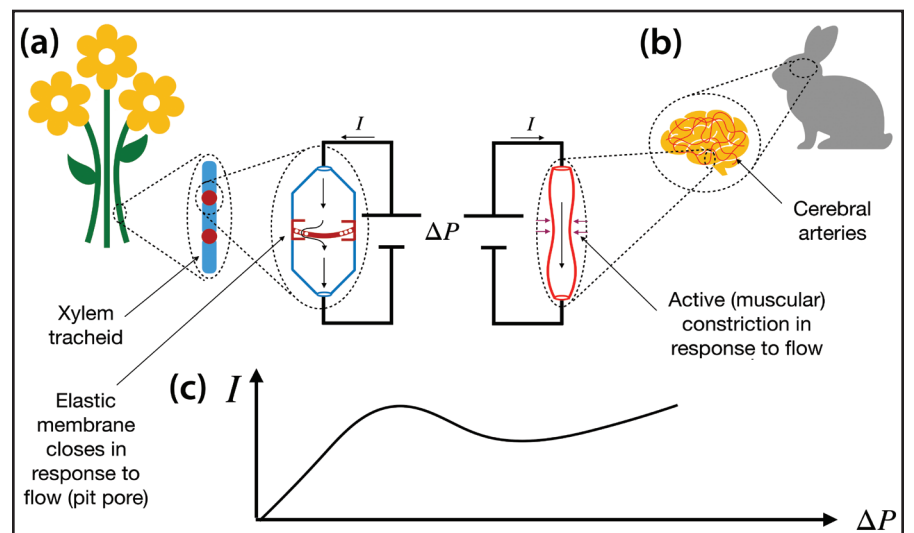
Here,  $\Gamma$  is a nonlinear function of  $\Delta P$  that may present a negative slope (see Figure 1c). In the biological systems that we model, the volume inside the network can change; for the sake of simplicity, we

account for this volume capacity at the nodes ( $V_i$ ). If the volume increases in one part of the network within the biological vasculature, it deforms the surrounding tissue and affects the pressure in nearby

regions. We model this effect by coupling volume accumulation and pressure:

$$V_i - 1 \propto \sum_k L_{ik} P_k,$$

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**Figure 1.** Nonlinear flow in plant and animal vasculature. **1a.** Zooming into the plant stem shows xylem tracheids and pit pores, which transport water from the roots to the leaves. **1b.** Zooming into the mammalian brain reveals the arteries that feed it. **1c.** When a pit pore [4] or cerebral artery [6] is isolated and connected to a pump, the flow ( $I$ ) that is measured as a function of pressure difference ( $\Delta P$ ) follows a nonlinear curve that reveals a region of negative slope (negative differential resistance). Figure courtesy of Miguel Ruiz-García.

## Multiscale Modeling of Dementia: From Proteins to Brain Dynamics

By Alain Goriely

At first, the signs were subtle; only a life of intimacy allowed his wife to notice the changes. At age 57, he had difficulty tying his necktie, could not properly handle the house finances, and seemed withdrawn. As these early lapses worsened, Mr. U, now aged 61, underwent a general neurological examination that appeared normal. However, a basic psychological test showed delayed recall and problems with episodic memory. A

magnetic resonance imaging (MRI) scan revealed broad cerebral atrophy and—together with advanced psychological tests—delivered the devastating diagnosis of probable Alzheimer’s disease. From then on, Mr. U experienced a well-known pattern of decline. He struggled with abstract reasoning, memory functions, and word retrieval, and could not properly visualize the world around him. At age 65, Mr. U exhibited global deterioration in his cognitive abilities — particularly verbal memory, language, motor control, face

recognition, and executive skills. Another MRI confirmed extended bilateral cerebral atrophy. Bouts of apathy, psychosis, and violent outbursts became more frequent.

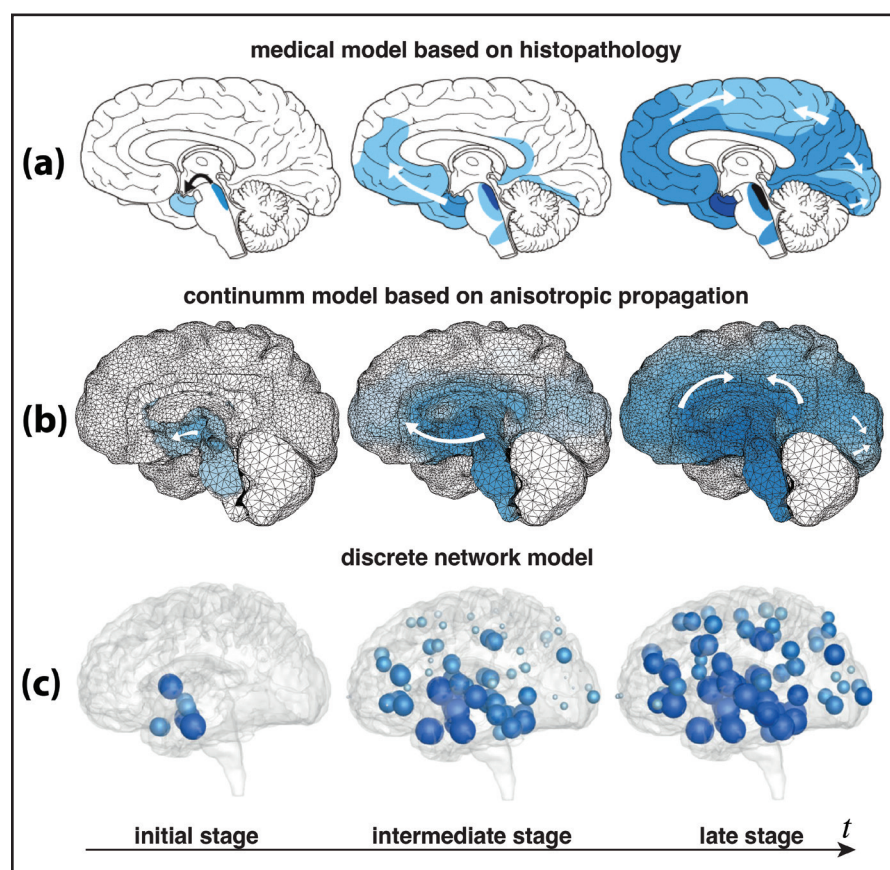
At age 70, Mr. U was a pale shadow of the man he once was. His wife could not manage his condition anymore and he was admitted to a nursing home. He died three years later from pneumonia.

### A Protein Story

Mr. U’s experience is unfortunately not unique, as the overall pattern of degeneration in Alzheimer’s patients is fairly homogeneous and systematic. The disease affects more than 50 million people worldwide and occurs in roughly one out of every nine adults over the age of 65. Unlike cancer and many viral and bacterial diseases, Alzheimer’s disease typically presents in codified stages that arise in most patients. This cognitive staging is associated with a systematic invasion of two key toxic proteins in the brain, which Alois Alzheimer identified in 1905: the well-known amyloid beta and the group of tau proteins that normally stabilize microtubules in axons.

Scientists believe that a misfolded version of tau acts as a template for healthy tau proteins and promotes the formation of increasingly sized oligomers, eventually leading to large aggregates that are evident in brain tissues after death [4]. While most drug trials focus on amyloid beta, the presence of toxic tau proteins is primarily correlated with brain atrophy and cognitive symptoms. The typical pattern of tau evolution—as measured through histological staining—is called Braak and Braak staging after neuroanatomists Eva and Heiko Braak, who first proposed the mechanism in 1991 [2]. It describes the disease’s evolution in six stages, beginning in the entorhinal cortex and evolving through the hippocampal region (which is associated with memory),

See **Dementia** on page 4



**Figure 1.** Progression of toxic tau proteins in the brain. **1a.** Medical staging based on histopathology (the analysis of postmortem brain slices). **1b.** Simulation of the anisotropic Fisher-Kolmogorov-Petrovsky-Piskunov (Fisher-KPP) model with the initial value in the entorhinal cortex. **1c.** Simulation of the network Fisher-KPP model with initial seeding at the entorhinal node. Figure adapted from [3].

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## 6 Ethical Concerns of Code Generation Through Artificial Intelligence

Many developers who release their code as open source also make their software available for community use with proper attribution and consent. However, artificial intelligence tools for code generation may replicate existing code and cause users to unknowingly violate copyright and licenses. Tim Davis and Siva Rajamanickam discuss this issue primarily in the context of GitHub Copilot.

## 8 Announcing the Newest SIAM Project NExT Fellows

As part of its dedication to the professional development of junior faculty, SIAM annually sponsors two Project NExT (New Experiences in Teaching) Fellows. Sachith Dassanayaka and Alice Schwarze—the 2023 SIAM Project NExT Fellowship recipients—collaborate with Kathleen Kavanagh to overview the program and discuss their goals and personal experiences in education.

## 8 On the Air

Atmospheric air pressure decreases roughly exponentially with height, under some assumptions. Mark Levi wonders how air pressure would change with depth in a shaft that is drilled through Earth's center. He explores this concept by first assuming the ideal gas law for air and taking the air temperature as constant, then addressing the role of gravity.

## 10 Thankful for the Commitment of the SIAM Community

Abby Addy joined SIAM in February 2022 as the Director of Development and Corporate Relations. She reflects on the generosity of SIAM members during her first year; notes the establishment of new programs and awards; discusses the wide-ranging impacts of donor initiatives; and encourages further conversation about philanthropy.

## 11 Taking the Plunge from Academia to Biotech

Though the division between academia and industry is becoming increasingly less opaque, information about industrial careers in biotechnology and pharmaceuticals is still somewhat scarce. A Q&A with applied mathematicians Andy Stein and Dean Bottino sheds light on various aspects of the biotech sector.

# Field-scale Modeling of Geological Carbon Storage

By Mohamad Jammoul, Mary F. Wheeler, and Mojdeh Delshad

Fossil fuels are the world's primary energy source and are expected to remain so for the foreseeable future. Carbon capture and storage (CCS)—which involves capturing carbon dioxide (CO<sub>2</sub>) and storing it underground—plays a key role in decarbonizing the power and industrial sectors. It also helps in meeting climate change mitigation targets as we transition into a lower-carbon energy world (see Figure 1).

## What is Carbon Sequestration?

CO<sub>2</sub> storage is the process of injecting captured CO<sub>2</sub> into geological formations such as deep saline aquifers, depleted oil and gas reservoirs, or unmineable coal seams. A major concern about carbon sequestration is the prediction of plume movement to ensure subsurface retention. CO<sub>2</sub> injection projects should assure safe storage in the subsurface for thousands of years. Primary containment mechanisms include structural trapping, dissolution, mineralization, and capillary trapping.

## Migration of CO<sub>2</sub> Plumes

Injected CO<sub>2</sub> remains at a supercritical state at the subsurface pressure and temperature. It is more buoyant than oil and water, and thus tends to migrate upwards. However, lower-permeability rock layers prevent buoyant CO<sub>2</sub> from reaching the surface. At the same time, CO<sub>2</sub>'s low viscosity (as compared to resident fluids) laterally moves it away from the injection wells. The heterogeneity in the rock formation—along with gravity forces—induces

a non-uniform migration of CO<sub>2</sub> (viscous fingers) as it continues to flow horizontally through the high-permeability layers and below the seal surface. After the injection of CO<sub>2</sub> stops, capillary and gravitational forces become more significant (see Figure 2, on page 5). As water starts to imbibe into the CO<sub>2</sub> plume, isolated CO<sub>2</sub> bubbles get trapped due to capillary forces; eventually, a significant fraction of the CO<sub>2</sub> plume is immobilized [10].

## Geochemical Reactions and Thermodynamic Effects

Another containment mechanism is the dissolution of CO<sub>2</sub> in brine. This process begins immediately after CO<sub>2</sub> comes in contact with water, slowly creating a denser mixture. The difference in density between the resident brine and CO<sub>2</sub>-rich brine causes instabilities in the system. The force that drives the CO<sub>2</sub> towards the surface is eventually eliminated, and the new mixture descends to the bottom of the aquifer as it forms gravity fingers. Geochemical reactions can also help immobilize CO<sub>2</sub> in the subsurface; the injected plume can react with existing minerals in the geologic formation, thus inducing precipitation of carbonates. This process occurs more slowly than other trapping mechanisms and might take place on a scale of tens or even hundreds of years [4].

Temperature changes during storage processes can impact the migration of CO<sub>2</sub> in the subsurface. For instance, varying temperatures alter fluid properties such as diffusion, density, and viscosity, which subsequently affect the storage dynamics across different scales. In fact, increases in

temperature and salt concentration decrease CO<sub>2</sub>'s solubility in brine and modify the interfacial tension, which in turn impacts hysteretic relative permeability and capillary pressure. Additionally, the drop in CO<sub>2</sub> temperature that is associated with the Joule-Thomson effect—which typically occurs in low-pressure reservoirs—induces the freezing of pore fluids or formation of hydrates, both of which can result in loss of injectivity [8]. Tracking these effects is one of the challenges that researchers face when developing models of multiphase flow in porous media.

## Geomechanics and Induced Seismicity

Temperature changes also induce geothermal stresses. Injected CO<sub>2</sub> is usually a lower temperature than the rock formation, and large differences in temperature between the injected fluid and formation can cause fractures and inadvertently lead to CO<sub>2</sub> leakage. Furthermore, the excessive increase in fluid pressure during the injection process might lead to rock failure. As such, evaluation of these stresses near the wellbore and seal rock layer is critical to project safety.

In addition, CO<sub>2</sub> injection affects the *in situ* fluid pressure and can induce seismic events. High injection rates may trigger open-mode fractures, while large injection volumes—even with low injection rates—can reactivate shear fractures and faults that generate earthquakes.

## Computational Science and the Geological Storage of CO<sub>2</sub>

The design of CO<sub>2</sub> storage projects aims to optimize CO<sub>2</sub> injection in the subsurface and assess the associated risks and consequences. In addition to the migration of CO<sub>2</sub>, numerical modeling must predict phase behavior, temperature changes, pressure buildup, geomechanical effects, and chemical reactions to ensure the safety of storage operations [5].

## Physics Modeling

The standard representation of the physical processes that contribute to CO<sub>2</sub> storage involves formulating them as a set of nonlinear partial differential equations (PDEs) [2]. Multiphase flow models simulate the migration of CO<sub>2</sub> by solving the conservation of mass equation for each component:

$$\frac{\partial(\phi \sum_{\alpha} \xi_{i\alpha} S_{\alpha} \rho_{\alpha})}{\partial t} + \nabla \cdot \sum_{\alpha} (\xi_{i\alpha} \rho_{\alpha} u_{\alpha} - \phi S_{\alpha} D_{i\alpha} \cdot \nabla(\rho_{\alpha} \xi_{i\alpha})) = \sum_{\alpha} q_{i\alpha}. \quad (1)$$

Here,  $\alpha$  refers to the phase and  $i$  refers to the component.  $S_{\alpha}$  is the saturation,  $\xi_{i\alpha}$  is the normalized mass fraction,  $\phi$  is the porosity,  $\rho_{\alpha}$  is the density,  $q_{i\alpha}$  is the rate of injection,  $u_{\alpha}$  is the flux, and  $D_{i\alpha}$  is the

See Carbon Storage on page 5

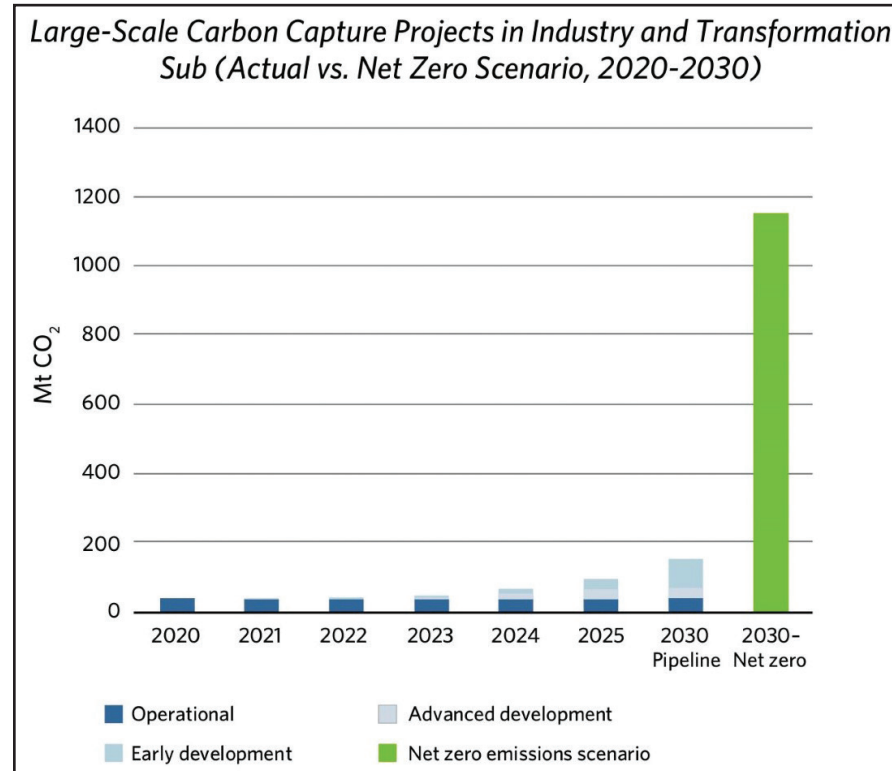


Figure 1. Comparison of the capacity of actual carbon capture projects versus the level of capture that is needed to achieve net-zero emissions. Figure courtesy of the International Energy Agency.

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# Broader Engagement Program Expands to the 2022 SIAM Conference on Mathematics of Data Science

By Malena Español, Shelby Horth, Mary Ann Leung, and Victoria Uribe

In 2015, Mary Ann Leung—president and founder of the Sustainable Horizons Institute<sup>1</sup> (SHI)—organized the first SHI Broader Engagement<sup>2</sup> (BE) program at a SIAM conference. The BE program offers financial assistance to members of underrepresented and underprivileged groups, allowing them full access to the robust programming at SIAM conferences. It also promotes mentorship, networking, and other activities to ultimately foster a sense of community and connect participants to one another. In addition, the program's various opportunities for scientists to volunteer, recruit, and learn encourage an overall feeling of inclusion and belonging.

The first BE program took place at the 2015 SIAM Conference on Computational Science and Engineering<sup>3</sup> (CSE15). Two years later, SHI began organizing Guided Affinity Groups (GAGs) during BE programming to enhance participants' conference experiences and heighten their relationships with SIAM. During daily GAG meetings, volunteers who are familiar with some of the conference's technical themes

recommend noteworthy sessions, answer any questions, and discuss conference presentations with attendees. Each group then shares their takeaways at the end of the week.

After a successful virtual event at CSE21,<sup>4</sup> BE returned with an in-person program<sup>5</sup> at the 2022 SIAM Conference on Mathematics of Data Science<sup>6</sup> (MDS22), which took place in San Diego, Calif., this September. Participating students had the

<sup>4</sup> <https://sinews.siam.org/Details-Page/growing-inspiring-and-diversifying-computational-science-and-engineering-through-broader-engagement>

<sup>5</sup> <https://shinstitute.org/be-mds-2022>

<sup>6</sup> <https://www.siam.org/conferences/cm/conference/mds22>

chance to explore recent advances in data science, advocate for science in their particular subfields, discuss their work with other attendees, contribute to their overall research profiles, and form meaningful relationships with professionals and/or future collaborators with similar interests.

At MDS22, volunteers managed the following six GAGs<sup>7</sup> on a variety of topics:

- Inverse Problems and Applications, led by Sean Ryan Breckling (Nevada National Security Site) and Malena Español (Arizona State University)

- Network Science: Connection, Computation, and Complex Systems, led

<sup>7</sup> <https://shinstitute.org/guided-affinity-groups-for-be-mds22>

by Philip Samuel Chodrow (Middlebury College) and Heather Zinn Brooks (Harvey Mudd College)

- Going Deep with Artificial Intelligence and Machine Learning for Science and Engineering, led by Alina Lazar (Youngstown State University) and Xiangyang Ju (Lawrence Berkeley National Laboratory)

- Implementing Artificial Intelligence in Healthcare: A Natural Language Processing Approach, led by Destinee Summer Morrow (Lawrence Berkeley National Laboratory)

- When Probabilistic Graphical Models Meet Deep Learning to Advance Machine Learning for Science, led by Talita Perciano (Lawrence Berkeley National Laboratory)

See **Broader Engagement** on page 6



Broader Engagement attendees and organizers gather for a group photo at a restaurant in the Old Town neighborhood of San Diego, Calif., during the 2022 SIAM Conference on Mathematics of Data Science, which took place this September. Photo courtesy of Angelica Valenzuela.

<sup>1</sup> <https://shinstitute.org>

<sup>2</sup> <https://shinstitute.org/the-broader-engagement-be-program>

<sup>3</sup> <https://archive.siam.org/meetings/cse15>

## Flow Networks

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where  $L_{ik}$  is the network's graph Laplacian. Finally, we must impose mass conservation at every node:

$$\frac{dV_i}{dt} = -\sum_k I_{ik}.$$

The previous equations form a system of nonlinear differential equations that we can apply to networks of any topology — i.e., each edge can connect any two nodes. Complex dynamical phenomena may thus emerge once we integrate the equations over time. When the network is large enough, it

can behave like an excitable system. An animation in the online version of this article demonstrates an example of this behavior, wherein we apply a constant direct current (DC) pump to the two sides of a rectangular network and allow the system to relax to a stationary situation (where all of the flows are constant). We then introduce a perturbation to the pressure boundary conditions, prompting the appearance of a travelling wave that moves from one side of the network to the other. We are unable to excite another wave in the presence of a previous one, which leads to a refractory time.

Yet contrary to other network models—in which the elements (edges or nodes) are intrinsically excitable—excitability emerges in our scenario as a collective phenomenon, given that our edges and nodes are simply passive elements that respectively conduct or store volume. Such behavior would be forbidden in a network of linear resistors because the flows within the network are uniquely determined by the boundary conditions; a perturbation at the boundary would instantaneously change the flows in the whole network, negating the possibility of observing travelling waves.

Another phenomenon that arises in these nonlinear flow networks is the appearance of self-sustained travelling waves (see Figure 2). Under the right circumstance (a certain range of model parameters) and with constant pressure boundary conditions (equivalent to a DC pump), the system does not find a stable stationary solution. Travelling waves nucleate at one contact and travel to the

other, recycling every time; these actions induce periodic oscillations in the current that runs through the pump [5]. Figure 2 depicts this behavior in a planar network with random connections and periodic spatial boundary conditions. The pump is connected to the blue and red nodes and imposes a constant pressure difference between them. Travelling waves nucleate around the blue node and move towards the red one until they disappear and recycle, generating periodic oscillations in the current (see Figure 2e). This behavior has an analog—called the Gunn effect—in the semiconductor realm, wherein negative differential resistance also leads to self-sustained oscillations of the current; in that case, however, the system is continuous and effectively one dimensional [2, 3].

To summarize, the nonlinear behavior of plant and animal vasculature inspired us to create a model for nonlinear flow networks of arbitrary topology. Our model displays a rich phenomenology that includes memory effects, excitability, and self-sustained oscillations, and we hope that it will enable further understanding of complex phenomena in the living realm. In the case of animal vasculature, the spontaneous emergence of hemodynamic fluctuations in the mammalian brain is particularly intriguing. When mice—or any mammal, for that matter—are resting or taking medication that suppresses brain activity, traveling waves of volume accumulation materialize in the arteries that surround the brain. Some researchers have suggested that a portion of these oscillations might have a non-neural origin [7]. Although this proposal is still under debate, it would be interesting to determine whether these waves are related to the negative differential resistance of the brain arteries, which would be reminiscent of the traveling waves that emerge in our theoretical model.

In the case of plant vasculature, it is especially striking that pit pores in the xylem transport network comprise a large region of negative differential resistance [4]. An exciting future research direction could investigate whether plants harness any of the collective phenomena that emerge when multiple nonlinear resistors are connected. For instance, we know that

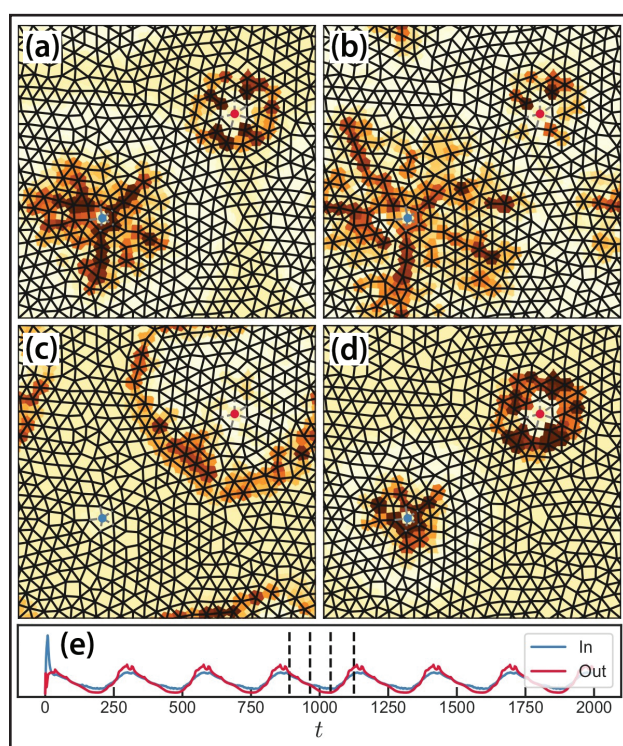
a pressure range wherein the flow is almost constant—independent of the amount of applied pressure—is present when many of these valves are connected in a series.

Ultimately, we hope that these results will motivate experimental researchers to build such systems in the laboratory. Harnessing the complex phenomenology of our model in practice could give rise to new and exciting technologies.

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**Figure 2.** Travelling waves in a nonlinear flow network. The planar network has random connections, an average node degree of 5.5, and periodic spatial boundary conditions. **2a–2d.** The area around each node is colored according to its volume ( $V_i$ ); darker colors correspond to higher volumes. The red and blue nodes maintain a constant pressure difference because they are connected to a direct current pump. Self-sustained waves emerge spontaneously, nucleating in the blue node and travelling to the red one to recycle again. **2e.** A plot of the current that travels from the pump into the blue node and the current that travels from the red node out to the pump. These quantities do not have to be equal because the volume inside the system can change. Dashed lines correspond to the snapshots in 2a-2d. See the online version of this article for an associated animation. Figure courtesy of Miguel Ruiz-García.



## Dementia

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the temporal lobe, the occipital lobe, and all regions of the neocortex. The lesions in each region worsen with time.

Alzheimer's disease is rather intimidating from a modeling perspective. Nevertheless, the systematic pattern of invasion through the brain—and the resulting cognitive effects—suggest that some simple underlying features of the brain may be responsible for the spatiotemporal pattern. Together with Ellen Kuhl of Stanford University, I therefore sought to obtain minimal mathematical models based on clear principles that can capture staging at the brain level as well as other characteristics of the disease, such as brain atrophy and changes in overall brain dynamics.

### Fisher-KPP Strikes Again

From a phenomenological point of view, we must consider three processes: transport, expansion, and saturation. During *transport*, toxic proteins move throughout the brain primarily along axonal bundles, which connect different regions and act as information highways. *Expansion* refers to the autocatalytic nature of the aggregation process, which leads to an initial exponential increase of small toxic populations. And *saturation* means that each region can only support a certain level of toxic proteins. A canonical model for such a process in a continuum medium is the celebrated Fisher-Kolmogorov-Petrovsky-Piskunov (Fisher-KPP) equation. If  $c(x, t) \in [0, 1]$  is the scaled concentration of the toxic protein, the equation reads

$$\frac{\partial c}{\partial t} = \nabla \cdot (\mathbf{D} \nabla c) + \alpha c(1 - c). \quad (1)$$

Here,  $\alpha > 0$  is the growth rate and  $\mathbf{D}$  is a transversely anisotropic diffusion tensor with a strong preferential direction along

the axonal bundle. Under generic conditions, we can obtain this model as a normal form of the full aggregation-fragmentation equations that track the evolution of differently sized oligomers [7]. The parameters can hence directly relate to the aggregation and clearance rates at the microscopic level.

After using MRI scans to obtain both the full brain geometry and the direction of axonal bundles, we began with an initial seed of toxic proteins in the entorhinal cortex and simulated the evolution of the brain's field (see Figure 1, on page 1). The results were striking. Without any other ingredients, the dynamics that we obtained from this minimal model recovered the disease's basic dynamics in great detail [8]. When we apply the same model to other neurodegenerative diseases that are associated with different toxic proteins—such as  $\alpha$ -synuclein for Parkinson's disease or TDP-43 for amyotrophic lateral sclerosis—it also reproduces their basic spatiotemporal patterns as well as the atrophy patterns obtained from finite-element simulations; the only difference is the region and extent of seeding. Despite the complexity and diversity of these diseases, universal features of progression emerge from the combination of an autocatalytic process and transport in an anisotropic medium.

### The Role of Topology

When such strong universal patterns appear, a natural question emerges: What essential features are responsible for the invasion pattern? Since we cannot further simplify the autocatalytic dynamics, we investigated the transport term and decided to test our hypothesis that the observed patterns are a consequence of the strong transport anisotropy along the axonal bundles. These bundles serve as more than information highways; they also efficiently carry toxic proteins across the brain. We can assess this idea by coarse graining the brain and considering multiple regions

and the connections between them. We then replace the full brain with a network called the *connectome*, wherein each node is a region and edges represent the possible connections between regions. This approach constitutes the basis for a large field of neuroscience, and various groups have successfully used the connectome to examine the effects of protein diffusion in the brain [6].

The natural discretization of the diffusion operator on a network is the weighted graph Laplacian  $\mathbf{L}$ , whose weights are proportional to the number of connections and inversely proportional to the distance squared between nodes. We then define  $c_i(t)$  as the concentration of toxic proteins at node  $i$ , which establishes the discrete Fisher-KPP as

$$\dot{c}_i = -\rho \sum_{j=1}^N L_{ij} c_j + \alpha c_i(1 - c_i), \quad (2)$$

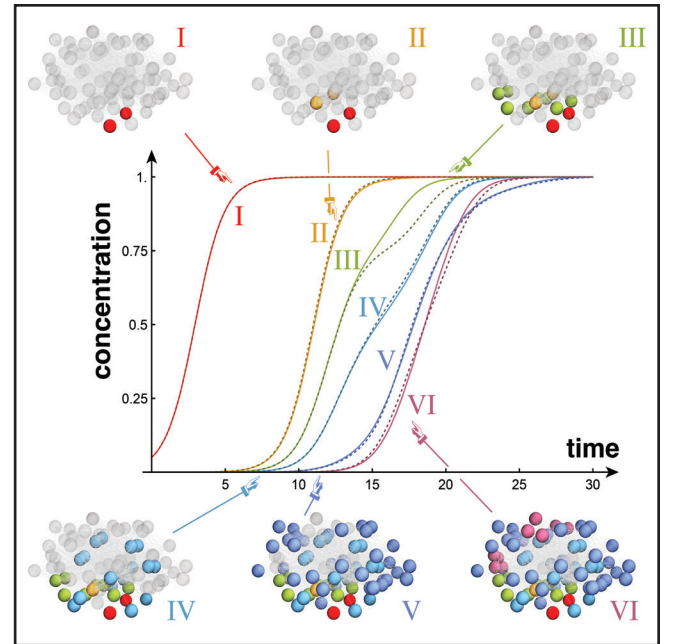
$$i = 1, \dots, N.$$

This system of nonlinear ordinary differential equations is an excellent approximation of the dynamics that are generated by the full nonlinear partial differential equations (1) with which we started [3]. Mathematically, there are two regimes of interest depending on the ratio  $\rho/\alpha$ . In the diffusion-dominated regime ( $\rho/\alpha \gg 1$ ), the system behaves mostly homogeneously and the concentration of toxic proteins uniformly increases in all regions (as evidenced in the propagation of amyloid beta). However, our systematic study of data from the Alzheimer's Disease Neuroimaging Initiative<sup>1</sup> used hierarchical Bayesian parameter inference to demonstrate that the evolution of tau proteins occurs in the growth-dominated regime ( $\rho/\alpha \ll 1$ ), where the primary seed invades each region. In this regime, we can implement a systematic nonlinear perturbation method to obtain an approximation of the solution (see Figure 2). We can also attach a metric to the graph based on the dynamics that provides a natural notion of propagation times between different regions [5]. Combining analytical and computational results revealed that brain topology strongly constrains the dynamics in the early stages of Alzheimer's disease; in the latter stages, a balance of protein kinetics and geometry controls the dynamics.

Despite its simplicity, our network model serves as a basic starting point to study many different aspects of Alzheimer's disease and test possible mechanisms. In more recent work, we considered local variations in parameters that are associated with brain inhomogeneity; identified topological signatures of the disease in graph space; and studied the coupling between amyloid beta and tau proteins, the role of clearance in the initiation and dynamics of Alzheimer's, and the interactions between the microvasculature and toxic proteins. In addition, we analyzed the perplexing brain activity dynamics in patients who typically show periods of hyperactivity followed by hypoactivity and a shift in brain wave frequencies. When coupled to so-called *neuronal mass models* for brain activity, the same model allowed us to test multiple hypotheses and conclude that local damage to particular groups of neuronal cells is most likely responsible for these observations [1].

### Modeling Matters

The difficulty of modeling Alzheimer's disease stems from its combination of multiple effects at different scales—from indi-



**Figure 2.** Average concentration of toxic proteins in each Braak region. The solid curves represent the numerical solutions and the dashed curves are their approximations, which result from a nonlinear perturbation expansion. Initial conditions ensure that the total concentration is 1/10 (Braak I) in the entorhinal cortex nodes and zero for all other nodes (parameters  $N=83$ ,  $\alpha=0.5/\text{year}$ , and  $\rho=0.01/\text{year}$ ). Figure adapted from [5].

vidual proteins to the entire brain—with interactions that transpire over decades in a highly complex environment. Yet this scenario is exactly the playground of modern applied mathematics. Models help us test hypotheses and identify key mechanisms that lead to possible therapeutic targets. In particular, we can match progression models to imaging data at the macroscopic level, to the parameters that enter aggregation-fragmentation models at the microscopic level, and to clearance rates at the cellular level. Such multiscale, multiphysics interactions are key to understanding and treating diseases like Alzheimer's. At the mathematical level, they represent a formidable and exciting intellectual challenge that synthesizes fields such as nonlinear partial differential equations, networks, dynamical systems, continuum mechanics, mathematical neuroscience, and topological data analysis.

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<sup>1</sup> <https://adni.loni.usc.edu>

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## Carbon Storage

Continued from page 2

diffusion-dispersion tensor. Darcy's constitutive law describes the flux for each phase in the porous medium:

$$u_\alpha = -K \frac{k_{ra}(S_\alpha)}{\mu_\alpha} (\nabla P_\alpha - \rho_\alpha g \nabla z). \quad (2)$$

Here,  $K$  is the absolute permeability of the porous rock matrix,  $k_{ra}$  is the relative permeability,  $\mu_\alpha$  is the viscosity,  $z$  is the depth,  $g$  is the gravitational force, and  $P_\alpha$  is the pressure. The resulting system of PDEs is closed by the capillary pressure relation and the constraint on phase saturation. Flash calculations that comprise a set of thermodynamic equilibrium equations provide the mole fraction of each component in every phase.

Heat transfer also plays an important role in such problems because thermal energy can affect phase behavior and mechanical stresses. The conservation of energy equation can predict the changes in temperature in the reservoir:

$$\frac{\partial(TU_T)}{\partial t} + \nabla \cdot \left( \sum_\alpha \rho_\alpha C_{pa} u_\alpha T - \lambda \nabla T \right) = q_H, \quad (3)$$

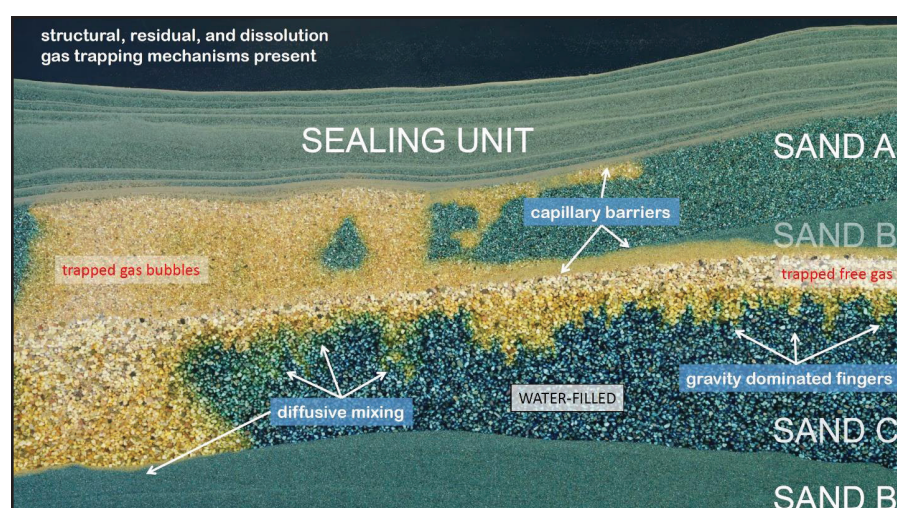
where  $T$  is the reservoir temperature,  $U_T$  is the effective heat capacity,  $C_{pa}$  is the isobaric molar specific heat,  $\lambda$  is the effective rock thermal conductivity, and  $q_H$  is the heat source/sink term.

Mechanical stresses and geochemical reactions can likewise impact  $\text{CO}_2$  storage processes. Researchers usually obtain geochemical deformations and stresses via elasticity solutions, with special treatment for handling fractures. Reservoir simulators can model different aqueous and mineral dissolution/precipitation reactions, but the main interest in storage simulations is the formation of carbonic acid and precipitation of calcium carbonate. Kinetic, equilibrium, or Monod models can represent these reactions [5].

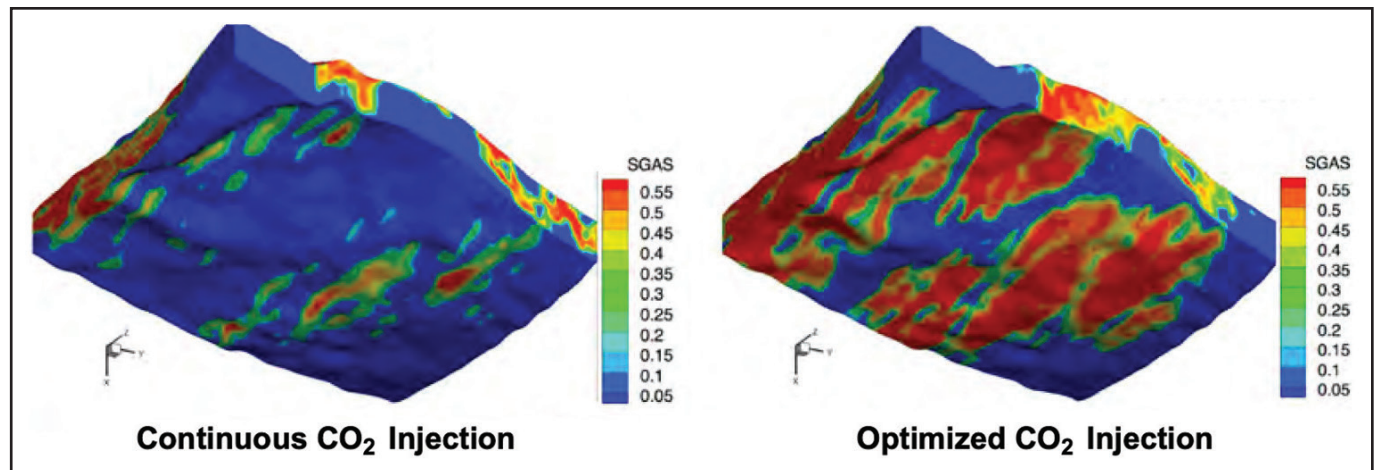
### Numerical Challenges

Accurate modeling of the aforementioned phenomena requires large-scale simulations of physical processes over long periods of time. However, such simulations pose a significant challenge due to the complexity of the coupled processes, broad range of temporal and spatial scales, and uncertainty of subsurface characterization [6].

Previous studies have utilized various numerical discretization schemes to solve the differential equations, including variants of the finite difference, finite volume, and finite element methods. The flow and transport equations typically require a local mass conservative scheme because violation of this property may lead to spurious sources and sinks, which cause substantial numerical inaccuracies and lead to overshoots and undershoots. Such problems can become exacerbated when chemical reactions are present in the system. Mixed finite element and finite volume schemes are popular tools for solving these equations because they enforce continuity of fluxes across element interfaces.



**Figure 2.** Experimental setup for carbon dioxide ( $\text{CO}_2$ ) injection. Structural, capillary, and dissolution gas trapping mechanisms are readily apparent. Diffusive mixing and gravity dominated fingers are also present. Figure courtesy of [9].



**Figure 3.** Comparison of the distribution of carbon dioxide ( $\text{CO}_2$ ) in the Cranfield reservoir. An optimized injection schedule leads to significantly more subsurface storage. Figure courtesy of [7].

The presence of distinct geological features—such as anisotropic permeability, heterogeneous layers, faults, and other internal boundaries—may require the use of unstructured or non-matching grids in local subdomains. Moreover, mesh refinement is necessary to capture transport phenomena like viscous fingering and diffusion.

The disparity between the space and time scales of different processes severely complicates modeling of the macroscale behavior of  $\text{CO}_2$  storage. The computational domain of a typical reservoir includes millions of grid cells that need to simulate  $\text{CO}_2$  dispersion and the accompanying processes for thousands of years. As such, the numerical performance of the reservoir simulator is a key factor in sequestration studies; using efficient algorithms, optimizing discretization methods, developing compatible solvers, and adopting large-scale parallelization strategies all help to enable field-scale simulations.

The uncertainty in geological characterization adds yet another level of complexity to subsurface reservoir modeling. To better assess the environmental risks, researchers usually report quantities of interest as confidence intervals via ensemble runs or Monte Carlo approaches that require thousands of simulations. However, the computational burden of high-fidelity simulations precludes their employment for such applications; even a single field-scale simulation can sometimes be computationally prohibitive.

### Practical Approaches

Site-specific conditions may permit researchers to simplify numerical and physical models in order to speed up calculations [1]. In deep formations, *ad hoc* correlations can estimate phase behavior when the changes in fluid properties are limited. Small temperature gradients warrant the assumption of an isothermal condition in the subsurface; likewise, formations with low stress sensitivity allow one to ignore the geomechanical calculations. Similarly, the reservoir's mineralogy indicates the need (or lack thereof) to model chemical reactions. Adoption of these assumptions relies on empirical parametrizations that are inferred from laboratory experiments.

From a numerical standpoint, researchers can use the hierarchy of distinct time scales to speed up the calculations by employing different coupling schemes for physical processes and adopting multirate formu-

lations. Scientists have applied reduced-order models and upscaling approaches to generate models with less grid points in space and time. These models require fewer computational resources and can survey the parameter space in optimization studies for field development (e.g., well placement) or operations like water- and surfactant-alternating-gas injections (see Figure 3). Researchers have also utilized reduced-order models in closed-loop reservoir management workflows for real-time assessment of sequestration operations based on sensor data.

### Looking Forward

The synergy between the generation of energy and minimization of associated drawbacks for the environment has become one of the foremost modern-day challenges. Geological CCS can help address this conundrum by bringing carbon under control and reversing rising emission levels. At the same time, the scientific fundamentals of  $\text{CO}_2$  sequestration are very similar to those of natural gas projects. Advances in the CCS field can therefore benefit other clean energy technologies, such as underground hydrogen storage [3]. Continued developments in modeling and monitoring capabilities for CCS projects will enable more efficient and cost-effective decision-making and help meet the world's energy needs.

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# Ethical Concerns of Code Generation Through Artificial Intelligence

By Tim Davis and  
Siva Rajamanickam

Machine learning models that are trained on large corpuses of text, images, and source code are becoming increasingly common. Such models—which are either freely available or accessible for a fee—can then generate their own text, images, and source code. The unprecedented pace of development and adoption of these tools is quite different from the traditional mathematical software development life cycle. In addition, developers are creating large language models (LLMs) for text summarization as well as caption and prompt generation. LLMs are fine-tuned on source code, such as in OpenAI Codex,<sup>1</sup> which yields models that can interactively generate code with minimal prompting. For example, a prompt like “sort an array” produces code one line at a time that a programmer can then either choose to accept or use to generate a match for an entire sort routine.

Examples of fine-tuned LLMs for code generation include GitHub Copilot<sup>2</sup> and

Amazon CodeWhisperer.<sup>3</sup> These models bring exciting possibilities to programmer productivity, bug detection during software development, and the translation of legacy code to modern languages. While the authors of these tools have addressed some potential issues in the codes—including bias and security implications—we want to highlight another pitfall in these fine-tuned models. The machine learning community is generally cognizant of matters like bias, but discussions about copyright and license issues in fine-tuning language models are far less common. In fact, the initial documentation for GitHub Copilot stated that “the code belongs to you” (this wording was recently revised).

SIAM members have invested considerable effort in the design and development of mathematical software packages that collectively build a software ecosystem that enables complex modeling and simulation on high-performance computing hardware. Several such open-source software packages are available at various levels of abstrac-

tion, from low-level dense linear algebra operations (i.e., BLAS and LAPACK) to sparse linear algebra libraries (i.e., CSparse, SuiteSparse, and Kokkos Kernels) and large frameworks (i.e., Trilinos) and ecosystems (i.e., xSDK). All of these libraries have well-defined interfaces and work smoothly together. They are also generally available both within their organizational GitHub accounts and through multiple other accounts, as permitted in their licenses. Many developers who release their code as open source also make their software readily accessible for community use (sometimes for profit) with proper attribution and consent of the copyright holders.

Since these codes are public, a human can intentionally copy code while knowingly violating copyright and licenses. If such a person actively asks an artificial intelligence (AI) tool to do so with a prompt like “sparse matrix vector multiply from Kokkos Kernels,” we would prefer that the system block these types of explicit requests. However, a bigger problem is that the AI system can put innocent users unintentionally in violation of copyright and

licenses. Here we demonstrate that GitHub Copilot emits CSparse<sup>4</sup> code (copyrighted by Tim Davis of Texas A&M University) almost verbatim, even with a generic prompt.

## GitHub Copilot Example

With a very simple sequence of prompts, GitHub Copilot emits 40 of the 64 functions from CSparse/CXSpase—a package that is protected by the GNU Lesser General Public License—which accounts for 27 percent of its 2,158 lines of code. The first prompt is “// sparse matrix transpose in CSC format”, followed by nine repetitions of enter, tab, ..., enter, and then control+enter. This prompt has no connection with the CSparse package (CSC is a common acronym for a sparse matrix data structure).

Copilot’s emitted code did not initially reproduce the CSparse copyright and license. But the prompt “// print a sparse matrix” did eventually cause Copilot to emit a near-verbatim copy of the CSparse `cs_print` function that included an incorrect

See Code Generation on page 7

<sup>4</sup> <https://github.com/DrTimothyAldenDavis/SuiteSparse>

<sup>1</sup> <https://openai.com/blog/openai-codex>

<sup>2</sup> <https://github.com/features/copilot>

<sup>3</sup> <https://aws.amazon.com/codewhisperer>

## Broader Engagement

Continued from page 3

- Optimize Everything!, led by Stefan Wild (Argonne National Laboratory).

Students also enjoyed daily breakfasts with their GAGs and SIAM leadership.

Participants of the MDS22 BE program attended panel discussions, delivered lightning talks to practice communicating their research, and partook in the Poster Session and Reception. Adrian De La Rocha Galan, a BE student from the University of Texas at El Paso, even received one of the meeting’s six Best Poster Awards. In addition, scientists from several national laboratories and universities throughout the U.S. organized multiple BE tutorials that were open to all conference registrants:

- Fundamentals of Accelerated Data Science with RAPIDS, a two-part session led by Xi Chen (University of Kentucky)

- Data Science with Julia and Julia for Python Programmers, both led by Johannes P. Blaschke (Lawrence Berkeley National Laboratory)

- Hands On High-performance Computing Crash Course, a two-part session led by Suzanne Parete-Koon and Leah Huk (both of Oak Ridge National Laboratory)

- Introduction to Graph Neural Networks, led by Alina Lazar (Youngstown State University) and Xiangyang Ju (Lawrence Berkeley National Laboratory)

- Best Practices and Tools for Secure Scientific Software Development, led by Nitin Sukhija (Slippery Rock University).

Upon the conclusion of MDS22, several BE participants shared testimonials about their experiences in the program. Shelby Horth, an undergraduate applied mathematics student at Wake Forest University, spoke highly of both her first BE experience and her first time at a conference. “It was inspiring to see so many like-minded individuals striving for success,” she said. “The abundance of support that I received from this incredible community definitely reinforced my enthusiasm for applied mathematics and data science. It was great to interact with such encouraging mentors and professionals across many disciplines, and to witness cutting-edge research from various domains. I made many new and hopefully long-lasting connections, and I can confidently say that this experience has motivated me to continue attending conferences and engaging with the opportunities that SIAM has to offer.”

Victoria Uribe, a Ph.D. student in applied mathematics at Arizona State University, had a similarly positive outlook. She had previously engaged in the virtual BE program during CSE21 and was glad to attend MDS22 in person. “The GAG breakfasts gave us an opportunity to network with other participants before the start of the daily sessions, and overall participation in the BE program provided us with a group of new friends with whom to attend the conference,” she said. “I was particularly excited for the tutorials and was not disappointed. The tutorial leaders were extremely friendly and supplied us with all of the materials

that we needed to work at our own pace. I am very thankful to have been a part of BE again and attended MDS22.”

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inverse problems, image processing, and materials science. Shelby Horth is an undergraduate student in applied mathematics at Wake Forest University. Mary Ann Leung is founder and president of the Sustainable Horizons Institute. Victoria Uribe is a Ph.D. student in applied mathematics at Arizona State University.



Broader Engagement program participants enjoy breakfast with their Guided Affinity Groups and SIAM leadership during the 2022 SIAM Conference on Mathematics of Data Science, which took place in San Diego, Calif., in September. Photo courtesy of Victoria Uribe.

## APPLICATIONS BEING ACCEPTED

### Gene Golub SIAM Summer School

The summer school will take place from July 30–August 12, 2023, at Lehigh University, Bethlehem, Pennsylvania U.S.

#### Quantum Computing and Optimization

By harnessing the properties of subatomic particles, quantum computing (QC) has the potential to radically transform our capability to solve extremely difficult decision-making and optimization problems for which no efficient classical algorithms exist. The goal for this program is to help build the next generation of QC researchers by bringing together QC and optimization experts and students in an inquiry-based learning environment. We will provide a concentrated review of necessary prerequisite math, optimization, and classical and quantum computing material. The QC-specific curriculum will then be broken into three parts: Foundations of QC, Quantum optimization techniques, and Advanced QC topics and applications. Students will work closely with lecturers to apply their learning by engaging in interactive seminars and labs.

The summer school will be held at Lehigh University, Bethlehem, PA, from July 30 to August 12, 2023. In-person attendance is required. Graduate and advanced undergraduate students highly motivated to learn QC and optimization techniques are encouraged to apply. Experience in QC or optimization is not required to join the program. Applications will be accepted beginning in December 2022.

For additional information, please visit [SIAMquantum.lehigh.edu](https://SIAMquantum.lehigh.edu) or contact [g2s3quantum-list@lehigh.edu](mailto:g2s3quantum-list@lehigh.edu).



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Application deadline: February 15, 2023.

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## Code Generation

Continued from page 6

copyright statement (wrong date, wrong version, wrong institution, and no license). The query “// sparse symbolic QR factorization” emitted a sparse upper triangular solve function from CSparse (the wrong method) that was prefaced with comments that contained an incorrect copyright and license. Copilot does not preserve license and copyright comments; instead, it treats them as mere text. Moreover, users are not warned that the discharged copyright and license statements can be incorrect.

Copilot’s first emitted function was nearly identical to `cs_transpose`. Figure 1 shows the original code from CSparse v2.0.1 (©2006 Timothy Davis), which uses Gustavson’s algorithm [2]. The code also appears in its entirety with permission in Davis’ *Direct Methods for Sparse Linear Systems*, which was published by SIAM in 2006 [1].

Figure 2 illustrates all of the changes in the code that Copilot produced. Yellow denotes the trivial changes: a few comments, the order of variable declarations (`w`, `m`, and `n`), and a single global replacement of `C` with `AT`. However, red indicates four changes in logic that affect the compiled code. The original code in Figure 1 is bug-free, but Copilot inserted a serious bug in Figure 2 that causes a segmentation fault (a security flaw). A naive Copilot user would likely miss this fatal flaw because the code’s execution would not always trigger it.

Copilot refers to many CSparse functions by their original names (the `cs` data structure as well as functions `CS_CSC`, `cs_salloc`, `cs_calloc`, `cs_cumsum`, and `cs_done`). Entering a subsequent empty prompt (control-enter+tab) often emits these functions verbatim, though doing so sometimes requires a prompt with the name that Copilot has already provided.

Microsoft (the owner of GitHub) distributes CSparse/CXSpase through many channels, respecting the software license and preserving copyright statements in each case. By discarding copyright and license information for CSparse/CXSpase and injecting bugs into a near-verbatim copy, Copilot sows confusion into Microsoft’s own code base.

Davis is communicating with the GitHub team about these issues. While developers are currently addressing certain problems, the inclusion of copyrighted open-source software in training data and its reproduction without the correct license or copyright remains unremedied. GitHub has announced plans for a forthcoming mechanism (arriving in 2023) that will provide links to software packages with attribution and license information when Copilot emits code that is a near-match.

### BigCode Project

Unlike GitHub Copilot, the BigCode project<sup>5</sup> excludes copyleft code from its training data and offers an opt-out option, though developers can only remove their own repositories. CSparse and many other widely used packages are often copied verbatim into other GitHub repositories (almost always while preserving copyright and license information), but neither Copilot nor BigCode provide attribution, copyright, or licenses for code that they emit. However, BigCode is actively working to amend this matter.

### OpenAI Codex

GitHub Copilot is based on OpenAI Codex. When given a similar prompt, Codex also produces `cs_transpose` essentially verbatim with no attribution, copyright, or license acknowledgment. In fact, the end user is unwittingly instructed to violate copyright; the OpenAI Sharing

<sup>5</sup> <https://www.bigcode-project.org>

& Publication Policy<sup>6</sup> states that “Creators who wish to publish their first-party written content ... created in part with the OpenAI API are permitted to do so,” under the condition that “the published content is attributed to your name or company.”

Furthermore, the OpenAI Content Policy<sup>7</sup> does not list copyright or license violations as one of its hazards, though it did previously offer the following warning (which has since been removed): “*Hallucinations*: Our models provide plausible-looking but not necessarily accurate information. Users could be misled by the outputs if they aren’t calibrated in how much they should be trusted. For high-stakes domains such as medical and legal use cases, this could result in significant harm.” We feel that stripping a code of its attribution, copyright, and license and injecting security flaws can result in significant harm in *any* domain, not just medical and legal settings.

### Possible Paths Forward

Despite the pitfalls, we do believe that it is possible to address the aforementioned issues and enable the future use of these tools within large, complex science and engineering codes. Most importantly, such fine-tuned models must allow for the correct attribution of the generated code and the proper copyright and license. We are excited by this potential development, as it would permit non-expert users to easily access some of our complex mathematical libraries. We would also like the programs to generate calls to libraries such as CSparse, rather than simply generating the code. Doing so would facilitate the use of these libraries as building blocks—as they were originally intended—instead of replicating the library

<sup>6</sup> <https://openai.com/api/policies/sharing-publication>

<sup>7</sup> <https://beta.openai.com/docs/usage-policies/content-policy>

code itself within multiple user codes. As such, the AI models must be able to distinguish versioning and interface changes. Finally, a true opt-out option that provides code owners with the choice to omit copies of their code in training would give owners more agency over their own work.

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```
#include "cs.h"
/* C = A' */
cs *cs_transpose (const cs *A, int values)
{
    int p, q, j, *Cp, *Ci, n, m, *Ap, *Ai, *w;
    double *Cx, *Ax;
    cs *C;
    if (!CS_CSC (A)) return (NULL); /* check inputs */
    m = A->m; n = A->n; Ap = A->p; Ai = A->i; Ax = A->x;
    C = cs_salloc (n, m, Ap [n], values && Ax, 0); /* allocate result */
    w = cs_calloc (m, sizeof (int)); /* get workspace */
    if (!C || !w) return (cs_done (C, w, NULL, 0)); /* out of memory */
    Cp = C->p; Ci = C->i; Cx = C->x;
    for (p = 0; p < Ap [n]; p++) w [Ai [p]]++; /* row counts */
    cs_cumsum (Cp, w, m); /* row pointers */
    for (j = 0; j < n; j++)
    {
        for (p = Ap [j]; p < Ap [j+1]; p++)
        {
            Ci [q = w [Ai [p]]++] = j; /* place A(i,j) as entry C(j,i) */
            if (Cx) Cx [q] = Ax [p];
        }
    }
    return (cs_done (C, w, NULL, 1)); /* success; free w and return C */
}
```

Figure 1. The original function `cs_transpose` from CSparse v2.0.1, ©2006 Timothy Davis. The yellow and red highlights identify areas that were subsequently altered in Copilot’s version of the code. Figure courtesy of Tim Davis.

```
// sparse matrix transpose in CSC format
// (9 lines of comments omitted here)
#include "cs.h"
cs *cs_transpose (const cs *A, int values)
{
    int p, q, j, *ATp, *ATi, *w, m, n, *Ap, *Ai;
    double *ATx, *Ax;
    cs *AT;
    if (!CS_CSC (A)) return (NULL); /* check inputs */
    m = A->m; n = A->n; Ap = A->p; Ai = A->i; Ax = A->x;
    AT = cs_salloc (n, m, Ap [n], values && Ax, 1= NULL, 0); /* allocate result */
    w = cs_calloc (m, sizeof (int)); /* get workspace */
    if (!AT || !w) return (cs_done (AT, NULL, w, 0)); /* out of memory */
    ATp = AT->p; ATi = AT->i; ATx = AT->x;
    for (p = 0; p < Ap [n]; p++) w [Ai [p]]++; /* row counts */
    cs_cumsum (ATp, w, m); /* row pointers */
    for (j = 0; j < n; j++)
    {
        for (p = Ap [j]; p < Ap [j+1]; p++)
        {
            ATi [q = w [Ai [p]]++] = j; /* AT(i,j) is the pth entry in A */
            if (ATx) ATx [q] = Ax [p];
        }
    }
    return (cs_done (AT, NULL, w, 1)); /* success; free workspace, return result */
}
```

Figure 2. The code that Copilot emitted, which began with the prompt “// sparse matrix transpose in CSC format” (colored in cyan). The red and yellow highlights illuminate the differences between the two versions; yellow represents trivial alterations and red represents significant changes in logic. Figure courtesy of Tim Davis.

DEPARTMENT OF ENERGY

# COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP

The DOE CSGF is open to senior undergraduates and students in their first year of doctoral study.



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The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) provides up to four years of financial support for students pursuing doctoral degrees in fields that use high-performance computing to solve complex problems in science and engineering.

The program also funds doctoral candidates in applied mathematics, statistics, computer science or computational science – in one of those departments or their academic equivalent – who undertake research in enabling technologies for emerging high-performance systems. Complete details and a listing of applicable research areas can be found on the DOE CSGF website.

Applications Due  
**1.18.2023**

### BENEFITS

- \$45,000 yearly stipend
- Payment of full tuition and required fees
- Yearly program review participation
- Annual professional development allowance
- 12-week research practicum experience
- Renewable up to four years

This equal opportunity program is open to all qualified persons without regard to race, color, national origin, sex, disability, or any other characteristics protected by law.





# Announcing the Newest SIAM Project NExT Fellows

By Kathleen Kavanagh, Sachith Dassanayaka, and Alice Schwarze

SIAM remains dedicated to the professional development of junior faculty, especially in the areas of teaching and applied mathematics education. The SIAM Activity Group on Applied Mathematics Education<sup>1</sup> (SIAG/ED)—which promotes the advancement and practice of courses, resources, and educational programs in applied math—is specifically committed to this goal. Beyond the efforts of SIAG/ED, SIAM also annually sponsors two Project NExT (New Experiences in Teaching) Fellows. Organized by the Mathematical Association of America<sup>2</sup> (MAA), Project NExT<sup>3</sup> is a professional development program for new or recent Ph.D.s in the mathematical sciences. The MAA website states that the program “addresses all aspects of an academic career: improving the teaching and learning of mathematics, engaging in research and scholarship, finding exciting and interesting service opportunities, and participating in professional activities.” Since the program’s commencement in 1994, the MAA has named



Sachith Dassanayaka of Wittenberg University.

more than 1,700 Fellows; in 2020, SIAM began to sponsor two Fellows per year.

Sufficient preparation for the workforce—whether it be an academic or business, industry, or government setting—begins with a solid applied mathematics education. The efforts of junior faculty members are particularly valuable in fostering a lasting appreciation of mathematics and inspiring all students to solve a variety of multifaceted, real-world problems. Unfortunately, not all recent Ph.D. recipients possess the necessary resources or training to thrive in academia and fully support their students. To mitigate this issue, Project NExT provides its Fellows with a

robust network of peers and mentors who offer guidance as they settle into their new careers.

During the first year of the Project NExT Fellowship, each cohort partakes in a range of workshops at both MAA MathFest<sup>4</sup> and the Joint Mathematics Meetings<sup>5</sup> (JMM). 2022 workshop topics included time management, vibrant and inclusive communities, the incorporation of modeling in differential equations, classroom orientation around inquiry, and preparation for careers in industry. In addition, the SIAM Project NExT Fellows are strongly encouraged to communicate with the SIAM Education Committee<sup>6</sup> and participate in its

<sup>1</sup> <https://www.siam.org/membership/activity-groups/detail/applied-mathematics-education>  
<sup>2</sup> <https://www.maa.org>  
<sup>3</sup> <https://www.maa.org/programs-and-communities/professional-development/project-next>  
<sup>4</sup> <https://www.maa.org/meetings/mathfest>  
<sup>5</sup> <https://www.jointmathematicsmeetings.org/jmm>  
<sup>6</sup> <https://www.siam.org/about-siam/committees/education-committee>

various activities, such as organizing SIAM-sponsored events at JMM and MathFest and attending SIAG/ED meetings.

The recipients of the 2023 SIAM Project NExT Fellowship are Sachith Dassanayaka (Wittenberg University) and Alice Schwarze (Dartmouth College). Both Fellows expressed their gratitude to SIAM for the opportunity and are eager to get started.

Sachith Dassanayaka is an assistant professor of data science at Wittenberg University, where he teaches statistics and data science courses for both major and non-major students. He earned his Ph.D. in mathematics with a concentration in statistics at Texas Tech University in the summer of 2022, and his dissertation focused on artificial intelligence pattern detection in information operation networks. In addition to expanding upon this project, Dassanayaka’s current research interests include data visualization, machine intelligence, computer networks and security, and the analysis of disinformation campaigns on social media via machine learning and natural language processing.

When he was a graduate student, Dassanayaka served as an event coordinator for the Texas Tech University SIAM Student Chapter; in this role, he helped organize events for both the campus and the outside community. As an educator, Dassanayaka now encourages his students to get involved with SIAM in order to maximize their learning. He appreciates SIAM’s sponsorship of his Project NExT

Fellowship and looks forward to attending future Project NExT workshops and meetings, ultimately contributing to a more inclusive mathematical community for undergraduate teaching.

Alice Schwarze is a postdoctoral researcher in the Department of Mathematics at Dartmouth College. She received a B.Sc. in



Alice Schwarze of Dartmouth College.

physics and a M.Sc. in theoretical physics from Technische Universität Berlin, and most recently a Ph.D. in mathematics from the University of Oxford in 2019. Prior to joining Dartmouth College, Schwarze worked as a postdoctoral researcher in the Department of Biology at the University of Washington.

Though she initially wanted to become a physicist, Schwarze eventually realized that her passion for building mathematical models extends beyond the realm of physics. In fact, most of her current research involves applications in biology or the social sciences. Schwarze is now at a point in her career where she feels confident in her status as an applied mathematician, and she credits SIAM for helping her realize that mathematics is a way of thinking, rather than just a set of theorems or methods. She is very thankful to have benefited from the SIAM Student Travel Awards program<sup>7</sup> and networking opportunities at previous SIAM conferences.

See Project NExT on page 10

<sup>7</sup> <https://www.siam.org/conferences/conference-support/siam-student-travel-awards>

## On the Air

Atmospheric air pressure decreases roughly exponentially with height (with some assumptions that are neither fully realistic nor preposterous). But how would air pressure change with depth in a shaft that is drilled through the center of the Earth?<sup>1</sup> For simplicity, let us assume the law of ideal gas for air and take the air temperature as constant. Later I will show that the pressure turns out to obey a normal distribution (see Figure 1):

$$p(x) = p(0)e^{-ax^2}, \quad (1)$$

where  $x$  is the distance to the Earth’s center and

$$a = cg/2R.$$

Here,  $R \approx 6.4 \cdot 10^6$  m is the Earth’s radius,  $g \approx 10$  m/sec<sup>2</sup>, and  $c = \rho/p$  is the coefficient of proportionality between the density and pressure at a fixed temperature. Taking this to be room temperature,

<sup>1</sup> Casting aside the impossibility of such a project.

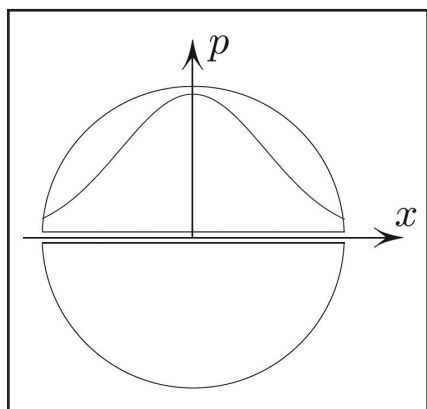


Figure 1. Atmospheric pressure inside a shaft that is drilled through a homogeneous planet obeys normal distribution (1).

$c \approx 10^{-5}$  sec<sup>2</sup>/m<sup>2</sup>. Substituting the expression for  $a$  into (1) relates  $p(0) = p_{\text{center}}$  to  $p(R) = p_{\text{atm}}$ :

$$p_{\text{center}} = p_{\text{atm}} e^{aR^2} = p_{\text{atm}} e^{cg/2R}.$$

Substituting the values of the constants yields

$$p_{\text{center}} > p_{\text{atm}} 10^{1,000}. \quad (2)$$

The super-astronomical estimate is laughably large; in truth,  $p_{\text{center}} < 10^7 p_{\text{atm}}$ . Generously speaking, my estimate (2) is off by 993 orders of magnitude!

What is the source of this preposterous answer? The big mistake was to assume the ideal gas law; this law breaks down once the density reaches that of liquid gas — which then becomes almost incompressible. The air behaves like ideal gas until it doesn’t.

### Gravity Is Greater Underground

Isaac Newton knew that the gravity inside a homogenous solid ball decreases linearly with depth until it reaches zero at the center. On our planet, however, the gravitational acceleration is highest not at the surface but rather at some depth — roughly halfway to the center. This is so because density is not constant and instead increases towards the center. By descending a mile underground, we gain a little bit of weight. This is especially clear in an extreme case where the entire mass of the planet is concentrated in a small concentric ball; the gravity would then be highest at the surface of the ball, which is under the planet’s surface. A related exercise for calculus students is to find the density distribution that yields constant  $g$  inside the ball.

### Derivation of (1)

For a strip of air (see Figure 2) in the shaft to remain in equilibrium, the weight must be balanced by the excess of pressure on the bottom over that on the top:

$$F_{\text{up}} - F_{\text{down}} = \text{weight}.$$

Dividing both sides by the thickness  $h$  and the area of the air column’s horizontal cross-section yields

$$-p'(x) = \rho(x)g(x). \quad (3)$$

Here,  $g(x)$  is the gravitational acceleration in the shaft at distance  $x$  to the Earth’s center. Let us treat the Earth as a homogeneous ball; the gravity then varies linearly with  $x$ , from zero to  $g$  at the surface where  $x = R \approx 6.4 \cdot 10^6$  m:

$$g(x) = \frac{g}{R}x. \quad (4)$$

Now the density of an ideal gas at a constant temperature<sup>2</sup> is in direct proportion to the pressure:  $\rho = cp$ . Substituting this and (4) into (3) gives

$$p' = -2axp, \quad (5)$$

where  $a = cg/2R$ . Separating the variables and integrating yields the normal distribution (1).

### A Paradox

Rising now above the ground, let me “prove” that the air pressure decreases with height — but not to zero! With the same

<sup>2</sup> If we can drill to the center of the Earth, maintaining constant temperature in the shaft will be easy by comparison.

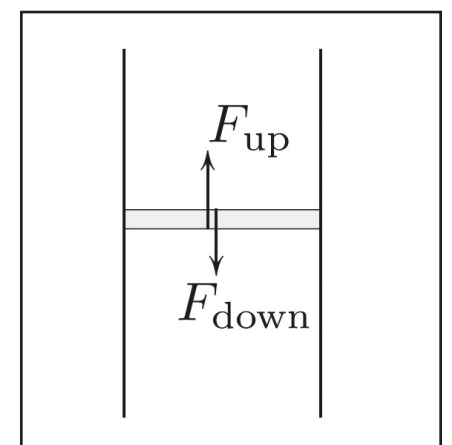


Figure 2. Derivation of an ordinary differential equation (5) for  $p(x)$ . The rate of change of  $p$  is in direct proportion to both gravity (and hence to  $x$ ) and density (and hence to  $p$ ), which explains (5).

assumptions as before and with gravity  $g(x) = \text{const.}/x^2$  above ground (where  $x$  is still the distance to the Earth’s center), the counterpart of (5) is

$$p' = -bp/x^2,$$

where  $b > 0$  is a constant. The general solution of this equation is  $p = ke^{b/x}$  with  $k > 0$ . So  $p \rightarrow k > 0$  as  $x \rightarrow \infty$ , ostensibly proving that the air pressure in outer space is positive. Of course, what this argument really proves is that the assumptions are wrong.

The figures in this article were provided by the author.

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



ATTENTION  
SIAM Math  
Modelers!

# GOT A PROBLEM?

## SIAM is Seeking Problem Ideas for Math Modeling Competition

### What is M3 Challenge?

MathWorks Math Modeling (M3) Challenge is an Internet-based, applied mathematics contest that takes place each year in February or March. High school juniors and seniors in the U.S. and sixth form students (age 16-19) in England and Wales may form and enter up to two teams of three to five students each per school. Teams are given 14 hours to solve an open-ended, applied math-modeling problem related to a real-world issue. Working collaboratively, students use math modeling to represent, analyze, make predictions and provide insight into current world issues. **Registration and participation are free.**

Past topics addressed issues such as substance abuse, food insecurity, climate change, car sharing, and modeling the cost, needs assessment, and placement of towers for maximizing access to the internet. View previous problem statements at [M3Challenge.siam.org/resources/sample-problems](https://M3Challenge.siam.org/resources/sample-problems).

The goal of the Challenge is to motivate students to study and pursue careers in STEM disciplines, especially applied mathematics, computational science, data science, and technical computing. The problem is revealed to students only after they login on their selected Challenge day. Solutions are judged on the approach and methods used and the creativity displayed in problem solving and mathematical modeling. Extra credit in the form of technical computing scholarship awards is available for teams who opt to submit code.

Winners receive scholarship prizes totaling \$100,000 (£75,000).

### Problem structure

Within the problem statement, there should be three questions:

- Question One: A warm up — every serious team can answer.
- Question Two: The guts — framed so that every team can have some success and many teams will cover it well.
- Question Three: The discriminator — many teams will do something, while only a few will have striking results.
- Data — data that is provided or easily found is desirable to encourage students to use coding and technical computing in solution papers.

### Honoraria

- \$50 for problems found suitable to add to the M3 Challenge problem reserve “bank”
- \$500 for problems selected from the reserve bank to be used as “the” Challenge problem

Watch a video that explains the Challenge in one minute!  
Go to YouTube and Search on “About MathWorks Math Modeling Challenge”

**M3** MathWorks Math  
Modeling Challenge  
A program of **siam**.

**\$100,000 (£75,000)  
in SCHOLARSHIPS**



### Required problem characteristics

- Accessibility to high school/sixth form students
- Suitability for solution in 14 hours
- Possibility for significant mathematical modeling
- Topic of current interest involving interdisciplinary problem solving and critical thinking skills
- Availability of enough **data** for a variety of approaches and depth of solutions (but no easily found answers)
- References identified that will be helpful for getting students started
- Submitted problem idea in the format of previous Challenge problems
- Potential to extend and enhance model using technical computing if a team chooses to do so.

Submit your ideas: [M3Challenge.siam.org/suggest-problems](https://M3Challenge.siam.org/suggest-problems)

Contact SIAM for more information: [M3Challenge@siam.org](mailto:M3Challenge@siam.org)

**M3Challenge.siam.org**

The National Association of Secondary School Principals has placed this program on the NASSP National Advisory List of Student Contests and Activities since 2010.



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# Thankful for the Commitment of the SIAM Community

By Abby Addy

If we haven't had a chance to meet yet, my name is Abby Addy and I joined SIAM in February 2022 as the Director of Development and Corporate Relations. My time at SIAM has been a whirlwind of activity thus far, but I've been deeply grateful for the warm welcome that I've received from the SIAM community and look forward to connecting with even more members in 2023.

One of my first endeavors at SIAM involved reaching out to our members to

hear their thoughts on the areas of support that are most meaningful to them. I received many great responses that addressed education; mentorship; research experience; equity, diversity, and inclusion; and more. These conversations have been essential in helping me form a thorough understanding of SIAM's top fundraising priorities — some have even led to exciting gift conversations that I hope to be able to share with you in the near future. If you are interested in discussing your thoughts on influential areas of development but haven't yet heard from me directly, please don't hesitate to get in touch. I'm always looking for further opportunities to engage our community!

We have been able to make an incredible amount of progress in just a few months because of dedicated members like you. We have recently seen the outcomes of generous gifts that established new programs and prizes—including the Renata Babuška Prize<sup>1</sup> and a program to support postdoctoral students, which SIAM will formally announce soon—and felt the positive impact of many first-time donors, returning contributors, and authors who graciously donate their royalties to SIAM. Our donor-supported initiatives—such as funding for student travel, which provided important opportunities for more than 200 students in 2022 alone—have wide-ranging impacts

<sup>1</sup> <https://sinews.siam.org/Details-Page/siam-establishes-the-renata-babu%25%a1ka-prize>

## Project NEXt

Continued from page 8

Schwarze believes that a sound mathematical foundation enables progress on many different research problems in numerous fields, including data science and machine learning. She is especially dedicated to reaching students who are motivated by strong, real-world applications and those who—due to gender, race, or other aspects of their identities—wrongfully believe that they do not belong in the mathematical community. Schwarze is grateful for Dartmouth's support as she develops an inclusive approach to teaching, and for the training that she will receive as a SIAM Project NEXt Fellow.

Candidates who wish to apply for the next round of Project NEXt Fellowships must submit a personal statement, research statement, one-page curriculum vitae, and letter of support from their department chair. Eligible applicants must have a recent Ph.D. in mathematics, statistics, math education, or another math-intensive field; a teaching position and experiences, attitudes, ideas, and leadership abilities that would positively contribute to the cohort are also critical. To be considered specifically for

that wouldn't be possible without your benefaction. For example, the generosity of donors to the James Crowley Fund for Student Support<sup>2</sup> has facilitated transformational experiences for students — notably providing lodging for attendees of the 2022 Graduate Student Mathematical Modeling Camp<sup>3</sup> at the University of Delaware and the 38th Annual Mathematical Problems in Industry Workshop<sup>4</sup> at Worcester Polytechnic Institute, both of which took place in June. Gifts from our community cover a wide variety of initiatives and have been instrumental in our success this past year, and we are deeply appreciative of your faith in our continued efforts. We look forward to recognizing all of our donors in new and exciting ways in 2023.

If you're considering philanthropically supporting SIAM this year but haven't yet made your gift, it's not too late! Gifts of all sizes have tremendous impact, and you can direct your gift to your preferred area of support.

To make a gift, visit SIAM's online giving page<sup>5</sup> or send a check payable to SIAM to the following address:

SIAM Development  
c/o Abby Addy  
3600 Market Street, 6th Floor  
Philadelphia, PA 19104

Please don't hesitate to contact me at (267)-648-3529 or [aaddy@siam.org](mailto:aaddy@siam.org) with any questions or comments, for assistance with your contribution, or just to chat. I'm looking forward to many more years of growth and success as a part of this inspiring organization. Wishing you and your families a happy and healthy holiday season!

*Abby Addy is the Director of Development and Corporate Relations at SIAM.*

<sup>2</sup> <https://www.siam.org/students-education/programs-initiatives/james-crowley-fund-for-student-support>

<sup>3</sup> <https://www.mathsci.udel.edu/events/conferences/gsmmc-2022>

<sup>4</sup> <https://labs.wpi.edu/cims/initiatives/mpi>

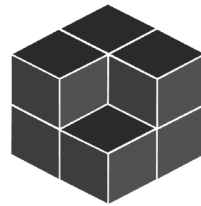
<sup>5</sup> <https://www.siam.org/donate>

SIAM sponsorship, candidates must note their SIAM membership on their applications. An MAA committee makes all final selections. The next application deadline is **April 15, 2023** — visit the program's website<sup>8</sup> for more information.

Even a single exceptional faculty member can have an extensive positive impact within the scientific community. SIAM is glad for the continued opportunity to advance applied mathematics education for the next generation of interdisciplinary problem-solvers.

*Kathleen Kavanagh is a professor of mathematics at Clarkson University and the Vice President for Education at SIAM. Sachith Dassanayaka is an assistant professor of data science at Wittenberg University whose ongoing research is based on disinformation campaigns on social media platforms. Alice Schwarze is a postdoctoral researcher in the Department of Mathematics at Dartmouth College whose research interests lie in the areas of biology and social science.*

<sup>8</sup> <https://www.maa.org/programs-and-communities/professional-development/project-next>



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## TOPICAL & HOT TOPICS WORKSHOPS

### Hot Topics: Algebraic Geometry in Spectral Theory – February 24-26, 2023

**Organizing Committee** > Steven Shipman, Louisiana State University; Frank Sottile, Texas A&M University

### Optimal Transport in Data Science – May 8-12, 2023

**Organizing Committee** > Shuchin Aeron, Tufts University; Markos Katsoulakis, UMass Amherst; James M. Murphy, Tufts University; Luc Rey-Bellet, UMass Amherst; Bjorn Sandstede, Brown University.

### Dynamics, Rigidity, and Arithmetic in Hyperbolic Geometry – May 15-19, 2023

**Organizing Committee** > David Fisher, Indiana University; Dubi Kelmer, Boston College; Hee Oh, Yale University; Alan Reid, Rice University.

### Tangled in Knot Theory – May 22-25, 2023

**Organizing Committee** > Simon Blatt, University of Salzburg; Elini Panagiotou, University of Tennessee; Philipp Reiter, Chemnitz University of Technology; Radmila Sazdanovic, North Carolina State University.

### Mathematical and Scientific Machine Learning – June 5-9, 2023

**Organizing Committee** > Marta D'Elia, Sandia National Lab; George Karniadakis, Brown University; Siddhartha Mishra, ETH Zurich; Themistoklis Sapsis, MIT; Jinchao Xu, Penn State University; Zhangqiang Zhang, WPI.

### Mathematical and Computational Biology – June 12-16, 2023

**Organizing Committee** > Wenrui Hao, Penn State University; Panos Kevrekidis, UMass Amherst; Natalia Komarova, UC Irvine; Marieke Juijjer, University of Oslo; Olivia Prosper, University of Tennessee; Leili Shahriyari, UMass Amherst; Nathaniel Whitaker, UMass Amherst.

### Modern Applied Computational Analysis – June 26-30, 2023

**Organizing Committee** > Anna Gilbert, Yale University; Roy Lederman, Yale University; Gilad Lerman, University of Minnesota; Per-Gunnar Martinsson, UT Austin; Andrea Nahmod, UMass Amherst; Kirill Serkh, University of Toronto; Christoph Thiele, University of Bonn; Sijue Wu, University of Michigan.

### Acceleration and Extrapolation Methods – July 24-28, 2023

**Organizing Committee** > David Gardner, Lawrence Livermore National Lab; Agnieszka Miedlar, University of Kansas; Sara Pollock, University of Florida; Hans De Sterck, University of Waterloo.

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BROWN



# Taking the Plunge from Academia to Biotech

Transitioning from academia to business, industry, and government used to seem like a black hole into which people and information would disappear. Nowadays the division between the two sectors is not as opaque, as more details—in the form of conference presentations, panels, and written and oral anecdotes—are readily becoming available. Yet because information and personal accounts about industrial careers in the biotechnology and pharmaceutical realm are still somewhat scarce, we asked applied mathematicians Andy Stein of Novartis Pharmaceuticals<sup>1</sup> and Dean Bottino of Takeda Pharmaceuticals<sup>2</sup> to offer readers a glimpse from beyond the event horizon.

**SIAM News:** Tell us a bit about your respective educational and career paths.

**Andy Stein:** I earned a bachelor's and master's degree in mechanical engineering from the Massachusetts Institute of Technology, then started my career in biotech during a summer internship at Novartis

(working with Dean Bottino) while I was pursuing my Ph.D. in applied mathematics at the University of Michigan. After completing a postdoctoral appointment at the Institute for Mathematics and its Applications (IMA) at the University of Minnesota, I joined Novartis full-time in 2009 and have worked there ever since.

**Dean Bottino:** I earned a bachelor's degree in mathematics from Hamilton College and a Ph.D. in applied mathematics from Tulane University, then completed a research instructorship at the University of Utah and a National Institutes of Health postdoctoral appointment at the University of California, Berkeley. My first biotech experience was at Physiome Sciences in 2000, after which I co-founded the BioAnalytics Group LLC in 2003; I next joined Novartis for seven years, Roche Pharmaceuticals for two years, and have been at Takeda from 2013 to present. I have spent the last 18 years working nearly exclusively in oncology.

**SN: What led you to make the transition from academia to biotech?**

**AS:** There was a lot that I loved about academia, but I couldn't figure out where I fit. I was hesitant to join an engineering department due to the pressure to bring in grants, and I was hesitant to join a math department because the only pure math class I had ever taken was real analysis, and the work that I was doing—and tend to still do—was very much focused on solving problems and light on mathematical proofs. I had enjoyed my summer internship at Novartis, so I applied for and accepted a full-time position at the end of my postdoc.

**DB:** During my academic work in mathematical biology, there always seemed to be an introductory paragraph that started with, "Cancer is bad. Indeed, let  $\tau_\gamma$  be a tensor field on the  $N$ -manifold  $\gamma \dots$ " In truth, I couldn't really see the connection between my work and explicit improvements to the human condition. I went into industry hoping to find a more direct link

between mathematics and its ability to improve the quality and duration of lives for people with diseases.

**SN: How can individuals know whether they will succeed in biotech?**

**AS:** The only way to really know is to try it, and I'd highly recommend an internship or industry postdoctoral appointment. I began my full-time career at Novartis as a "visiting scientist," which basically meant postdoc. It paid slightly less than a standard full-time position, but I could conduct more focused work on scientific problems—much like what I was accustomed to in academia—and was able to publish. Communication and teamwork are much more important in industry than in academia, and deriving novel mathematical results is less so. If you can answer critical questions using high school math and easily explain your answers to the team, everyone will greatly appreciate you. But if you prove a new result or develop a new method that your team can't understand and that doesn't help them solve a valuable problem, no one will care.

**DB:** Academia is great if you aspire to be the best <adjective><adjective><adjective> mathematician on Earth (remove one adjective if you're a rock star). But if you like applying math to solve important and interesting problems in medicine—irrespective of the math's "fanciness"—and you enjoy working with large teams on issues that are much too big for one person to tackle, then biotech could very well be for you.

**SN: What is your typical day like?**

**AS:** It's a mix of coding in R, attending meetings (either one-on-one conversations or team meetings), reading papers, putting together presentations, and going for walks to think. Since the start of the pandemic, I have been going into the office about once a week; while there, I conduct mini hackathons with the other pharmacometrician on my team to develop tools that will help the entire department.

**DB:** My answer is similar to Andy's, but I'm not as good as he is at getting out of meetings. Some days I just go from meeting to meeting, either to mentor junior modelers or lead cross-disciplinary teams toward some shared goal that involves mathematical modeling. Other days I do hands-on tasks like building models, fitting them to data, and reporting the results.

**SN: What coursework should graduate students pursue to prepare for a career in biotech or pharmaceuticals?**

**AS:** You should learn to code. Python and R are good choices, but know that you'll probably have to learn a new language at some point. I knew MATLAB when I joined Novartis and used it for a while, but my group and field moved heavily into R so I eventually made the switch.

See *Academia to Biotech* on page 12

## CAREERS IN MATHEMATICAL SCIENCES

## Thomas J.R. Hughes won William Benter Prize in Applied Mathematics 2022



Professor Thomas J.R. Hughes

Professor Thomas J.R. Hughes, Peter O' Donnell Jr. Chair in Computational and Applied Mathematics and Professor of Aerospace Engineering and Engineering Mechanics, University of Texas at Austin, US, won the William Benter Prize in Applied Mathematics 2022.

Professor Hughes, a phenomenal leader in the field of computational science, engineering and mathematics, created isogeometric analysis, a novel approach to integrating computer-aided design (CAD) and computer-aided engineering (CAE). The ingenious idea is to derive finite element basis functions from CAD, which has revolutionised numerous engineering applications. His fundamental paper on this topic has been cited over 6,000 times on Google Scholar and is widely referred to throughout industry, national labs and academia.

Variational multiscale methods (VMS) and stabilised methods are the groundbreaking results of Professor Hughes' research in computational fluid dynamics (CFD). They overcome a fundamental mathematical obstacle, the Babuska-Brezzi condition, and have enabled the construction of widely used methods for simulating viscous compressible flows. VMS is leading to new turbulence models and multiphase flow algorithms.

Additionally, Professor Hughes applied his expertise in computational mechanics to a different

field: blood flow modelling. This work has evolved into the concept of "predictive medicine". The underlying methodology has been commercialised to provide non-invasive, patient-specific, coronary disease diagnosis based on CFD.

Among his many prestigious awards, Professor Hughes has received the ASME Medal from the American Society of Mechanical Engineers (ASME), the John von Neumann Medal from the U.S. Association for Computational Mechanics (USACM), and the Gauss-Newton Medal from the International Association for Computational Mechanics (IACM).

There are two awards under the name of Professor Hughes: the Thomas J. R. Hughes Medal of USACM, and the Thomas J.R. Hughes Young Investigator Award of ASME.

Professor Hughes is a member of the US National Academy of Sciences, the US National Academy of Engineering, and the American Academy of Arts and Sciences, and is a foreign member of the Royal Society of London. He has been a plenary lecturer at the International Congress of Mathematicians.

The William Benter Prize will be presented during the opening ceremony for the International Conference on Applied Mathematics (ICAM 2023), which is co-organised by CityU's Liu Bie Ju Centre for Mathematical Sciences (LBJ) and the Department of Mathematics.

The William Benter Prize in Applied Mathematics was set up by LBJ in honour of Mr William Benter for his dedication and generous support to the enhancement of the University's strengths in mathematics. The prize recognises outstanding mathematical contributions that have had a direct and fundamental impact on scientific, business, finance and engineering applications. The cash prize of US\$100,000 is given once every two years.

– City University of Hong Kong

### Nominate Your Students for the SIAM Student Paper Prize

The 2023 SIAM Student Paper Prize will be awarded to the student authors of the three most outstanding papers accepted for publication in SIAM journals between February 15, 2020 and February 14, 2023. The award is based on the merit and content of the students' contributions to the papers. Each recipient will receive a cash prize of \$1,000, a SIAM Student Travel Award, and free registration for the 2024 SIAM Annual Meeting — where the awards will be presented.

Nominations will be accepted until **February 15, 2023**. Visit <https://www.siam.org/student-paper-prize> for full eligibility requirements, necessary materials, and further details. Contact [prizeadmin@siam.org](mailto:prizeadmin@siam.org) with questions.



# Making Up for Lost Time in SIAM Membership

By Richard Moore

As COVID-19 approaches endemic stability and we gradually resume our pre-2020 routines, my thoughts turn to members of our community who may have missed out on valuable opportunities over the last few years. Students in particular had fewer chances to build collaborations and friendships through in-person classes, present their research and network at in-person conferences, visit labs and institutions in their own countries and beyond, physically intern at companies, and so forth. In short, they faced difficulties when attempting to develop their communities and careers outside of the narrow focus of their coursework and theses.

SIAM's student membership numbers have been slower to recover from the COVID-19 blip than other categories.

Almost all students have access to free SIAM membership<sup>1</sup> through either their participation in one of the more than 200 SIAM Student Chapters<sup>2</sup> or their institution's status as a SIAM Academic Member;<sup>3</sup> yet despite this perk, student membership is currently at 76 percent of its pre-pandemic total. As a result, many students are not receiving significant discounts on SIAM conferences and publications, getting involved in SIAM-funded student chapter activities, connecting with each other at conference "Student Days" and other SIAM networking events, learning about career fairs and professional development happenings, and beginning

<sup>1</sup> <https://www.siam.org/membership/join-siam/individual-members/student>

<sup>2</sup> <https://www.siam.org/students-education/student-chapters>

<sup>3</sup> <https://www.siam.org/academic-members>

their journeys toward leadership positions in the SIAM community.

Outreach membership,<sup>4</sup> which is available to individuals in countries that the World Bank has designated as "developing," has also not yet recovered to pre-pandemic levels. SIAM now offers an outreach registration rate at all virtual and hybrid conferences; starting in 2023, outreach members will also be entitled to free membership in a SIAM Activity Group<sup>5</sup> of their choice. These advantages add significant value to an already heavily discounted membership rate.

SIAM membership delivers a high return on investment in each of its categories, but students and outreach members undoubtedly benefit the most. So why haven't these numbers bounced back as quickly? The answer is not entirely clear, but I suspect that a combination of exhaustion over COVID-19-related disruptions and fewer opportunities to attend conferences is to blame. Rising levels of inflation and—for outreach members—an unfavorable exchange rate with the U.S. dollar certainly do not help, but the discounts to conferences, books, and journals far outweigh these deterrents.

What can the rest of us do to bolster student and outreach participation? Spread the word! Regular SIAM members can nominate two students for free membership. Make sure that the students you nominate are aware of the many exciting activities that are scheduled for 2023, including the following:

- The 2023 SIAM Conference on Computational Science and Engineering,<sup>6</sup> which will take place in Amsterdam, the

Netherlands, from February 26 to March 3 (with Student Days<sup>7</sup> and a Hackathon<sup>8</sup>)

- The 2023 SIAM Conference on Applications of Dynamical Systems,<sup>9</sup> which will take place in Portland, Ore., from May 14-18 (with the Workshop Celebrating Diversity)

- The 2023 Graduate Student Mathematical Modeling Camp, which will take place at the University of Delaware from June 7-10

- The 2023 Mathematical Problems in Industry Workshop, which will take place at the New Jersey Institute of Technology from June 12-16

- Two virtual SIAM Career Fairs on April 4 and October 11.

We should also ensure that our colleagues in outreach countries know about the outreach rate at upcoming hybrid conferences — such as the 2023 ACM-SIAM Symposium on Discrete Algorithms,<sup>10</sup> which will be held in Florence, Italy, from January 22-25. SIAM membership will ensure access to all available discounts for this and other future events.

2023 will be a year full of new experiences that help us make up for lost time by reconnecting with old friends and colleagues, forming new collaborations, and expanding the boundaries of our professional careers. I look forward to ringing in the year with all of you.

*Richard Moore is the Director of Programs and Services at SIAM.*



Lina Sorg (left), the managing editor of SIAM News, poses with Richard Moore, SIAM's Director of Programs and Services, at the 2022 SIAM Conference on Mathematics of Data Science, which took place this September in San Diego, Ca. SIAM photo.

## Academia to Biotech

Continued from page 11

**DB:** I was an anti-statistics snob in graduate school, but that attitude (and the resulting exclusively deterministic skillset) did not serve me well in biotech. All key decisions are made under uncertainty and involve noisy sparse data, interpatient variability, and prediction uncertainty. I had to pick up a lot of stats on my own and wish that I had learned more of it in school—like nonlinear regression, survival analysis, and statistical physics—in addition to deterministic math.

**AS:** Oh yeah, stats is a good one. Along with all of those analysis techniques, stats also teaches design. Let's say that you want to create a study to answer a question; how can you do so in a systematic way and account for as many confounding factors as possible? This type of project falls under the framework of "causality" and is one of the hardest topics I've encountered, just because of how counterintuitive everything can be.

**SN:** What do you miss about academia, and what are you glad to have left behind?

**AS:** I miss being able to submit for publication any interesting results that I find. Now, if I'm working on a drug that has billions of dollars of revenue, uses data from hundreds of patients, and was developed by dozens of people, much more stakeholder management is required in order to publish. I've partially addressed this challenge by focusing on the development of new methodologies and trying to use data from drugs that are already in the literature. But regardless, maintaining all of these relationships and following the correct operational procedures can be exhausting.

In academia, I found it quite hard to select a single problem on which to work; I couldn't figure out how to prioritize or when to give up on something that was too difficult. I like that there is a natural focus in industry — I want to help my team quickly

determine whether a drug works and if so, how to optimally dose it and get it approved as quickly and efficiently as possible. Within that framework, I'm free to be as creative as I can when coming up with solutions.

**DB:** Sometimes I miss teaching and working with students, but those interactions have been replaced by mentoring other modelers and explaining my thinking to non-mathematicians, which I greatly enjoy. The main thing that I don't miss about academia is balancing my time between teaching and research; I liked both but hated the constant feeling that I was neglecting one or the other at any given moment.

**AS:** I also miss working with students, but I've found that it is possible to get involved in those type of endeavors if they're important to you. I've participated in various collaborations with academia, including the IMA's Math-to-Industry Boot Camp<sup>3</sup> and a New Jersey Institute of Technology Workshop on Mathematical Problems in Industry.<sup>4</sup> I enjoyed these so much that Novartis has twice hosted a two-week Academia-Industry Hackathon, during which students learned about basic drug development concepts for a few days and then worked on relevant problems.

**SN:** The ladder to success in academia typically involves publishing papers, receiving grants, and teaching and mentoring students. What is the "currency" for success in the biotech industry?

**AS:** There are many different currencies for success. Some easily quantifiable measures are salary, job title, and number of direct reports. Other currencies include the drugs that you've worked on and advanced, and sometimes the publications that you've written. Certain things are harder to measure but perhaps even more important, such as the quality of

<sup>3</sup> <https://cse.umn.edu/ima/math-industry-boot-camp>

<sup>4</sup> <https://web.njit.edu/~lcumming/MPI2019/MPI2019home.php>

your relationships with your collaborators. More than anything else, "relationship currency" will probably help you achieve the career that you want. Unlike in academia, there's no obvious tenure-adjacent goal in industry. This means that it's up to you to pursue what's important to your career and life. This is not necessarily easy to figure out, and I've shared further thoughts on this topic on my website.<sup>5</sup>

**DB:** In my opinion, the main currency is the ability to use principled quantitative thinking to impact key decisions in drug programs. There is not a big emphasis on novelty, at least not on being "first but wrong." You get additional points for working well across disciplines and operating outside of your comfort zone.

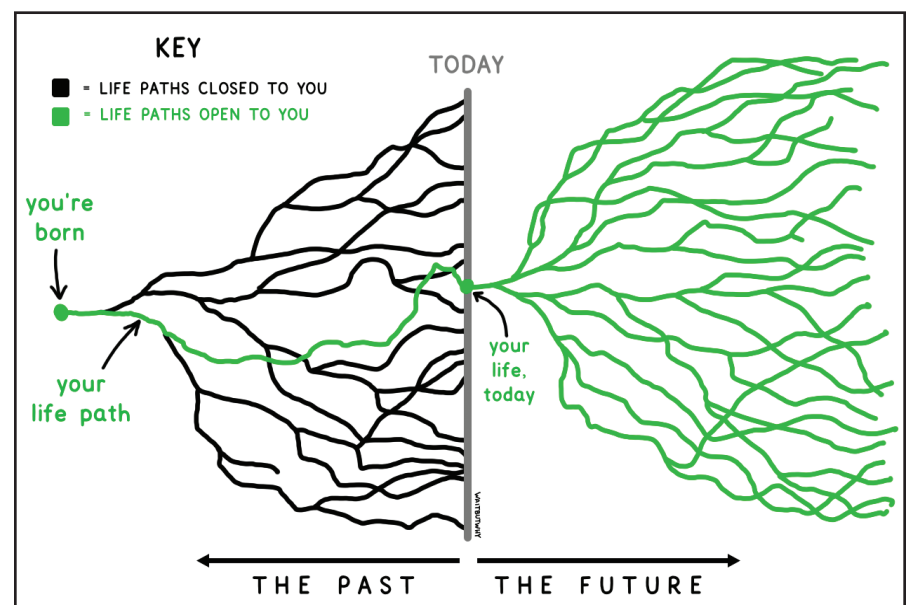
**SN:** Do you have any advice for academicians whose students might be interested in biotech?

<sup>5</sup> <https://sites.google.com/site/andrewsteinphd/career-advice>

**AS:** In the drug development field, it is not uncommon for people to leave industry and return to academia. Those people are often particularly good researchers and teachers because they understand both theory and practice, and they can be good resources for your students (see Figure 1).

**DB:** Sometimes it's hard when a bright young person doesn't want to follow in your footsteps — I've been there too! But don't take it personally; like biotech, academia is not for everyone. Encourage your students to network and seek out industry internships, then give them the time and space to go all in. Shorter commitments, such as weeklong industrial-academic workshops like the Fields Institute's Systems Modeling in the Pharmaceutical Industry Problem Solving Workshop,<sup>6</sup> can also give students a feel for whether they want to try a lengthier internship.

<sup>6</sup> <http://www.fields.utoronto.ca/activities/19-20/systems-modeling>



**Figure 1.** As long as students and early-career researchers continue to stay curious, they are likely to find rewarding careers regardless of whether they ultimately opt for industry or academic paths. Figure courtesy of Tim Urban at Wait But Why, <https://twitter.com/waitbutwhy/status/1406980353986809861>.