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Special Issue on Computational Science and Engineering

This ***special issue*** *explores content from the 2021 SIAM Conference on Computational Science and Engineering and other research in CSE.*

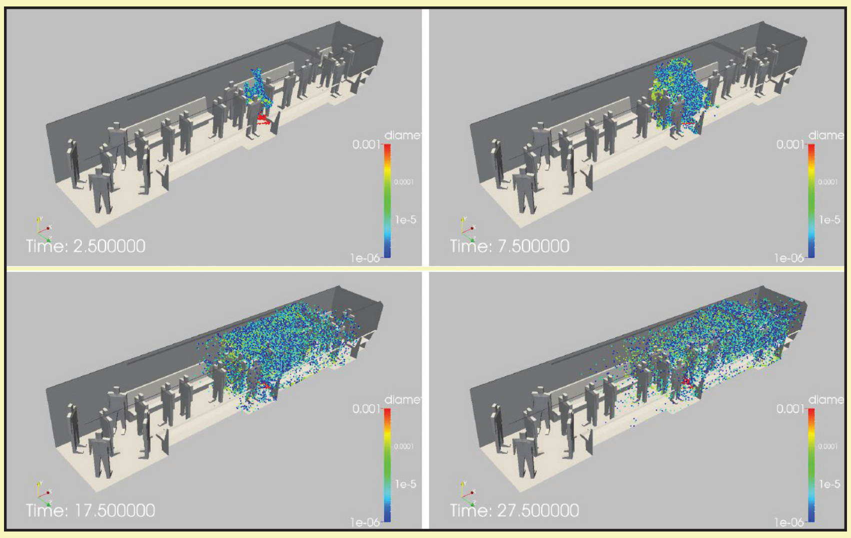

Figure 2. *Sneezing in a subway car. The sneezing occurs in the middle of the car, towards the right. The particles that are emitted by the sneezing passenger are colored according to the logarithm of the diameter, with red representing the largest particles and blue representing the smallest particles. Note the quick dispersion of particles due to the air conditioning ventilation; some particles enter the left portion of the subway car. The health implications are obvious. Figure courtesy Rainald Löhner and Harbir Antil.*

In an article on page 5, Rainald Löhner and Harbir Antil describe the physical assumptions, ensuing ordinary and partial differential equations, and associated numerical schemes for the movement of large and small viral droplets.

The Optimality of Bayes' Theorem

By Tan Bui-Thanh

Inverse problems are pervasive in scientific discovery and decision-making for complex, natural, engineered, and social systems. They are perhaps the most popular mathematical approach for *enabling predictive scientific simulations* that *integrate observational/experimental data, mathematical models, and prior knowledge*. While indirect data provide valuable information about unknown parameters and the physical problem itself, such data are typically limited and therefore unable to sufficiently infer the parameters. Conversely, the prior encodes *a priori* knowledge about the parameters and its bias is thus unavoidable.

Of the many frameworks that facilitate uncertainty quantification in inverse solutions, the Bayesian paradigm is perhaps the most popular.[1] The Bayesian approach combines prior knowledge (via prior distribution of the parameters) with observational data (via the likelihood) to produce the posterior probability distribution as the inverse solution. The following two-part question hence arises: *Is this method of using observed information from data the best way to update the prior distribution? If so, in what sense?* Answering these queries yields insight into Bayes' theorem and brings to light meaningful interpretations that are otherwise hidden.

Here we utilize three different perspectives—two from information theory and one from the duality of variational inference—to show that Bayes' theorem is in fact an optimal way to blend prior and observational information. To that end, let us use $\mathbf{m}$ to denote the unknown parameter of interest, $\pi_{\text{prior}}(\mathbf{m})$ for the prior density (or distribution), $\pi_{\text{like}}(\mathbf{d}|\mathbf{m})$ for the likelihood of $\mathbf{m}$ given observable data $\mathbf{d}$, and $\pi_{\text{post}}(\mathbf{m}|\mathbf{d})$ for the posterior density. Every student of the Bayesian inference framework presumably knows that according to conditional probability [1], Bayes' formula—the sole result of Bayes' theorem—reads

$$\pi_{\text{post}}(\mathbf{m}|\mathbf{d}) := \frac{\pi_{\text{like}}(\mathbf{d}|\mathbf{m}) \times \pi_{\text{prior}}(\mathbf{m})}{\mathbb{E}_{\pi_{\text{prior}}}[\pi_{\text{like}}(\mathbf{d}|\mathbf{m})]}, \quad (1)$$

[1] A Google search for "Bayes' theorem" returns 7,510,000 results.

See **Bayes' Theorem** *on page 2*

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Space Exploration and Data Science

By Simon Mak and C.F. Jeff Wu

In his famous 1962 address at Rice University about U.S. space efforts to reach the moon, President John F. Kennedy declared that "the exploration of space will go ahead…and it is one of the great adventures of all time." This adventure has become even more of a reality in recent years, as modern breakthroughs in mathematical modeling, scientific computing, and data science have inspired numerous pioneering achievements that were only dreams in the past.

A crucial part of space exploration is the design and development of high-performance rocket propulsion systems, and a central component of such systems is the rocket injector. This device enables the intermixing of fuel and oxidizer prior to combustion; Figure 1 displays a schematic of a simplex swirl injector [1, 2, 6, 10]. Liquid oxygen is injected into a gaseous fuel environment via the inlet slots on the left, then swirled along the injector wall and propelled out for combustion. The design space consists of $p=5$ parameters: injector length L, injector radius R_n, inlet slot width δ, tangential inlet angle θ, and the distance between the inlet and the headend $\triangle L$ (one can easily extend the methods that we propose for more complex design settings with additional parameters). The goal is to identify parameter designs that ensure good mixing of fuel and oxidizer, which translates to a fuel-efficient and robust combustion performance.

In order to explore potential injector designs, engineers must conduct experiments over the desired parameter space. Traditional *physical* experiments are prohibitively expensive due to high prototyping costs and the harsh requirements of operating conditions [4]. Because these experiments rely on optical diagnostics for measurements, they offer minimal insight into the underlying physiochemical mechanisms [9]. Due to recent advances in scientific modeling, numerical simulations are becoming a reliable alternative to physical tests. These so-called *computer* experiments can provide more salient features of the flow and combustion dynamics within the injector [7]. They also allow for significant savings in prototyping and experimental costs.

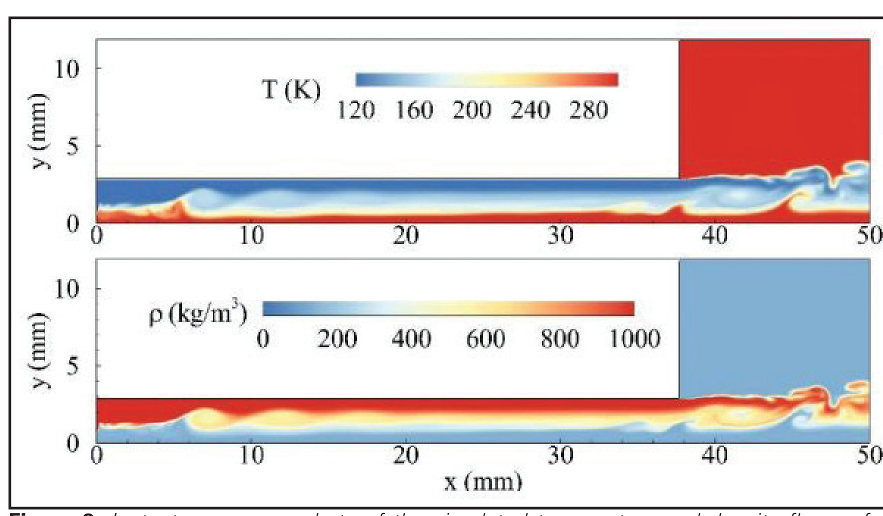

Figure 2. *Instantaneous snapshots of the simulated temperature and density flows of an injector design. Figure courtesy of [10].*

To reliably capture the rich physics within the turbulent flow, a sophisticated multiphysics computational fluid dynamics (CFD) model is necessary for simulation purposes. We begin with the well-known Navier-Stokes equations, which express the conservation of mass and momentum for Newtonian fluids. Then we model thermodynamic properties via the Soave-Redlich-Kwong equation of state, which correlates fluid pressure, temperature, and density under high-pressure conditions. The large eddy simulation (LES) framework achieves turbulence closure. Figure 2 depicts instantaneous snapshots of the simulated temperature and density flows of an injector design.

However, a key limitation of CFD-based design exploration is that these flow simulations are computationally expensive. For a fine grid of 100,000 mesh points, a high-fidelity flow simulation that uses LES can take roughly 30,000 central processing unit (CPU) hours to obtain statistically meaningful data. This restriction greatly limits the number of potential designs that are sampled on the parameter space, particularly given the number of geometric attributes and operating conditions for survey. We utilized a *surrogate modeling* approach to address this limitation. Surrogate modeling consists of two steps. One first performs simulations at a carefully selected set of design points on the parameter space, then fits a predictive model using the simulated flows as training data. The fitted model serves as a *surrogate* for the expensive LES code, thus enabling efficient exploration of the parameter space.

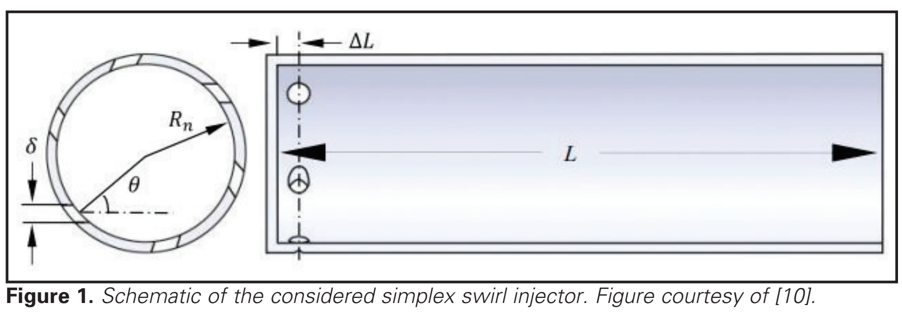

Figure 1. *Schematic of the considered simplex swirl injector. Figure courtesy of [10].*

See **Space Exploration** *on page 4*

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Bayes' Theorem

Continued from page 1

where $\mathbb{E}_{\pi_{\text{prior}}}[\cdot]$ denotes the expectation under the prior distribution. Bayes' formula (1) provides a simple formula for the posterior as the product of the prior and likelihood. Indeed, it is so simple that deep insights are perhaps neither necessary nor possible. In fact, most researchers likely never wonder why such a simple framework is so effective for many statistical inverse problems in engineering and the sciences.

Calculus of variations tells us that if an optimizer for some objective functional exists, it has to satisfy the first-order optimality condition (equation) that indicates that the first variation of the objective functional at the optimum must vanish. The equation form of Bayes' formula (1) triggers our curiosity and prompts us to wonder whether *Bayes' formula is the first-order optimality condition of some objective functional*. To approach this question, we note that the prior encodes our prior knowledge/belief before we see the data. From the point of view of information theory, we should elicit the prior so that its discrepancy relative to the updated distribution $\rho(\mathbf{m})$ (to be found) is as small as possible. That is, if we believe that our prior is meaningful, the information that we gain from the data in $\rho(\mathbf{m})$ should not be significant. The relative loss or gain between two probability densities is precisely captured by the relative entropy, also known as the Kullback-Leibler (KL) divergence [3]: $D_{\text{KL}}(\rho\,|\,\pi_{\text{prior}}) := \mathbb{E}_{\rho}\left[\log\left(\frac{\rho(\mathbf{m})}{\pi_{\text{prior}}(\mathbf{m})}\right)\right]$. When the updated distribution $\rho(\mathbf{m})$ is identical to the prior $\pi_{\text{prior}}(\mathbf{m})$, the KL divergence is zero — i.e., the prior is perfect. But when $\rho(\mathbf{m})$ deviates from the prior $\pi_{\text{prior}}(\mathbf{m})$—e.g., when the data provides additional information or strengthens some information in the prior—the KL divergence is positive.

Since the observational data $\mathbf{d}$ is the other piece of information in the posterior's construction, we wish to match the data as well as possible while avoiding overfitting. One way to do so is to look for $\rho(\mathbf{m})$ that minimizes $-\mathbb{E}[\log(\pi_{\text{like}}(\mathbf{d}|\mathbf{m}))]$, which is a generalized mean squared error (MSE) that comes from using the updated distribution to predict the data.

At this point, we see that a competition exists between the prior knowledge and the information from the data in terms of constructing the updated distribution. On the one hand, the updated distribution should be close to the prior if we believe that the prior is the best within our subjective elicitation. On the other hand, the updated distribution should be constructed in such a way that the data is matched well under that distribution. We argue that the optimal updated distribution should compromise these two sources of information so that it captures as much of the limited information from the data as possible while also resembling the prior. We can construct such a distribution by simultaneously minimizing the KL divergence and MSE (see Figure 1 for a demonstration) [2], i.e.,

$$\min_{\rho(\mathbf{m})} D_{\text{KL}}(\rho|\pi_{\text{prior}}) - \mathbb{E}_{\rho}[\log(\pi_{\text{like}})]. \quad (2)$$

The beauty here is that the optimization problem (2) is convex, its first-order optimality condition is precisely Bayes' formula (1), and its unique updated distribution is exactly Bayes' posterior $\pi_{\text{post}}(\mathbf{m}|\mathbf{d})$.

We can also achieve the optimality of Bayes' formula (1) from an information conservation principle [5]. In this approach,[2] we divide the information—with respect to the updated distribution $\rho(\mathbf{m})$—into the input information $\mathbb{E}_{\rho}[\log \pi_{\text{prior}}(\mathbf{m}) + \log \pi_{\text{like}}(\mathbf{d}|\mathbf{m})]$ that is provided by the prior $\rho(\mathbf{m})$ and likelihood $\pi_{\text{like}}(\mathbf{d}|\mathbf{m})$, and the output information $\mathbb{E}_{\rho}[\log \rho(\mathbf{m}) + \log \mathbb{E}_{\pi_{\text{prior}}}[\pi_{\text{like}}(\mathbf{d}|\mathbf{m})]]$ that is provided by the updated distribution $\rho(\mathbf{m})$ and evidence $\mathbb{E}_{\pi_{\text{prior}}}[\pi_{\text{like}}(\mathbf{d}|\mathbf{m})]$. The optimal updated distribution is the one that minimizes the difference between the output and input information — it is exactly Bayes' posterior $\pi_{\text{post}}(\mathbf{m})$, at which the difference is zero [5]. In other words, Bayes' posterior is the unique distribution that satisfies the information conservation principle (see Figure 2 for a demonstration).

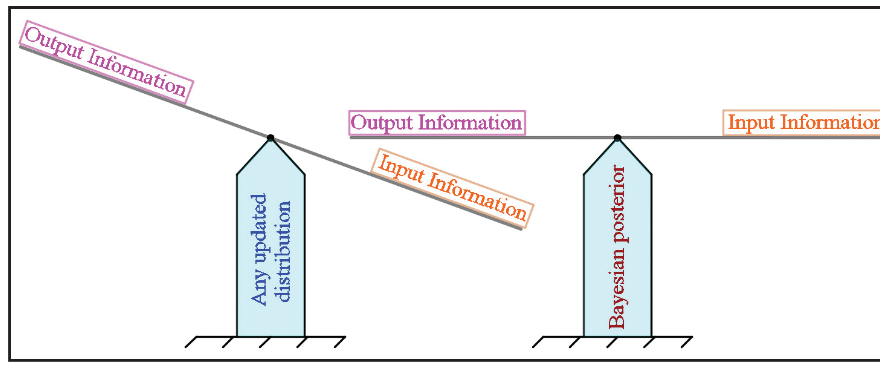

Figure 2. *Bayes' posterior minimizes the output information and is the only distribution that conserves the information. Figure courtesy of Hai Nguyen.*

Next, we show that the optimality of Bayes' formula (1) is also apparent from a duality formulation of variational inference [4]. Under mild conditions on $\pi_{\text{prior}}(\mathbf{m})$, $\rho(\mathbf{m})$, and a large class of functions $f(\mathbf{m})$, the following inequality holds true:

$$-\log \mathbb{E}_{\pi_{\text{prior}}}[e^{f(\mathbf{m})}] \leq$$
$$\mathbb{E}_{\rho}[-f(\mathbf{m})] + D_{\text{KL}}(\rho\mid\pi_{\text{prior}}).$$

The equality occurs when the right-hand side of the formula attains its minimum and the unique optimizer $\rho(\mathbf{m})$ satisfies $\rho(\mathbf{m}) \times \mathbb{E}_{\pi_{\text{prior}}}[e^{f(\mathbf{m})}] = e^{f(\mathbf{m})} \times \pi_{\text{prior}}(\mathbf{m})$. Taking $f(\mathbf{m}) = \log(\pi_{\text{like}}(\mathbf{d}|\mathbf{m}))$, we immediately conclude that the optimal $\rho(\mathbf{m})$ is the Bayes' posterior $\pi_{\text{post}}(\mathbf{m})$. In this case, the right-hand side is exactly the objective functional (2). The objective functional's minimum is the negative log evidence (the left-hand side of the formula); this is achieved only at Bayes' posterior (see Figure 1).

Here we show that Bayes' formula has a firm foundation in optimization. In particular, one can view the formula as the first-order optimality condition for three different yet related optimization problems: (i) simultaneous minimization of the information gain from the prior and the MSE of the data, (ii) minimization of the output and input information discrepancy, and (iii) minimization of the upper bound of a variational inference problem. This material yields additional insight into the Bayesian inference framework and paves the way for the development of optimization approaches for Bayesian computations.

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[2] The approach in [2] was discovered independently of [5].

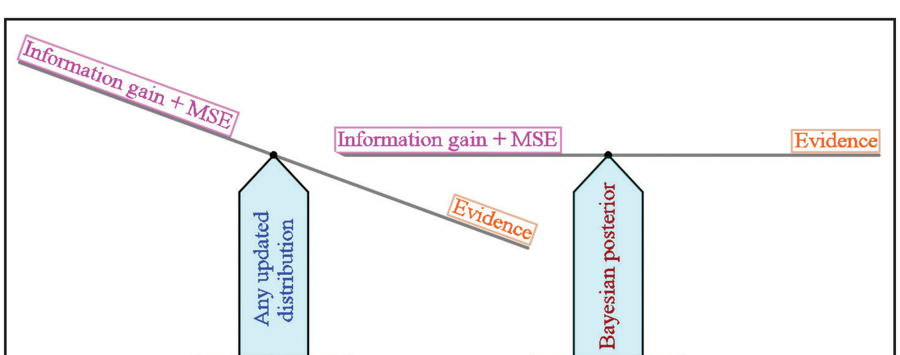

Figure 1. *Bayes' posterior minimizes the sum of information gain and mean squared error (MSE), and is the only distribution that balances information gain + MSE with the evidence. Figure courtesy of Hai Nguyen.*

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Three-Part Panel Series at CSE21 Explores Equity, Diversity, and Inclusion in the Workforce

By Lina Sorg

The last several years have seen increased attention to issues of equity, diversity, and inclusion (EDI) in applied mathematics and computational science. Nevertheless, women, persons with disabilities, Blacks and African Americans, Hispanics and Latinos, and American Indians and Alaska Natives are still underrepresented in science and engineering fields across the U.S.[1] In response, organizations around the country are taking active steps to support these communities in the workforce, understand the unique challenges they face, and engage in direct conversation to invoke positive change.

The 2021 SIAM Conference on Computational Science and Engineering (CSE21),[2] which took place virtually earlier this year, featured a three-part panel that addressed EDI in CSE-related careers. The seven panelists—who have experience in academia, industry, and national laboratories—were divided into two groups. Members of the first group shared their personal experiences as minorities in CSE, while those in the second detailed the ways in which their respective institutions are working to foster a more diverse culture. A live discussion with all panelists followed both sessions. Mary Ann Leung of the Sustainable Horizons Institute served as the moderator, and Ron Buckmire of Occidental College—SIAM's Vice President for EDI—delivered the opening remarks.

Stories from Underrepresented Members of the CSE Community

Sally Ellingson of the University of Kentucky, Derek Jones of Lawrence Livermore National Laboratory (LLNL), and Bonita Saunders of the National Institute of Standards and Technology (NIST)—also a member of the SIAM Board of Trustees—served on the first panel. Ellingson began with some background about herself. After earning dual undergraduate degrees in computer science and mathematics as a first-generation college student at the Florida Institute of Technology, she determined that she wanted to pursue further education. While working an office job after graduation, Ellingson received a competitive monetary offer for a fellowship. As a single mother, she decided to leave home with her daughter, move away from her support system, and pursue her Ph.D. "It was a scary transition," she said. "I actually did not tell anyone in the program that I had a kid and was a single parent. I had nightmares that people would find out and I would lose my fellowship. I felt like I had to go and prove myself a bit before I was comfortable talking about it, but of course I had lots of support once I did."

Jones grew up in rural Kentucky and had limited access to science, technology, engineering, and mathematics (STEM) outreach during his youth. He was one of only a few Black students at his school, and recalls paging through textbooks and wondering why none of the computer scientists or mathematicians looked like him. But when Jones encountered people from other backgrounds while earning his undergraduate degree at the University of Kentucky—including Ellingson, who took him under her wing—they exposed him to a number of inspiring research projects. "It really has enriched my life," he said. "I didn't have a clear picture as to what my role [in STEM] would ultimately be until I began to meet mentors."

1 https://ncses.nsf.gov/pubs/nsf21321
2 https://www.siam.org/conferences/cm/conference/cse21

Saunders was also often one of the only Black people in her departments, both throughout the course of her career and as an undergraduate at William and Mary (W&M). "In a way I've gotten used to it over the years," she said. "You have to be willing to be the only one. Some people want to be around people who are like themselves and have the same experiences. But that's something I've always been open about, working with different people and going to school with different people."

Saunders' perspective is especially unique because she was born around the time of Brown v. Board of Education—the 1954 Supreme Court case wherein justices unanimously ruled that racial segregation in U.S. public schools was unconstitutional—and even attended segregated schools until high school. She went on to become the valedictorian of her integrated high school class and decided to pursue teaching — a common profession for Black women at the time. Though she completed the student teaching requirements at W&M, Saunders ultimately chose to attend graduate school to study mathematics. It was not until she enrolled at Old Dominion University for a master's degree—and was automatically admitted to the Ph.D. program because she was a promising student—that Saunders began to feel recognized. "It would have been nice if someone had noticed me along the way and encouraged me," she said. "I think that's the big thing, just being aware and not only looking at students who look like yourself."

Ellingson echoed this sentiment and stressed the importance of engaged, encouraging mentors. When participating in an Integrative Graduate Education and Research Traineeship,[3] she had a program manager who was especially dedicated to his mentees' personal growth. He served as a strong advocate, made sure Ellingson received adequate support, stepped in to mitigate a difficult group project situation, and even helped her find a new babysitter.

Jones then described the value of EDI programs, especially those that support funding and education. However, he noted that people of color often feel ashamed to receive money for school if it comes from a diversity scholarship or fellowship and is not purely merit based. "Everybody starts off at a different point in life, and we have plenty of data to say that people of color are definitely starting behind in that race," he said. "It's not mutually exclusive with academic abilities either. You can be diverse and also academically talented."

Strategies for EDI at CSE-based Organizations

The second group of panelists included Scott Collis of Sandia National Laboratories (SNL), Lesia Crumpton-Young of Morgan State University (MSU), Bruce Hendrickson of LLNL, and Maria Klawe of Harvey Mudd College. Klawe, who has been president of Harvey Mudd for 15 years, immediately began working to increase diversity within the student body upon her arrival. As a result, Harvey Mudd launched the President's Scholars

3 http://www.igert.org

A three-part panel during the 2021 SIAM Conference on Computational Science and Engineering (CSE21), which took place virtually in March, featured seven speakers who discussed their experiences with underrepresentation and suggested strategies to effectively diversify the workforce. Top row, left to right: Sally Ellingson of the University of Kentucky, Derek Jones of Lawrence Livermore National Laboratory (LLNL), and Bonita Saunders of the National Institute of Standards and Technology. Bottom row, left to right: Scott Collis of Sandia National Laboratories, Lesia Crumpton-Young of Morgan State University, Bruce Hendrickson of LLNL, and Maria Klawe of Harvey Mudd College.

Program[4] — a full-tuition scholarship for STEM students who come from backgrounds that are traditionally underrepresented at the college. Recipients are selected based on their leadership capabilities and ability to diversify the student body. Though the scholarship is not defined by race, most recipients are people of color. "It's had a huge impact and was relatively easy to do," Klawe said. "We had to give up some tuition income, but the way we structured this as a leadership award meant that those students who came had proportionately more impact."

In a similar vein, LLNL offers Employee Resource Groups[5] that cultivate and enhance a diverse and inclusive workforce via recruiting, mentoring, and networking efforts. "These entities provide a safe space and welcoming environment for a diverse group of individuals," Hendrickson said. "They also make it a more attractive environment for us to recruit and bring people with diverse backgrounds into the laboratory."

In addition, LLNL regularly participates in conferences like the Blackwell-Tapia Conference[6] and the Grace Hopper Celebration of Women in Computing.[7] "These are opportunities for us to recruit, engage, and learn about and understand the environments and particular challenges that individuals from nontraditional backgrounds have to overcome," Hendrickson continued. "We can then adjust our work environment and our processes to be more inclusive."

Crumpton-Young is the provost and Senior Vice President for Academic Affairs at MSU, where 75 percent of the student body is Black. "Most of the policies that I'm working with start at a place where I found myself as a student," she said. "Our policies really work on creating a sense of belonging for our students and faculty." Crumpton-Young was the first African American woman to earn a Ph.D. in engineering from Texas A&M University, where advisors initially encouraged her to pursue a less rigorous major. As a result of her own experiences, she strives to create an environment where students feel like their peers and educators expect them to succeed. She also helps prepare students of color for workplace situations where they will not comprise the majority and thus might feel less comfortable being their authentic selves.

4 https://www.hmc.edu/admission/afford/scholarships-and-grants/merit-based-scholarships/presidents-scholars-program
5 https://diversity.llnl.gov/groups
6 https://mathinstitutes.org/diversity/blackwell-tapia-conference
7 https://ghc.anitab.org

Collis noted that SNL is working to define "excellence" in a broader sense by moving away from focused job postings with particular skillsets in favor of a wider recruiting approach. "We're casting a broad net by emphasizing skills such as teaming and the ability to take on work and be innovative," he said. "That's really been empowering for us in terms of identifying more diverse pools of candidates." SNL has also created several postdoctoral fellowships that emphasize these characteristics, including the Jill Hruby Fellowship in National Security Science and Engineering[8] and the Sandia Data Science Postdoctoral Fellowship.[9]

Collis then stressed the importance of implicit bias awareness training within hiring committees and promotion evaluation committees. Though such training might inspire difficult conversations, these dialogues are crucial for growth. "Be courageous enough to have that difficult discussion," Crumpton-Young added. "Don't just ignore the elephant in the room. Address every elephant in every room."

Klawe encouraged faculty members and administrators to listen to their students, especially those who have had challenging paths to success. "Just listening to people talk about what it's like to be a Black person, or a Black gay person, or a Latinx person, and how entering the Mudd community felt to them was really helpful," she said. "It's hard to advocate for someone if you don't understand where they're coming from." Hendrickson remarked that although some people believe that efforts towards diversity and inclusion fall solely on management, this is not the case. The challenge—one of sustained, steady, and consistent discussion and openness—belongs to everybody.

A robust follow-up session the next morning allowed panel attendees to further explore ideas from the previous day and pose questions directly to the speakers. One key takeaway was the consensus that diversity should be inherent in the workforce; establishing a welcoming sense of inclusivity is the first step. "The work we need to do is inclusion first," Hendrickson said. "Diversity is not sustainable unless we can solve the inclusion and cultural challenge. And everyone needs to help."

Lina Sorg is the managing editor of SIAM News.

8 https://www.sandia.gov/careers/career-possibilities/students-and-postdocs/fellowships/jill-hruby-fellowship
9 https://www.sandia.gov/careers/career-possibilities/students-and-postdocs/fellowships/data-science-fellowship

Space Exploration

Continued from page 1

We employed the proper orthogonal decomposition (POD) to build this flow surrogate model [1, 2, 6, 10]. Researchers frequently employ the POD in experimental physics to decompose a turbulent flow into its component coherent structures. When $f_\theta(s,t)$ is the simulated flow at design setting θ—where s and t are spatial and temporal variables—the POD yields the following decomposition:

$$f_\theta(s,t) \approx \bar{f}_\theta(s) + \Sigma_{k=1}^{K} \beta_{k,\theta}(t)\phi_{k,\theta}(s).$$

Here, $\bar{f}_\theta(s)$ is the time-averaged flow at design setting θ, $\mathcal{S}(\theta)=\{\phi_{k,\theta}(s)\}_{k=1}^{K}$ is the set of orthonormal spatial modes, and $\mathcal{T}(\theta)=\{\beta_{k,\theta}(t)\}_{k=1}^{K}$ is the set of time-varying coefficients. We can extract these spatiotemporal POD features via a singular value decomposition from the simulated flow snapshots.

To predict the flow $f_{\theta_{\text{new}}}(s,t)$ at a new design setting θ_{new}, we first build two surrogate models: one for predicting the spatial modes $\mathcal{S}(\theta_{\text{new}})$ and one for predicting the time-varying coefficients $\mathcal{T}(\theta_{\text{new}})$. We construct both models using Gaussian processes—a flexible Bayesian nonparametric predictive model—and train them with the extracted spatiotemporal POD features from simulated flows. We can utilize decision trees [10] and kernel smoothing methods [2] to further learn the changing physics over the parameter space, such as the boundary between jet and swirl injectors. Once we predict the spatial modes and time-varying coefficients, we can then reconstruct the corresponding flow prediction at the new design setting θ_{new} via the aforementioned decomposition.

Next, we examine the performance of this flow surrogate model on four test injector designs that were taken over a broad parameter space that contains the RD-0110 [8] and RD-170 [3] engines. We trained our model with flow simulations at $n=30$ design settings from a sliced Latin hypercube design. Figure 3 presents the simulated flow snapshots from LES and predicted flow snapshots at different times. The predictions appear to successfully capture the large-scale features of the instantaneous flow, including the spray angle and the liquid film along the injector wall. The key advantage of this surrogate model is the savings in computation time. After simulating the initial $n = 30$ training runs, we can train our model using 150 CPU hours. With the trained model, we can generate the flow prediction at a new design setting in approximately 30 CPU hours. This outcome provides significant (1,000-fold) computational reduction when compared to a full CFD simulation, which requires 30,000 CPU hours per setting; it thereby allows engineers to more efficiently explore the desired parameter space.

These results, while promising, likely only scratch the surface of an exciting and emerging interdisciplinary field. In order to tackle the unavoidable challenges of this ambitious space travel adventure, practical solutions must reflect sophisticated developments and integration of state-of-the-art methods in scientific modeling, applied mathematics, and data science. Such interdisciplinary efforts collectively serve as a catalyst for furthering scientific progress and in turn spur novel methodological development.

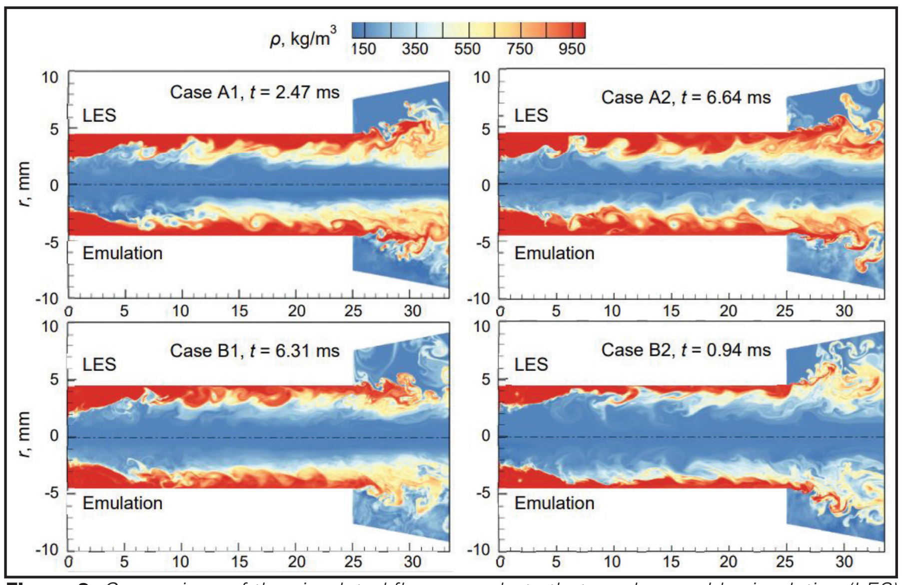

Figure 3. *Comparison of the simulated flow snapshots that use large eddy simulation (LES) and predicted flow snapshots from our surrogate model for four test injector designs. Figure courtesy of [2].*

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High-Fidelity Simulation of Pathogen Propagation, Transmission, and Mitigation

By Rainald Löhner and Harbir Antil

The current COVID-19 pandemic has stimulated a renewed interest in pathogen propagation, transmission, and mitigation [1–3, 9]. In particular, the relative impact of transmission via "large droplets" versus "small droplets" or aerosols—combined with possible changes to existing heating, ventilation, and air conditioning (HVAC) systems, building floorplans, pedestrian traffic management, and the installation of ultraviolet (UV) lights—has been the topic of thorough debate over the last year and a half. Natural and forced convection, the presence of moving pedestrians or objects, and accurate computation of droplets in airflow motion in the context of HVAC systems are all key requirements for the development of quantitative predictions of pathogen propagation, transmission, and mitigation in the built environment. Numerical techniques that satisfy these requirements have reached high degrees of sophistication and offer a quantum leap in accuracy when compared to simpler probabilistic models [6, 7].

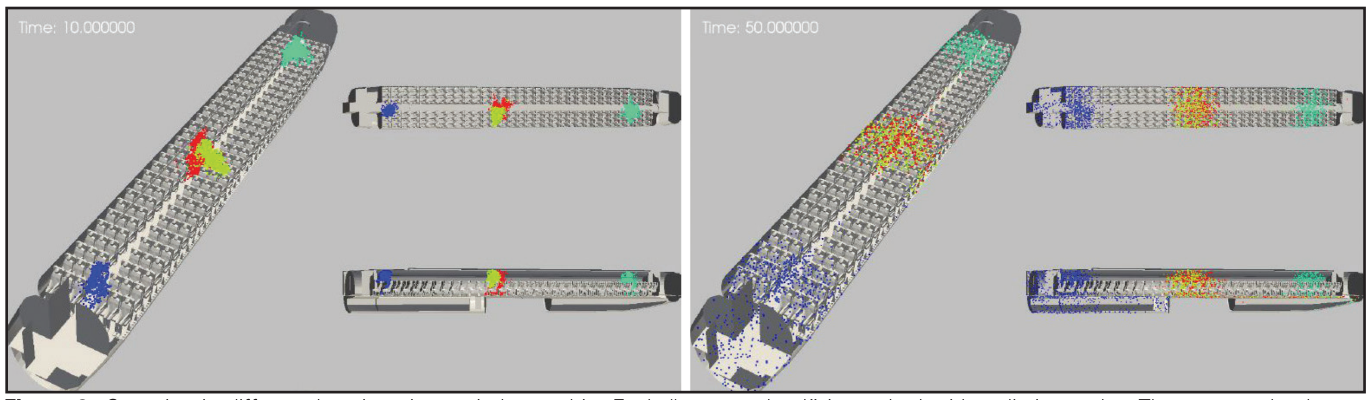

Figure 3. *Sneezing in different locations in an airplane cabin. Each "sneeze cloud" is marked with a distinct color. The sneeze clouds stay localized within two to three seats/rows of their origin, making the airplane cabin a much safer environment than the subway car in Figure 2. Figure courtesy of the authors.*

Mitigation Techniques

When developing pathogen mitigation or elimination strategies, one must visualize the movement of the droplets that carry the pathogen:

– *Larger* $(1\,\mathrm{mm} \geq \mathrm{d} \geq 0.1\,\mathrm{mm})$ droplets follow a ballistic path, are not significantly slowed by the surrounding air, and drop and attach to the floor or any surface in a time of approximately $O(1)$ seconds without considerable evaporation. Spitting saliva is one such example.

– *Smaller* $(d < O(0.01)\,\mathrm{mm})$ droplets are immediately slowed by the surrounding air, evaporate in a fraction of a second, and are transported by the air itself. One can conceptualize these aerosolized droplets as (invisible) cigarette smoke or sprays (e.g., hair spray or deodorants).

Figure 1 summarizes a list of common mitigation techniques and evaluates their effectiveness for a variety of transmission/infection mechanisms.

Procedure Measure	Large Droplets (spitting)	Small Droplets (cigarette smoke)	Person-Air-Person	Person-Surface-Person
2m/6ft Distance	✓ (green)	✓ (yellow)	✓ (yellow)	✓ (green)
Face Masks	✓ (green)	✓ (yellow)	✓ (yellow)	✓ (green)
Periodic Hand Cleaning	✓ (green)	✗ (red)	✓ (yellow)	✓ (green)
Plexiglass Shields	✓ (green)	✓ (yellow)	✓ (yellow)	✓ (green)
1-Way Person Traffic	✓ (yellow)	✓ (green)	✓ (green)	✓ (yellow)
2x Daily Cleaning	✓ (green)	✓ (yellow)	✓ (yellow)	✓ (green)
Nightly UV Cleaning	✓ (green)	✓ (yellow)	✓ (yellow)	✓ (green)
Maximize Fresh Air in HVAC	✗ (red)	✓ (green)	✓ (green)	✗ (red)
Hard UV Lamps in HVAC Ducts	✗ (red)	✓ (green)	✓ (green)	✗ (red)
HEPA Filters in HVAC Ducts	✗ (red)	✓ (green)	✓ (green)	✗ (red)
Upper Room UV Cleaning	✗ (red)	✓ (green)	✓ (green)	✗ (red)

Figure 1. *Common procedures that mitigate the spread of pathogens. Green indicates effective measures, yellow designates somewhat effective measures, and red marks ineffective measures. Figure courtesy of the authors.*

Physical Modeling of Aerosol Propagation

When solving the two-phase equations, one can best represent air (as a continuum) with the Navier-Stokes equations. These equations describe the conservation of momentum, mass, and energy for incompressible Newtonian flow and are given by

$$\rho \mathbf{v}_{,t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla p = \nabla \cdot \mu \nabla \mathbf{v} + \rho \mathbf{g} + \beta \rho \mathbf{g}(T - T_0) + \mathbf{s}_v, \quad (1)$$

$$\nabla \cdot \mathbf{v} = 0, \quad (2)$$

$$\rho c_p T_{,t} + \rho c_p \mathbf{v} \cdot \nabla T = \nabla \cdot k \nabla T + s_e. \quad (3)$$

Here, ρ, $\mathbf{v}$, p, μ, $\mathbf{g}$, β, T, T_0, c_p, and k respectively denote the density, velocity vector, pressure, viscosity, gravity vector, coefficient of thermal expansion, temperature, reference temperature, specific heat coefficient, and conductivity. In addition, $\mathbf{s}_v$ and s_e are momentum and energy source terms (e.g., due to particles or external forces/heat sources). One can obtain both the viscosity and conductivity for turbulent flows either from additional equations or directly via a large eddy simulation (LES) assumption through monotonically-integrated LES. Adding the appropriate advection-diffusion equations with source terms allows researchers to attain the concentration of pathogens, age of air, and possible UV radiation.

We model the droplets/particles—which are relatively sparse in the flow field—with a Lagrangian description, which monitors and tracks individual particles (or groups of particles) in the flow. This allows for an exchange of mass, momentum, and energy between the particles and the air. The position $\mathbf{x}_p$, velocity $\mathbf{v}_p$, and temperature T_p of each particle are given by ordinary differential equations (ODEs) of the form

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \quad (4)$$

$$\frac{d\mathbf{v}_p}{dt} = \mathbf{f}(\mathbf{v}, \mathbf{v}_p, \ldots), \quad (5)$$

$$\frac{dT_p}{dt} = s(\mathbf{v}, \mathbf{v}_p, T, T_p, \ldots). \quad (6)$$

Empirical relationships that depend on both the particle and flow variables yield the terms on the right-hand side [4, 6, 7].

The Navier-Stokes equations are integrated using FEFLO via a so-called projection scheme [4] that is comprised of an "advective predictor" and a subsequent Poisson solver to re-establish incompressible flow. The Lagrangian particles are integrated with an explicit fourth-order Runge-Kutta scheme, and immersed body techniques handle the presence of moving, inhaling, and exhaling pedestrians [4, 6].

Modeling Pedestrian Motion

Modeling pedestrian motion has been the focus of research and development for more than two decades [5, 8]. An example simulation with moving pedestrians to assess pathogen propagation and/or mitigation options is presented here. This simulation utilizes the PEDFLOW model [5].

Necessary information from computational fluid dynamics (CFD) codes consists of pathogen distribution and the spatial distribution of temperature, smoke, and other toxic or movement-impairing substances in space. We interpolate this information to the computational crowd dynamics code at every timestep to properly calculate the visibility/reachability of exits, routing possibilities, smoke, toxic substance or pathogen inhalation, and any other flow field variable that the pedestrians require.

Illustrative Examples

The following examples are by no means exhaustive or unique; the simulation of aerosol transmission via high-fidelity CFD techniques has received considerable attention in recent years, and researchers worldwide have carried out such work with both commercial and open-source software. Further cases with videos and descriptions are available online.[1]

See **Pathogen Propagation** *on page 7*

[1] https://cfd.science.gmu.edu/research/projects/covid-19-spread-of-diseases-in-the-built-environment

Celebrating the DOE's Office of Advanced Scientific Computing Research

As per its website, the mission of the Advanced Scientific Computing Research (ASCR) program is "to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena [that are] important to the Department of Energy (DOE)." ASCR's prehistory dates back to John von Neumann's advocacy for increased mathematics and computing activity after the Manhattan Project in the 1940s. Since its inception, ASCR and its predecessor organizations have played a pivotal role in shaping the entire discipline of computational science through investments in basic research, leadership-class facilities and computers, and workforce development programs, among other initiatives. ASCR has also intersected with SIAM in many ways throughout the decades — providing a block grant to support SIAM conferences, funding SIAM members' research, and much more. The program's full history is available in *ASCR@40: Highlights and Impacts of ASCR's Programs*.[1] To our knowledge, this 115-page report is the most comprehensive history ever written on the topic and is thus highly recommended for scientists, students, and science historians.

The following text is an abridged excerpt from chapter six of *ASCR@40*, entitled "Lessons Learned and Challenges of the Future." It has been lightly edited for brevity and provides readers with a thorough overview of previous takeaways, current issues, and potential concerns regarding the future of applied mathematics and computational science.

Lesson 1: A Compelling and Consistent Vision Can Drive Scientific Revolutions

ASCR and its predecessor organizations have consistently believed that computing is a key driver of science. This sustained commitment drove nearly all of ASCR's investments, including the development of advanced mathematical techniques, the evolution of computer architecture, the creation of state-of-the-art networking capabilities, an array of innovative computer science concepts, the creation and support of powerful software libraries, and an interdisciplinary workforce. The integration of these capabilities with DOE applications has driven a scientific revolution.

In partnership with scientists at DOE laboratories, ASCR has displayed an admirable focus at key points of technological evolution. It recognized the importance of parallel computing well before the community broadly embraced the technique, and funded critical work to navigate the transition to parallelism. ASCR also appreciated the emerging importance of data science and the critical role of uncertainty quantification as researchers incorporated computer models into decision-making. Collaborations between knowledgeable program managers and the research community have enabled a clear vision and sustained commitment, which are essential to overall progress in these areas.

[1] https://computing.llnl.gov/misc/ASCR@40-11.2020.pdf

Lesson 2: Diverse Funding Models Are Required for Diverse and Impactful Outcomes

ASCR has employed a wide variety of different funding models over the years: short- versus long-term, open-ended versus narrowly targeted, large collaborations versus single investigators, and so forth. Graduate and postdoctoral fellowships have helped build the required workforce and attract top scientists to DOE laboratories. Sustained investments in single principal investigators and small teams have enabled fundamental mathematical and computer science advances, while larger, cross-institutional investments have inspired interdisciplinary collaborations.

Software is an essential element of ASCR's capabilities. Competitive processes drive excellence and innovation, but mechanisms that sustain long-term assets in research and software are also essential. Networking, high-performance computing (HPC) facilities, and HPC platforms require yet another funding model. This broad ecosystem of funding modalities has facilitated ASCR's greatest successes.

Lesson 3: Workforce Investments Have Been Critical

When working on methodologies that universities had not yet embraced, ASCR invested in workforce development initiatives. The Computational Science Graduate Fellowship[2] has been the most visible and transparently successful effort in this regard, but postdoctoral positions at many laboratories have also been hugely impactful. These investments have staffed DOE laboratories and led to broader achievements in industry and academia.

Lesson 4: Partnerships Are Essential

Complex challenges require interdisciplinary teams that encompass diverse areas of expertise. These scientific partnerships are best enabled by programmatic partnerships. For example, Scientific Discovery through Advanced Computation[3] (SciDAC) helped overcome organizational barriers and inspired new kinds of science. ASCR has also embraced additional partnerships; for example, the Exascale Computing Project[4] maintains a close partnership with the National Nuclear Security Administration.[5]

[2] https://www.krellinst.org/csgf/about-doe-csgf

Lesson 5: Testbeds and Platform Access Funding Models Are Important

At points of architectural uncertainty, investing in small testbed systems is critical for understanding the strengths and weaknesses of different designs and making informed decisions about future directions. Larger "early access systems," wherein users can try full-scale applications and adapt them for the next generation of machines, are particularly beneficial. These steps build confidence in the architectures and allow vendors to learn from early adopters. ASCR has embodied this approach by funding codesign centers on the path to exascale systems.

As growth in the scale of the largest systems outpaces that of widely-available commercial systems, ASCR must continue to invest in the research and development (R&D) that is necessary to build and deploy energy-efficient systems with increased scientific capabilities. To do so, ASCR should keep investing in pathfinding R&D—such as the PathForward program—and non-recurring engineering efforts that are associated with the acquisition of specific systems.

Though scientific computing centers at universities and national laboratories have tried to finance medium- to large-scale systems by charging users for access, this business model does not work for large-scale leadership systems. To advance the state of the art in HPC, the funds to purchase computers must be appropriated and system access should be free for users.

Challenge 1: Technology Disruptions

The vast majority of supercomputer performance improvements in the past several decades have resulted from shrinking microelectronics and faster clock speeds. As these performance drivers come to an end, researchers must find new ways to squeeze additional performance gains from machines. Although the scientific community is embracing simple heterogeneity, future machines will be much more complex. We are entering an era of great change, so strategic clarity and vision—along with sustained investments in creative individuals and high-risk concepts—will be essential.

Challenge 2: Funding Balance

The rapid emergence of data science and machine learning (ML) in scientific workflows comprises another dramatic shift in the ASCR landscape. With finite dollars, how should ASCR balance support of new areas with continued support of areas of historical strength? Strategic clarity will again be critical when making these hard choices.

Challenge 3: Software Stewardship

The community has long struggled to identify a good model for sustained support of key elements in the software ecosystem. ASCR must recognize that software is a scientific facility that requires sustained investments in maintenance and support. A simultaneous need for investments in improved software engineering practices reflects ongoing, profound changes in the development and maintenance of modern scientific software. Such technology is often the product of large, dispersed teams and leverages a diverse suite of libraries and tools. These trends complicate development, but researchers can manage them through disciplined software engineering processes like thorough documentation, comprehensive regression suites, and issue tracking.

[3] https://www.scidac.gov
[4] https://www.exascaleproject.org
[5] https://www.energy.gov/nnsa/national-nuclear-security-administration

Challenge 4: Broader Partnerships

The SciDAC program is rightly regarded as a visionary success in building transformative, interdisciplinary partnerships across various scientific domains. There is a growing opportunity for simulation and ML in other areas of the DOE, including organizations that have different value systems and funding models than the Office of Science. How can ASCR partner with this broader group of entities to maximize impact?

Challenge 5: A Sought-after Workforce

Generational and technological changes will require fresh approaches to workforce issues. Computational scientists have vastly more opportunities in industry and academia than in the past, which increases competition for talent with DOE laboratories.

Challenge 6: New Roles for Computing to Advance Science

For many years, ASCR's primary goal was to enable more rapid, detailed, and accurate simulations. But in the last several decades, it has broadened its activities to support collaborative technologies and data-centric research and development endeavors. These investments have empowered scientific advances that are quite different from modeling and simulation. As science continues to evolve, ASCR will need to adapt to new roles for scientific computing.

One clear current trend is the explosive growth of ML and artificial intelligence (AI). ASCR researchers are exploring new computing workflows in which simulations and AI work together to generate novel insights. Moving forward, ASCR intends to nurture scientific ML with both fundamental and applied investments. These new workflows will likely drive innovative thinking about the design and usage models for advanced computers.

Another trend is the rapid growth in data streams from DOE user facilities, including light sources, accelerators, and telescopes. The demands associated with the volume and velocity of these data streams require advanced computing. Scientists are increasingly utilizing HPC to analyze experimental data in real time and combine experiments with simulation. As with AI, this trend will presumably motivate fresh thinking about the nature of advanced computing platforms and their integration with data sources and human decision-makers.

Since its establishment, ASCR has played a central role in creating and shaping the field of computational science. This area faces enormous opportunities and challenges in the coming years, and ASCR is poised to continue its pivotal role in advancing the discipline.

SIAM News thanks editor-in-chief Hans Kaper of Georgetown University and Bruce Hendrickson of Lawrence Livermore National Laboratory—who is also co-chair of the Advanced Scientific Computing Advisory Committee Subcommittee on the 40-year History of ASCR—for their review of and contributions to this piece.

Incorporating Ethical Discussions in the Mathematics Classroom

By Joe Skufca

As mathematics, computational science, data science, and other tangential fields become increasingly involved in situations with large societal impact, researchers in these areas are beginning to recognize the need for sound ethical reasoning in their professions. Maurice Chiodo and Dennis Müller's recent *SIAM News* article[1] [3] about ethical questions in the context of COVID-19 modeling serves as an example. Our community is well versed in the ethics of *scholarship*, but our professional training likely did not address the *ethical applications* of our work. Here, I provide some tested resources to guide the incorporation of ethics-based questions and materials into existing classes or seminars.

Why Ethics Now?

Some fields (law or medicine, for example) have a formalized understanding of *ethical standards*, but mathematics does not. However, a number of professional organizations in the mathematical sciences acknowledge the need for such standards. Efforts like the Cambridge University Ethics in Mathematics (EiM) Project[2]—and the two corresponding EiM conferences[3] in 2018 and 2019—serve as flagship standards in working towards community-wide awareness. Of course, a simple "code of ethics" is not sufficient; *ethical awareness* should be integral to professional preparation. Many higher educational institutions recognize this necessity and are making ethics an explicit component of their curricula. Chiodo has been a continuing leader in this space for the last several years [2]. His webpages[4] at Cambridge contain a wealth of resources, and several of the forthcoming examples stem directly from (or were inspired by) his course notes.

ETHICS IN MATHEMATICS

When we were developing a new data science major at Clarkson University, most of the coursework was already in place. As such, I told our administration that we only needed two new courses: (i) an introductory course in data science and (ii) *a course in ethics*. In addition to embedding ethics across the entire curriculum, we decided that the major would include a three-credit ethics course that is taught by a math professor.

The following exercises are student favorites from the aforementioned ethics course. Some provide background material and are appropriate for inclusion as part of a sequence (perhaps in a seminar course), but most are standalone items. Several can easily be incorporated into standard math classes. Many of these topics apply across multiple levels and might even serve as backdrops for larger faculty discussion.

Background Materials

For the Instructor: Bonnie Shulman's "Is There Enough Poison Gas to Kill the City? The Teaching of Ethics in Mathematics Classes" [6] is a great starting point to help instructors design a framework that addresses ethical issues within mathematics curricula. This article is especially valuable for faculty members who are still exploring whether they want to include ethics in their teachings.

Background Definitions: The Internet Encyclopedia of Philosophy's article about ethics[5] provides an excellent summary of key terms in the field. I recommend equipping students with this *standard terminology* to inform their reading, ease discussions, and facilitate their consideration of multiple viewpoints (i.e., "That is the *utilitarian* argument, but how might your argument change if you take a *duty ethics* perspective?").

See **Ethical Discussions** *on page 8*

[1] https://sinews.siam.org/Details-Page/questions-of-responsibility-modelling-in-the-age-of-covid-19

[2] https://www.ethics.maths.cam.ac.uk

[3] https://www.ethics.maths.cam.ac.uk/conferences

[4] https://www.dpmms.cam.ac.uk/~mcc56

[5] https://iep.utm.edu/ethics

Pathogen Propagation

Continued from page 5

Sneezing in Subway Car

An obvious vector for pathogen contamination and spread is mass transport, as passengers are in extremely close proximity and airflow might result in considerable mixing. We therefore chose to analyze a sneeze in a subway car. The flow enters through two parallel slits in the ceiling and exits through the ceiling at both ends of the car. A detailed STL triangulation yielded the geometry [2]. An immersed technique was used for the passengers, who were located randomly throughout in the car; the mesh had approximately 10^7 elements.

As one might expect, the flow field is highly turbulent. Figure 2 (on page 1) illustrates the distribution of particles after a sneeze in the middle of the car by someone who is facing one end. The large red particles follow a ballistic path and fall to the ground. The air quickly stops the green particles of size $d = 0.1\,\mathrm{mm}$, which then sink slowly towards the floor in close proximity to the person who is sneezing. The blue particles, which are even smaller, rise with the cloud of warmer air that is exhaled by the sneezing individual and disperse much further at later times.

Sneezing in an Airplane Cabin

The air flow in airplane cabins has been a media focal point throughout the COVID-19 pandemic. Given that the air in planes is renewed much more often than in air-conditioned buildings—one exchange every two minutes versus one exchange every 12-15 minutes—people would likely assume that airplanes are much safer. Indeed, influenza studies have shown that the "radius of transmission" on a plane is limited to two-three rows; large droplets that move from surfaces to hands and then to noses/eyes/mouths are the most common route of infection. Nevertheless, regions of stagnant flow could be conducive to pathogen transmission. This prompted us to analyze flow and sneezing in a Boeing 737-500.

Unlike older models, the flow in this cabin enters through two parallel slits in the ceiling that are close to the windows, moves towards the center, and exits through holes in the floor below the windows. A detailed STL triangulation once again yielded the geometry [3], and the mesh had approximately $0.89 \cdot 10^9$ elements. The run was carried out to one minute of physical time, which required approximately 24 hours on nearly 8,000 cores. Different "sneezing positions" were also considered, and only the smaller particles—which move much further—were accounted for. Figure 3 (on page 5) depicts the movement and extent of the "sneeze clouds" that originated at different positions. Each of these clouds is marked with a unique color, and the clouds remain bounded to two-three seats/rows in every direction. This result is qualitatively in line with studies of influenza and COVID-19 transmission on airplanes.

Corridor with Pedestrians

This example considers a corridor of size $10.0\,\mathrm{m} \times 2.0\,\mathrm{m} \times 2.5\,\mathrm{m}$. Both entry and exit sides have two doors, each of size $0.8\,\mathrm{m} \times 2.0\,\mathrm{m}$. For the purpose of climatisation, four entry vanes and one exit vane are placed in the ceiling. The vertical air velocity for the entry vanes is set to $v_z = 0.2\,\mathrm{m/sec}$, while the horizontal velocity is set as increasing proportionally to the distance of the vane's center to a maximum of $v_r = 0.4\,\mathrm{m/sec}$. The CFD mesh has approximately $3.5 \cdot 10^6$ elements of uniform size, and two streams of pedestrians enter and exit through the doors over time.

The case shown here considers two pedestrian streams in counterflow mode. Figure 4 indicates that the different velocities between walking pedestrians—and particularly counterflows—lead to large-scale turbulent mixing, therefore enhancing the spread of pathogens that emanate from infected victims. More cases/options are available in [6].

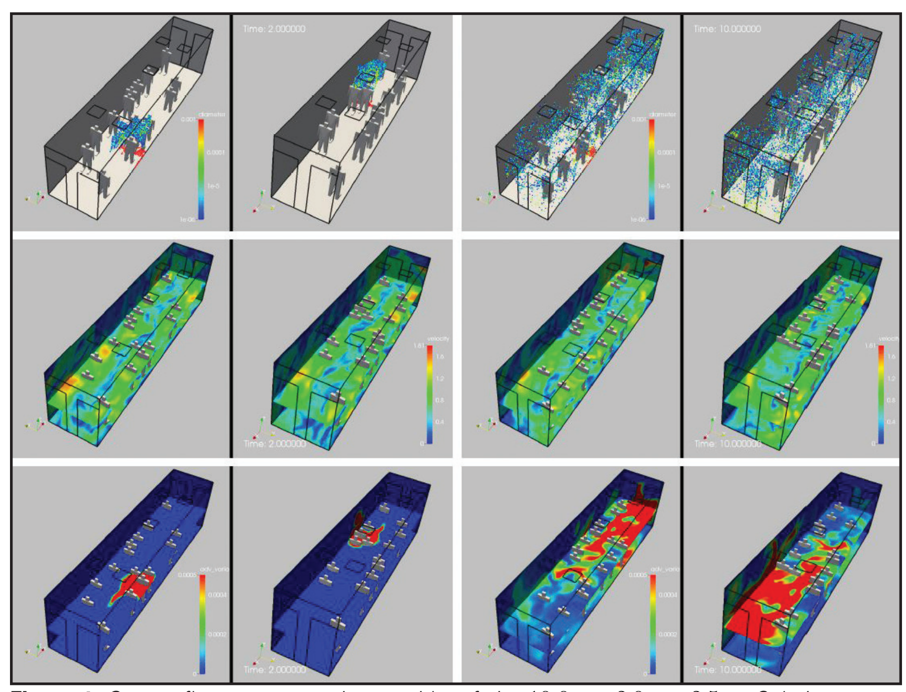

Figure 4. *Counterflow movement in a corridor of size* $10.0\,\mathrm{m} \times 2.0\,\mathrm{m} \times 2.5\,\mathrm{m}$. *Solutions are at* $t = 2.00\,\mathrm{sec}$ *and* $t = 10.00\,\mathrm{sec}$. *As before, the particles are colored according to the logarithm of the diameter, with red representing the largest particles and blue representing the smallest particles. The very strong mixing effect is due to the large-scale turbulence that is generated by the moving pedestrians and their wakes; this leads to a much higher propagation and transmission of pathogens in such environments. Figure courtesy of the authors.*

Outlook

As with any technology, further advances are clearly possible. The list is long, so we just mention the following areas for further development:

– Improved knowledge of the infectious dose that is required to trigger infection/illness

– Improved boundary conditions for HVAC exits

– Improved modeling of particle retention and movement through cloths (e.g., for masks).

The basic physical phenomena—and the partial differential equations and ODEs that describe them—have been known for more than a century, and solvers have advanced considerably over the last four decades. Nevertheless, we need a vigorous experimental program to complement and validate the numerical methods and establish firm "best practice" guidelines.

Acknowledgments: The authors acknowledge the help of Mika Gröndahl, a graphics editor at *The New York Times*, for the detailed STL models and thoroughly researched boundary conditions of the subway train car and airplane cabin. These runs would have been either impossible or meaningless without his efforts.

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Math in the World, from Mosquitoes to Gerrymanders

Shape: The Hidden Geometry of Information, Biology, Strategy, Democracy, and Everything Else. *By Jordan Ellenberg. Penguin Press, New York, NY, May 2021. 480 pages, $28.00.*

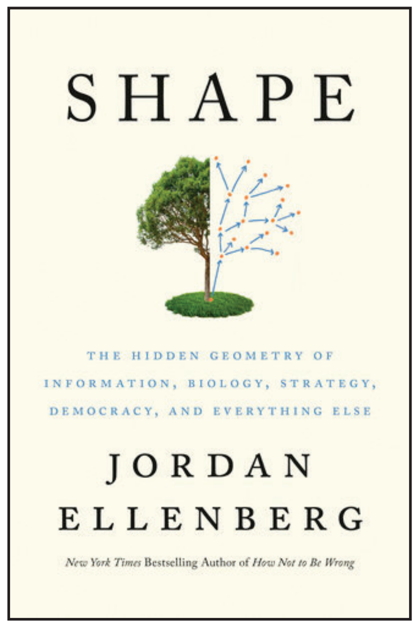
BOOK REVIEW
By Ernest Davis

Seven years ago, Jordan Ellenberg's *How Not to Be Wrong*—which explained the importance of mathematics for a popular audience—was a runaway success and earned both critical praise (including a review by me in *SIAM News*[1]) and a place on *The New York Times'* Best-Seller list. His new book, *Shape*, has raised the game; it seems to me even better than his last.

Ellenberg is an enviably skillful writer. His explanations of technical material are simultaneously crystal clear, patient, complete, and entertaining. He is also an exceptional raconteur. Ellenberg's many biographical and historical passages are skillfully integrated with the mathematical content, and he recounts them in a way that seems leisurely—as if he had all the time in the world to tell readers about a curious story or fun anecdote—but never drags. His inclusions of himself in the commentary are unfailingly tasteful — enough to make the narrative vivid and personal but never so much as to appear egotistical.

Ellenberg is witty yet balanced. His accounts of historical events and people are clear-eyed but sympathetic. His descriptions of contentious topics—such as artificial intelligence (AI) and gerrymandering—are scrupulously fair. Ellenberg loves math but is fully aware of the limitations of the mathematical viewpoint and the occupational vices of mathematicians. He writes that *"Mathematicians are prone to an imperial tendency: We often see other people's problems as consisting of a true mathematical core surrounded by an irritating amount of distracting domain-specific knowledge, which we impatiently tear away to get as quickly as possible to 'the good stuff.'"*

Incidentally, Ellenberg has a particular affinity for poetry. As such, he discusses both poets who engaged with mathematics—such as William Wordsworth and Rita Dove—and mathematicians who wrote poetry, including William Rowan Hamilton and James Joseph Sylvester.



Shape: The Hidden Geometry of Information, Biology, Strategy, Democracy, and Everything Else. By Jordan Ellenberg. Courtesy of Penguin Press.

What is actually in *Shape*? Well, the book contains a chapter on Euclidean proof, with a discussion of its impact on figures like Wordsworth, Abraham Lincoln, and Thomas Jefferson. A second chapter explores the question, "How many holes does a straw have?"—which was apparently a hot topic on the internet in 2014—with discussions of Henri Poincaré (a leading figure throughout the book) and Johann Benedict Listing, a lesser-known 19th-century savant. Yet another chapter addresses symmetries and geometric transformations in the context of Poincaré and Emmy Noether.

Ellenberg then moves on to the theory of random walks. He begins with Ronald Ross' analysis of mosquitoes' transmission of malaria, passes through Karl Pearson, Poincaré, Albert Einstein, and Andrey Markov, and concludes with Claude Shannon's use of Markov chains to generate English text. Three chapters focus on AI, game playing, and machine learning, with an excursion into cryptography. A chapter on metric spaces ends up mostly examining the vector representation of words that are used in AI programs. Two chapters detail prediction and include a long discussion of the attempts to predict the course of the COVID-19 pandemic. One chapter describes nearly geometric sequences and eigenvalues, while another delves into graph connectivity.

Next comes a true masterpiece: Ellenberg's chapter on districting and gerrymandering. He covers the implications, history, law, and relevant algorithmics. He also addresses the difficulty of determining what is fair and reasonable; the various suggested mathematical objectives for districting and criteria for gerrymandering detection; and the strengths and flaws of each topic. This chapter is very long—almost twice the length of all the others—but exceptionally clear, absorbing, and of course important.

I did find one aspect of the book disappointing: there is very little geometry after the introduction and first three chapters, which comprise only 63 of 425 total pages of content. *Shape* includes a lot of math of all kinds, but game trees, Markov chains, cryptographic codes, integer sequences, graphs, and so forth do not constitute geometry. Even the geometric considerations in the section on gerrymandering—such as district requirements for spatial compactness—are largely peripheral. There are very few *shapes*, other than the shapes of Congressional districts: some triangles, rectangles, circles, and occasional passing references to ellipses, hyperbolas, Alexander's horned sphere, and such.

This seeming uninterest in spatial and visual aspects of math manifests itself in other ways as well. There is a really beautiful proof of Fermat's little theorem $a^p = a \bmod p$ if p is prime[2] that I had never seen before, but the book has no proofs of geometric theorems beyond the *pons asinorum* and a dissection proof of the Pythagorean theorem. There are 100 pages on AI—mostly as applied to language—but barely a reference to computer graphics, computational geometry, or solid modeling. As I mentioned, the text contains a lot of poetry, but the only work of visual art that Ellenberg acknowledges is Salvador Dali's *Crucifixion: Corpus Hypercubus*. The subtitle promises "the hidden geometry of…biology," but *Shape* fails to comment on the marvelous geometric forms that living organisms create and only remarks on the flight of mosquitoes, spread of disease, and network structure

See **Math in the World** *on page 9*

[1] https://sinews.siam.org/Details-Page/everyday-problems-shot-through-with-mathematics

[2] The book gives the proof only for the case $a = 2$, but the generalization is immediate.

Ethical Discussions

Continued from page 7

Establishing a Professional Ethics Standard: The recording of Anna Alexandrova's talk at the 2018 EiM meeting, entitled "How to Build an Ethics: Lessons for Mathematics from Other Fields,"[6] presents an expert philosopher's interpretation of an important meta-question: *How can the professional community of mathematicians collectively move forward?* Alexandrova notes that "No research, no matter how pure, is immune from social responsibility."

Pondering the Impact of Abstraction: In "The Ethics of Mathematics: Is Mathematics Harmful?" [4], Paul Ernest argues that the standard method of abstraction—moving from the "real world" to mathematical equations, which is typical in math classes—may have adverse effects on mathematics students. This text can inspire some thought-provoking discussions about the profession as a whole.

Single-Lesson Resources

Not Just "Avoiding Doing Bad:" There are many examples of "unethical mathematics," especially in the context of data science, but fewer opportunities to highlight "good" behavior. Chad Topaz (Williams College) delivers an excellent talk about several projects at the Institute for the Quantitative Study of Inclusion, Diversity, and Equity.[7] His October 2020 presentation[8] at the Vanderbilt Postdoctoral Association Symposium offers an inspiring glimpse of the possibilities that emerge when one engages with the *good side* of ethics.

Laws and Ethics: *Ethical behavior* and *legal behavior* are not the same concepts, but some standards do become encoded into statute. On a day-to-day basis, mathematicians typically do not have to worry about the *legality* of their work. In the field of data science, however, this issue arises much more frequently. Patrick Hall and Ayoub Ouederni provide a short list of questions to consider with regard to the increasing scrutiny of the legalities of data-driven work [5].

Mathematics Provides Solutions: Our math majors really enjoy learning about *differential privacy*, which I introduce in the backdrop of its adoption by the U.S. Census Bureau[9] [1]. Plenty of web resources offer varying levels of sophistication in their explanations, so I recommend that educators select one or two to tailor to their classes.

Case Study: Uber Surge Pricing: This topic—a class favorite—always generates hearty discussion among the students. I typically begin with a short news story[10] that highlights the greedy side of surge pricing and encourages a certain viewpoint. Next, I present a 20-minute talk by Dawn Woodward of Uber[11] about the underlying mathematical principles.

Industry Case Study 1: The Volkswagen emissions scandal,[12] wherein the company installed "cheat devices" in their cars, inspires much conversation. I ask the students to think about how many people might have been involved and what levels of ethical culpability may have been at play. We consider whether some participants could have been "fooled" into going along, how others might have been willfully ignorant, and what ethical shortfalls are associated with such ignorance.

Industry Case Study 2: In the 1970s, a design flaw in the Ford Pinto[13] resulted in an increased risk of explosion and fire in the instance of rear-end collision. Based on actuarial analysis of overall cost, Ford initially decided to pay settlements for the expected lawsuits rather than recall and fix the design. In this case, the mathematicians/actuaries did precisely what their job required. The company eventually made the recall, but only after this analysis became public and a judge awarded $125 million in punitive damages.

Milgram Experiment: Students often begin to think that when the ethical answer in a particular situation seems obvious, people should be expected to "do the right thing." I show a short video about the Milgram experiment[14]—the famous study at Yale University that asked subjects to administer shocks to other participants as part of a supposed "learning" exercise—to demonstrate people's inclination towards obedience of authority.

Embedding Ethics Into a Calculus I Course: A final example, pulled directly from Chiodo's notes, suggests the following problem: *There is an oil rig in the ocean near a straight shoreline. Somewhere on the shore, there is an oil refinery. The rig is 100 kilometers (km) from the nearest shore point. You are asked to design the optimal route for an oil pipe from the rig to the refinery. The pipe costs $100,000/km under water and $40,000/km on land. Please compute the optimal route for the pipe.*

At some point, students will likely indicate that they need to know the refinery's distance down the shore. Give them the information and follow up with a conversation about the aspects that they might not be considering in their decision (as they will almost certainly choose to simply minimize cost).

Bringing It to the Classroom

Many mathematicians agree that we need more ethical understanding within our profession. To achieve an increased sense of ethical mindfulness, we must instill the rising generation with an awareness of ethical issues that they might encounter in the workforce. Consequently, *the critical first step is making ethical discussions an important component of existing courses.*

The aforementioned resources offer some "easy starts" for educators who are looking to explore ethics-based curricula. Hopefully these examples will provide a template for developing such modules *in any course that focuses on applications*. Just a few simple questions can help both students and teachers develop and flex their ethical muscles.

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[6] https://youtu.be/3e-E_SYK8Dg
[7] https://qsideinstitute.org
[8] https://youtu.be/9VM30uZ6PLI

[9] https://www.census.gov/content/dam/Census/newsroom/press-kits/2019/jsm/presentation-deploying-differential-privacy-for-the-2020-census-of-pop-and-housing.pdf
[10] https://youtu.be/LHYWuhxK04g
[11] https://youtu.be/GyPq2joHZv4
[12] https://en.wikipedia.org/wiki/Volkswagen_emissions_scandal
[13] https://en.wikipedia.org/wiki/Ford_Pinto#Legal_cases

[14] https://youtu.be/9DxSKTSoA_E

A New IEEE 754 Standard for Floating-Point Arithmetic in an Ever-Changing World

By James Demmel and Jason Riedy

Since 1985, most computational scientists—or anyone who uses floating-point (FP) arithmetic—have assumed that their computing platforms implement arithmetic operations according to the Institute of Electrical and Electronics Engineers (IEEE) 754 Standard for Floating-Point Arithmetic. This standard has made it much easier for researchers to write correct and portable code, since computers no longer round results or handle exceptions with the level of variety that existed among companies such as Digital Equipment Corporation, IBM, Cray, and Intel in 1985. Almost all differences became user-controlled under the standard, which also defined interchange formats to ease data porting between platforms and debugging efforts. The 2019 version of the IEEE standard provides new capabilities for reliable scientific computing, fixes bugs, and clarifies exceptional cases in operations and predicates.

The ever-changing world of technology motivates IEEE to periodically update all of its standards. One can only imagine an arithmetic standard that was (literally) set in stone and still uses base 60 instead of binary [6], as we do for keeping time. Beyond the few inevitable bug fixes, what changes in the world motivated updates in the most recent version of the IEEE 754 standard [4]? And what changes are still underway, unpredictable, and left to future versions of IEEE 754 or other arithmetic standards?

At a high level, one significant change is the burgeoning demand for reliability. Increasingly more groups now depend on computing to make important decisions. Sometimes it takes a disastrous rocket launch [2], naval propulsion failure [8], or robotic car crash [7] (see Figure 1)—all caused by faulty exception handling—to rouse public attention. The growing prominence of autonomous devices like cars and health monitors makes reliability even more critical.

One corresponding change in IEEE 754 is the addition of several new recommended operations: augmented addition, subtraction, and multiplication. Augmented addition takes two arguments—x and y—and returns two results: $h = x + y$ rounded in a new way, and $t = (x + y) - h$ exactly. Here, h stands for head and t stands for tail, since (barring exceptions) $h + t = x + y$ exactly; h represents the leading bits of the sum (the head) and t represents the trailing bits (the tail). The new rounding mode for this specific instruction rounds h to the nearest FP number, breaking ties toward zero (as opposed to the nearest even number, which is the standard approach). This new instruction accelerates two high-level operations that both support reliability.

Augmented addition is also known as two sum, which programmers have long used to simulate double precision via single or quadruple via double [5]. When done appropriately, performing some operations in higher precision can significantly improve the error bounds and increase a calculation's reliability. For example, Donald Knuth's original algorithm for computing h and t costs six FP operations. A "fast" version requires three operations, assuming that $|x| \geq |y|$. Neither algorithm handles exceptional cases uniformly. But if one implements augmented addition

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Figure 1. *"Impact" of poor exception handling for a driverless robotic car. Figure courtesy of [7].*

in hardware, it requires only one or two instructions and provides both significant speedups and uniform exception definitions.

The new definition of augmented addition employs a novel (for binary) rounding mode—rounding halfway cases to the nearest result that is smaller in magnitude (i.e., towards zero)—to support a new use case: bitwise reproducible FP summation [1]. Parallel and vector processing is now ubiquitous, and codes can no longer assume a fixed summation order. Because FP addition is not associative, the final results can differ substantially between runs. A prior *SIAM News* article[1] summarizes real-life applications that range from debugging efforts to the detection of underground nuclear tests [3]. A portable algorithm uses the fast two-sum algorithm and bitwise-reproducibly sums n numbers—independent of the summation order—in approximately $9n$ FP operations and $3n$ bitwise operations in the common case [1]. Hardware-accelerated augmented addition reduces this calculation to $4n$ or $6n$ FP operations and no bitwise operations. Unlike rounding to nearest even, fixing the rounding mode to be independent of the result eliminates the bitwise operations. With parallel synchronization overhead, the utilization of four to six operations per entry enables programmers to make all summations reproducible by default with negligible cost.

Another requirement for reliability is "consistent exception handling." This concept's definition may depend on context, but everyone agrees that computing the maximum or minimum of an array of numbers should yield the same result regardless of the argument order. Due to an oversight on the interaction of two sections in IEEE 754-2008, the definition of max and min did not have this property when one argument is a "signaling NaN." These old definitions are deprecated in the 2019 standard, and new suggested operations guarantee that min and max are associative.

Ensuring that higher-level software behaves consistently and portably with exceptional values requires work that falls outside of standard IEEE 754 arithmetic. For example, the reference implementation of the Basic Linear Algebra Subprograms (BLAS) routine NRM2—which computes the 2-norm of vector x—may return NaN if two or more entries of x equal infinity and no NaNs; some releases, like Intel's Math Kernel Library, have repaired this issue. The reference implementation of the BLAS routine ISAMAX, which returns the index of the largest entry in terms of absolute value of input array x, returns $\mathrm{ISAMAX}([0, \mathrm{NaN}, 2]) = 3$ and $\mathrm{ISAMAX}([\mathrm{NaN}, 0, 2]) = 1$. Even more examples of this phenomenon exist in BLAS and other widely used software. Carefully defining "consistency"—and automating the identification and repair of such cases—is a work in progress.

An interesting challenge when defining consistency is that not all high-level languages agree on the definitions of basic operations. For example, multiplying two complex numbers $x = (\mathrm{Inf} + i * 0)$ and $y = (\mathrm{Inf} + i * \mathrm{Inf})$ yields $(\mathrm{NaN} + i * \mathrm{NaN})$ in `Fortran` and $(-\mathrm{NaN} + i * \mathrm{Inf})$ in `C`. Backward compatibility may prevent languages from agreeing on the correct answer. Fortunately, the `C` and `Fortran` standardization committees are currently updating their definitions of max and min to match the new IEEE standard.

Other novel recommended operations in the IEEE 754 standard include "payload" operations to read or write information that is stored in the fraction bits of a NaN—which allow more customized exception handling—as well as the previously-undefined trigonometric functions $\tan\mathrm{Pi}(x) = \tan(\pi * x)$, $\mathrm{asinPi}(x) = \mathrm{asin}(x)/\pi$, and $\mathrm{acosPi}(x) = \mathrm{acos}(x)/\pi$. The standard also explains additional exceptional cases, such as the menagerie of x^y functions. Clarifications and additions to decimal arithmetic focus on the "quantum" that formalizes useful fixed-point aspects like dollars and cents. These items and other details are discussed in corresponding IEEE documents.[2]

Now we turn to the future. During the standard's finalization, there was an explosion of 16-bit and smaller precisions for

See **IEEE 754 Standard** *on page 11*

[1] https://sinews.siam.org/Details-Page/reproducible-blas-make-addition-associative-again

[2] https://grouper.ieee.org/groups/msc/ANSI_IEEE-Std-754-2019

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of the circulatory system. Many years ago, my father Philip Davis decried the disappearance of the visual and spatial sense from mathematics [1]; it is dismaying to see this tendency in a book by an eminent geometer that is entitled *Shape*.

Nevertheless, this is at most an objection to the title. *Shape* is a wonderful book; it is superlatively well written and full of history, mathematics, and much else. Readers that range from professional mathematicians to people who disliked geometry in high school can enjoy and learn from the material.

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SIAM Advocates for Research Growth as Biden Administration Releases Funding Request

By Eliana Perlmutter

A new administration and Congress in Washington, D.C., mean new priorities for the federal agencies that support applied math and computational science. Over the last few months, the SIAM Committee on Science Policy[1] has been championing federal support for these research areas. President Biden supports research and development funding at non-defense agencies; this is reflected in his first budget proposal to Congress, which was released with full details on May 28, 2021. The Biden administration's policy and budget priorities include public health, climate and clean energy, innovation, education, and racial equity.

In April, the SIAM Committee on Science Policy and Science Policy Fellowship recipients[2] conducted virtual meetings with congressional offices to advocate for robust funding to support applied mathematics and computational science research at the National Science Foundation (NSF), Department of Energy (DOE), Department of Defense (DOD), and National Institutes of Health (NIH). SIAM representatives also engaged in discussions about agency updates with relevant federal agency leaders, including Juan Meza, Director of the Division of Mathematical Sciences at NSF; Barbara Helland, Associate Director of the Office of Science's Advanced Scientific Computing Research (ASCR) program at DOE; Bindu Nair, Director of DOD's Basic Research Office; and Jean-Luc Cambier, Program Director of DOD's Basic Research Office.

After these discussions about the Biden administration's initial plan and priorities, the fiscal year (FY) 2022 budget request offered additional details.[3] Unrestrained by legally imposed budget caps for the first time in a decade, President Biden proposed an 18 percent boost in discretionary spending for a total of $1.522 trillion. This budget is a sharp contrast to the Trump administration, which prioritized defense spending and proposed major cuts to other domestic programs. Overall, the FY 2022 budget would significantly increase funding for research and development programs that are of interest to the mathematics and computational science communities. The notable exception is a 13 percent proposed cut to basic research within the DOD Science and Technology (S&T) programs. Some budget proposals require the creation of new agencies, which will be a bigger lift in the narrowly divided Congress. Other proposed increases are consistent with existing legislation to invest in research and development for national competitiveness.

Though the budget proposal would increase funding for fundamental research at key science agencies, it focuses primarily on use-inspired research, translation, and the development and deployment of technology. For example, the proposal would establish a new NSF Directorate for Technology, Innovation, and Partnerships (TIP);[4] create a new Advanced Research Projects Agency for Health (ARPA-H) within NIH; allocate $500 million for a new Advanced Research Projects Agency for Climate (ARPA-C); and increase funding for applied energy development and demonstration projects at DOE by $5.8 billion. The budget proposal would also continue to grow investments that began under the Trump administration for emerging technology areas, such as quantum information science (QIS), artificial intelligence (AI), microelectronics, and advanced computing.

The Biden administration proposes major increases across NSF in both administration research and education priority areas, as well as core programs. Overall, Research and Related Activities would grow by 18 percent from the FY 2021 estimated level, while Education and Human Resources would grow by 16 percent. The budget request recommends an increase of $110 million—or seven percent—for the Mathematical & Physical Sciences Directorate and an increase of 16 million—or 6.5 percent—for the Division of Mathematical Sciences. If enacted by Congress, the Office of Advanced Cyberinfrastructure in the Computer & Information Science & Engineering Directorate would see an increase of $22 million, or 9.4 percent. Across both the new Directorate for TIP and existing NSF directorates, NSF would continue to prioritize critical technologies like AI, QIS, wireless research, advanced manufacturing, and biotechnology while simultaneously adding additional priorities in climate change and clean energy research.

The Biden administration's FY 2022 budget request would provide the DOE's ASCR program office with $1.04 billion, a $25 million—or 2.5 percent—increase from the FY 2021 enacted level. As the demands of the Exascale Computing Project (ECP) continue their planned decrease, the request for ASCR re-emphasizes foundational research to advance AI, QIS, and strategic computing initiatives that will increase the competitive advantage of U.S. industry. It also includes a new focus to address climate change and develop a clean energy future. Within ASCR, the proposal would provide the Mathematical, Computational, and Computer Science Research account with a $33 million—or 12.7 percent—increase above the FY 2021 enacted level. This account includes $51 million—a five percent increase—for Applied Mathematics Research activities that conduct basic research in scalable algorithms and libraries; multiscale and multi-physics modeling; and integration of scientific modeling, data, and AI/machine learning with advanced computing to promote efficient data analysis.

The request also recommends $86 million—a 12.9 percent increase—for Computational Partnerships, which primarily support the Scientific Discovery through Advanced Computing (SciDAC) program and in FY 2022 would support plans for the transition of mission-critical ECP applications into SciDAC. Furthermore, the administration would provide an unspecified increase for the Computational Science Graduate Fellowship program to fund additional fellows and expand participation from members of underrepresented groups.

The budget request suggests funding basic research (6.1) at DOD at $2.3 billion, which is a 13 percent decrease from the FY 2021 enacted level. Overall, the S&T accounts (6.1-6.3) would see a $2.1 billion

See **Funding Request** *on page 12*

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

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

[3] https://www.whitehouse.gov/omb/budget

[4] https://www.nsf.gov/about/budget/fy2022/pdf/52_fy2022.pdf

Panel Discussion at CSE21 Offers Advice to Mid-Career Mathematicians

By Lina Sorg

The mid-career point is an exciting time for researchers in science, technology, engineering, and mathematics (STEM). As experienced scientists settle into their professions, they begin to think more diligently about future research or occupational directions, professional and personal opportunities, and broader community engagement. A panel discussion at the 2021 SIAM Conference on Computational Science and Engineering,[1] which took place virtually earlier this year, offered guidance to applied mathematicians and computational scientists at the mid-career stage. Hans De Sterck (University of Waterloo), Katherine J. Evans (Oak Ridge National Laboratory), Sarah Knepper (Intel Corporation), Damian W. Rouson (Sourcery Institute and Sustainable Horizons Institute), and Mayya Tokman (University of California, Merced) comprised the panel, which attracted over 120 attendees in various phases of their careers.

The session began with a conversation about the seemingly universal fear of plateauing at the mid-career point. Tokman acknowledged that this type of stagnation is more likely to occur for individuals in academia who have had particularly strong early careers and are exhausted from working towards tenure. Upon achieving tenure, mentorship and other support systems within universities are typically less strong than in early-career settings. These factors—when combined with the temptation to relax a bit—can collectively cause burnout.

To combat a prospective slump, Tokman advised attendees to consider their passions and brainstorm ways to best exercise the newfound flexibility of tenure. "Think about possible new directions that might be a bit more risky," she said. "Being able to say no [is important] as well, because the amount of service requests is going to grow quite significantly." Increased participation in committees, groups, and other volunteer activities is typically expected of professors with tenure. However, one should also maintain personal research projects, as these endeavors determine promotion eligibility.

Evans affirmed that nearly everybody plateaus at some point in their career, simply due to the evolutionary nature of STEM. "We're in computing and math, and architectures and other things will change," she said. "You'll find that what you've been working on will change too. To stay current and fresh, you need to learn more skills." Acquiring these skills sometimes involves working on larger, more complex projects. Knepper urged mid-career scientists not to get discouraged if they feel like they are accelerating at a slower pace, which often happens with long-term assignments.

Rouson offered a counterpoint to these perspectives and suggested that plateauing does not necessarily have to be a bad thing if it helps individuals slow down and reevaluate their priorities, especially in industry. In this sense, the mid-career period can be an appropriate time to set future goals. "One important thing to consider is, what are you passionate about?" Rouson said. "Does that necessarily align with rising in an organization?" For instance, moving into an administrative position is likely not in the best interest of someone who wants to conduct technical research.

CAREERS IN MATHEMATICAL SCIENCES

Knepper, however, recently transitioned from software engineering to a managerial role and is enjoying the different responsibilities. Though she spends less time coding, she can now explore strategies to promote productivity, team culture, and diversity and inclusion. This career shift offered Knepper more opportunities to support the types of changes that she wants to see in the workforce.

Discussion then turned to tactics for handling regrets about previous work-related choices. Rather than regret any of his decisions, Rouson chooses to see every problem as an opportunity. Knepper agreed, encouraged attendees to think in terms of lessons learned, and spoke about a challenging project in her past as an example. Although she spent more time on the project than she would have liked before ultimately giving it to another team with a better fit, it taught her valuable lessons about logically managing transitions.

Evans reminded participants to take risks despite the possibility of failure. She also warned that stakes can feel higher at the mid-career stage. "They forget to tell you that taking risks by nature means that some of them will not pan out and you will fail," Evans said. "When you fail at something, that's part of the deal." Coming to terms with the reality that failure is always a potential outcome made it easier for her to process and accept disappointments.

De Sterck admitted that envisioning the effective coexistence between a career and family is sometimes difficult — a concern that is relevant at all levels of experience. Mid-career scientists should carefully consider the ramifications of major workplace decisions to ensure that they align with the expectations of one's personal life. For example, De Sterck changed institutions—effectively moving his family to a new continent—six months before his second child was born. "In hindsight, maybe that was not the best time to do that," he said. "It's not that I think we shouldn't have done it, but it's good to be aware of what you're going to have to go through if you're in such a situation."

Increasing demands on one's time—in terms of both occupation and personal/familial responsibilities—necessitate effective work strategies. Evans advocated for time blocking as the best way to get things done. She suggested that researchers cluster their meetings and schedule several lengthy blocks of time for uninterrupted work; this approach is especially valuable for coding projects, during which distractions like phone calls or emails are especially disruptive.

As individuals advance in their careers, they may find that balancing "fun" aspects of research with the need to manage and mentor students can become overwhelming. De Sterck recommended that professors always maintain a good sense of their students' basic technical abilities, and noted that he generally tries to preserve at least one project for which he does a significant amount of the technical work himself. Version control systems like GitHub allow professors and mentors to collaborate and stay connected with students and postdocs, especially as new hardware arises.

In some ways, having a cohort of multiple students allows more senior mathematicians to partake in a wider variety of projects than at the early-career stage. Yet as researchers accumulate more students over the years, they typically have less time to devote to each one individually. Tokman initially had seemingly unlimited hours to spend with her first graduate student; now she has much less time to split between several graduate students, which was a challenging adjustment. She encouraged attendees to enlist a second advisor or even a postdoc when they have limited time to dedicate to their cohort. "We need to take the idea of raising the next generation very seriously," she said. "Mentorship in our field is very important."

Next, panelists discussed the viability of changing institutions at the mid-career stage. Tokman admitted that it is often quite difficult to move within academia at this point, and advised participants to do so before reaching tenure. Academics should ideally start thinking about this type of transition in advance and try to give talks or get involved at institutions where they might want to make connections. De Sterck added that most people who switch universities after tenure are pursuing specific leadership positions. "If you think that you will be moving, having a really strong research track method is the most important," he said.

Rouson indicated that the exact opposite is true in industry, as he witnesses frequent movement in Silicon Valley. "If you like moving, then maybe industry is the place to be," he said. Knepper mentioned that she has been with Intel for 10 years, which is atypically long for an industrial position. She indicated that employees sometimes even return to a previous organization at a later date to advance within the company and obtain new skills.

The speakers agreed that individuals who are looking to diversify their activities should seek out volunteer opportunities. After gaining tenure, De Sterck became involved with SIAM activity groups and conference committees. "If you're interested in helping to organize things, I think it's a great way to contribute to the community," he said. Evans and Tokman echoed this sentiment and urged attendees to volunteer with SIAM, particularly if they are considering future leadership positions in academia or within science in general.

As the session concluded, the panelists reminded everyone that mid-career mathematicians are not done learning and should not be afraid to reach out to their own mentors or establish new connections. It is also important that they continually evaluate their own priorities and change their focus or direction accordingly. "You need to think about which things you're doing to advance your career, which things you're doing for your department, and which things you're doing just to be liked," Tokman said. "Time is precious, and you can't spread yourself too thin."

Lina Sorg is the managing editor of SIAM News.

[1] https://www.siam.org/conferences/cm/conference/cse21

IEEE 754 Standard

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machine learning (ML) applications. IEEE 754-2008 formalized binary16 (which has 10 bits of precision plus one implicit bit, five bits of exponent, and one sign bit) with input from graphics hardware manufacturers. ML applications benefit from a wider exponent range to represent smaller probabilities, thus leading to formats like Google's bfloat16 (with 7(+1) bits of precision, eight bits of exponent, and one sign bit). Other ML architectures implement different partitionings of the 16 bits, and researchers are investigating the use of even fewer bits to accelerate both ML training and inference.

ML optimizations are one example in which understanding arithmetic requirements is important for novel architectures. Other architectures work by distributing the FP load between control processors and memory-side processors. In the past, programmers have failed to ensure the reliability and reproducibility of these results for smart network interfaces that only accelerate the Message Passing Interface (MPI) and similar standards. Although distributed hardware supports newer memory-centric programming interfaces—which are intended to be transparent to programmers—they must accommodate the same semantic assumptions as sequential codes. Furthermore, developing arithmetic that is more amenable to low-power and high-error situations like interstellar probes requires additional end-to-end analysis.

Some incredibly novel architectures are pushing the limits of current numerical analysis. Bridging the gap between analog computing (like quantum) and the binary domain is an open field with many historic precedents. Advances in stochastic and semi-stochastic arithmetic also accentuate all of the issues that accompany the composition of different rounding and truncation methods. Though this matter lies beyond IEEE 754 and possibly beyond the rectilinear interval standard IEEE 1788.1, it still merits consideration.

Many opportunities exist for students and other researchers in these areas. It is also important to remember that not everything must live within one standard. IEEE 754 does not limit other ideas; instead, this evolving standard supports and inspires comparison. We encourage your undoubtably vigorous comments — perhaps some aspects will appear in IEEE 754-2029 or other future editions. We all have work to do!

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James Demmel is a professor of mathematics and electrical engineering and computer sciences (EECS) at the University of California, Berkeley. He is the former chair of the Department of EECS. Jason Riedy is a member of the technical staff at Lucata Corporation, where he applies novel memory-centric architectures to data analysis problems. Both Demmel and Riedy were part of the 2019 IEEE 754 Standard Committee.

Growing, Inspiring, and Diversifying Computational Science and Engineering through Broader Engagement

By Mary Ann Leung and Jasmine Pineda

The COVID-19 pandemic forced most of the world to reinvent collaboration amid dire circumstances, and SIAM staff and the organizers of the 2021 SIAM Conference on Computational Science and Engineering (CSE21)[1]—which took place in March—certainly rose to the occasion. SIAM reimagined the conference in a virtual format by implementing new and engaging online platforms that allowed members of the CSE community to connect and discuss innovative research from their own individual workspaces. CSE is critical to the advancement of pressing scientific issues that require inter- and multidisciplinary work. When individuals who seek to solve the world's greatest problems—regardless of their professional or academic journeys—work together, the possibilities for scientific discovery are limitless. The Sustainable Horizons Institute's[2] (SHI) Broader Engagement (BE) program[3] endeavors to widen these possibilities.

In 2015, Mary Ann Leung—president and founder of SHI—initiated BE@CSE to encourage student participation while she was serving on the CSE15 Organizing Committee.[4] Since then, SHI has continued the program at each subsequent CSE meeting. BE offers financial support to members of underrepresented and underprivileged groups, affording them full access to the rich technical material at CSE conferences. It also fosters a sense of community and belonging through mentorship, networking, and other activities that connect participants with each other. In addition, the program promotes inclusion by providing opportunities for scientists to volunteer, recruit, and learn.

[1] https://www.siam.org/conferences/cm/conference/cse21
[2] https://shinstitute.org
[3] https://shinstitute.org/siam-cse21-broader-engagement-program
[4] https://archive.siam.org/meetings/cse15

Over the last six years, BE participation has increased from just a handful of students in 2015 to more than 100 in 2021. In 2017, BE began organizing Guided Affinity Groups to strengthen participants' connections with SIAM, enhance their conference experience, and provide psychosocial support. Volunteers with expertise in one or more of the conference's technical themes lead daily group meetings to suggest sessions of interest, answer questions, and discuss recent talks. At the end of the week, each group presents their findings. BE@CSE continues to evolve and improve with each meeting.

BE@CSE21 was very successful despite the challenges of a virtual conference format. Throughout the conference, 47 BE participants presented posters and four individuals spoke about their research during a BE minisymposium. Participants made long-lasting connections with seasoned scientists via the mentor-protégé mixer and BE networking session (see Figure 1), both of which took place in an online platform that was customized by BE committee member Aimee Maurais (Massachusetts Institute of Technology).

The popularity of Guided Affinity Groups[5]—which allowed students to join one of 10 groups that spanned a wide range of topics from quantum computing to machine learning—soared at CSE21. Group members especially enjoyed chatting about their conference experiences and offering advice to each other. Christine Vaughan (Iowa State University) discussed her involvement in the "Meshes and Particles and GPUs Oh My!" group, which was led by Ann Almgren (Lawrence Berkeley National Laboratory). "I particularly enjoyed being part of a small Guided Affinity Group where I was able to check in daily with other participants and learn about how they navigated the conference," Vaughan said. "As a young researcher, I find these interactions with my peers to be so helpful."

[5] https://shinstitute.org/guided-affinity-groups-for-be-cse21

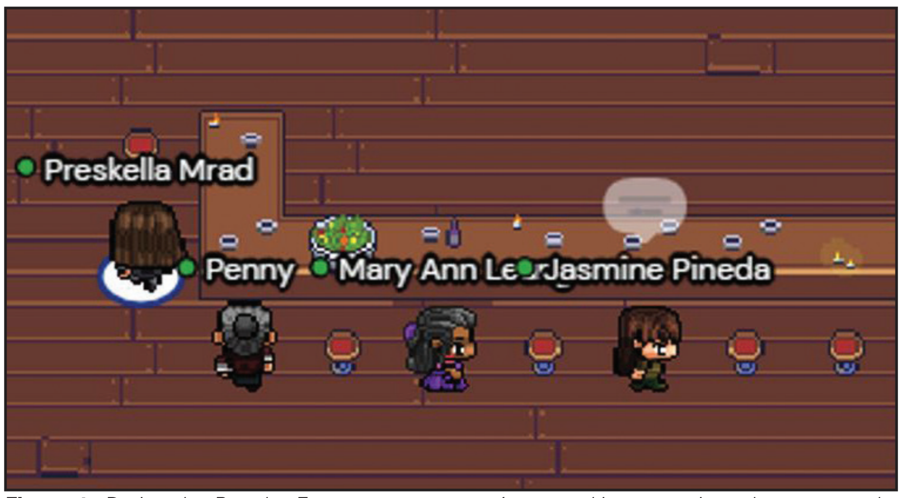

Figure 1. *During the Broader Engagement program's networking event in gather.town at the virtual 2021 SIAM Conference on Computational Science and Engineering, Preskella Mrad (University of Texas at Dallas) and Penny Wu (Arizona State University) chat with Mary Ann Leung and Jasmine Pineda of the Sustainable Horizons Institute about their conference experiences.*

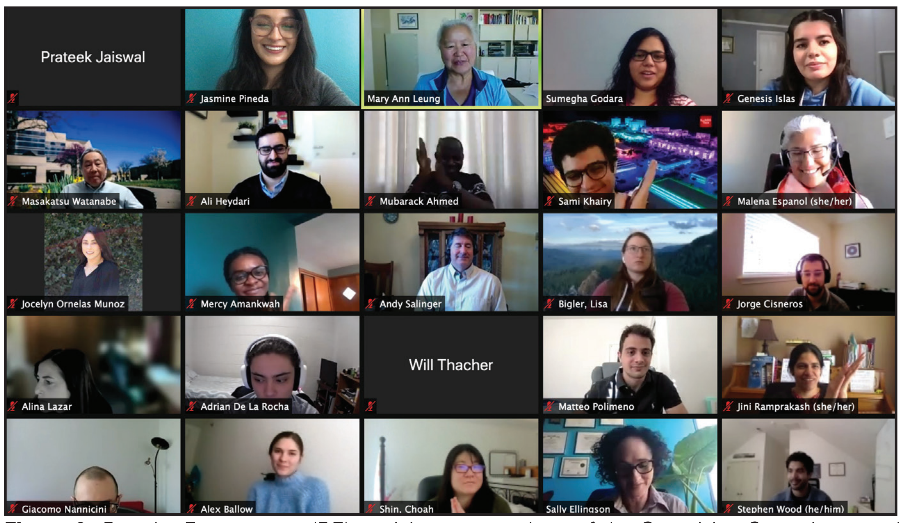

Figure 2. *Broader Engagement (BE) participants, members of the Organizing Committee, and staff from the Sustainable Horizons Institute celebrate during the BE wrap-up session at the 2021 SIAM Conference on Computational Science and Engineering, which took place in March.*

Although technical topics were the primary focus of most conversations, leaders also extended their advice and professional networks to their groups. "My group had a wonderful leader who helped connect us with her network, gave us amazing advice and suggestions, and instilled so much confidence in us," Vaughan continued. "She was incredible and has already made lasting impacts in our scientific lives."

All Guided Affinity Groups presented their takeaways during the BE wrap-up session (see Figure 2). This year's presentations included creative displays and heartfelt messages about the program's positive impacts. Andy Salinger's (Sandia National Laboratories) "Impacting Science and Engineering Applications with Computational Science" group used a scale from 0 (fundamental) to 1 (applied) to rate the talks they attended. Participants analyzed their own interests on the spectrum to better understand the type of research they might want to pursue. The "Inverse Problems and Applications" group, which was led by Malena Español (Arizona State University), explored the virtues of being part of a diverse group comprised mostly of women, ethnic minorities, and a community college student. Participants reviewed advice from guest speakers about applying for fellowships and degree programs.

BE also collaborated with conference organizers to provide a meeting-wide panel series on challenges and best practices for equity, diversity, and inclusion (EDI) in CSE.[6] The first part of the panel featured scientists at varying career stages who discussed their perseverance through the difficulties of finding one's place in CSE as a member of an underrepresented group. After reflecting on his journey and successes, panelist Derek Jones (Lawrence Livermore National Laboratory) drew some conclusions. "As a minority, I felt proud because I got to do really interesting work even though I wasn't well represented," he said. "Hopefully in the future we can help change that."

[6] See "Three-Part Panel Series at CSE21 Explores Equity, Diversity, and Inclusion in the Workforce" on page 3.

The second portion of the panel showcased organizational leaders who are actively working on EDI initiatives. They shared successes and challenges in their efforts to catalyze change within institutions that have long operated the same way. During the third and final session, panelists engaged in constructive conversation about EDI and brainstormed strategies for moving forward.

For many BE participants, CSE21 was the first conference that they ever attended. The goal of BE was thus to provide a positive and inclusive experience so that CSE21 would not be their last. The program continues to inspire and alter trajectories to ensure that SIAM's CSE community is both diverse and inclusive. Miandra Ellis (Arizona State University) reflected on the connections she made during the conference, which boosted her confidence and provided a new perspective on self-worth. "I interacted with professionals in my field and learned about both their research and their journey to becoming the researchers they are today," she said. "This shattered my preconceptions about successful mathematicians being people without doubt who knew that they belonged from the first time they saw an equation. This evolution in the way that I viewed successful mathematicians was further supported by my mentoring experience. The discussions I had with my mentor about how to approach the post-graduate career period helped to dispel notions that I had about my worth being tied to my ability to graduate with a job offer in hand."

The BE program thanks everyone who participated in this year's activities at CSE21 and looks forward to continued engagement with the SIAM community at future conferences.

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Funding Request

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decrease; the administration instead prioritized advanced technology research and prototyping. This reflects DOD's overall FY 2022 goal to deliver fieldable capabilities to troops more quickly and efficiently. The Army, Navy, and Air Force basic research accounts would respectively decrease by $79 million, $48.3 million, and $45.6 million when compared to FY 2021 enacted levels. Given these and other DOD cuts, the administration's flat toplines for defense spending, and razor-thin Senate and House voting margins, Congress will likely struggle to add appropriations to make up for requested cuts.

The budget request would fund NIH at $52 billion in FY 2022, an increase of $9 billion—or 21 percent—above the FY 2021 enacted level. $6.5 billion of this proposed increase would help establish ARPA-H, the aforementioned entity within NIH that would use nontraditional research and development approaches to invest in highly innovative science that has the potential for transformative breakthroughs. If established, ARPA-H could reshape the nation's biomedical research enterprise. The Biden administration would also invest in new research priorities that are related to climate change's impacts on human health, in addition to research that aims to eliminate health disparities and improve health equity.

Given the whole-of-government interest in climate change, SIAM convened a task force to draft recommendations for Congress and federal agencies about areas of research and education that are related to climate change, environmental resilience, and clean energy and would benefit from involvement of the applied math and computational science communities. The resulting task force report includes recommendations for many agencies that are related to climate, energy, and resilience—including the U.S. Department of Agriculture and U.S. Department of Transportation—as well as agencies like NSF and DOE that are historically more connected to applied mathematicians and computational scientists. The timing of this report aligns with federal agency planning to develop and implement initiatives—such as a new internal NSF climate committee—that progress President Biden's climate agenda, as well as efforts by the Democratic-led Congress to advance climate legislation while in the majority and in control of the presidency.

The FY 2022 budget request formally initiated the congressional appropriations process. However, the timing of passing final FY 2022 appropriations remains uncertain. Furthermore, the late start to the appropriations process increases the likelihood of a stop gap funding measure, known as a continuing resolution, to avoid a government shutdown and continue to fund federal agencies beyond September 30 — the end of FY 2021. SIAM will stay abreast of the FY 2022 appropriations cycle and its impact, advocate for strong funding for applied mathematics and computational science programs at relevant agencies, and keep members informed.

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