Research in Inverse Problems and Training in Computational Science: A Reflection on the Importance of Community

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As we strive to create a more diverse and inclusive scientific community, it is worth reflecting on the importance of mentors, collaborators, role models, and friends. This is my story. From collaborators who have guided me to new and exciting research directions to mentors who have provided much-needed support and perspective, it is my "village" (i.e., the close members of my scientific community) that has been critical in shaping my professional journey. This article is a retrospective of the people and experiences that have had significant impacts on my research portfolio, on my teaching and mentoring of students, and on my involvement in the scientific community. It begins in 2006 when, as a second-year Ph.D. student in the Department of Mathematics and Computer Science, Emory University, I was awarded the Department of Energy Computational Science Graduate Fellowship.

As we celebrate the 30th year of the Department of Energy (DOE) Computational Science Graduate Fellowship (CSGF) program, I take a moment to reflect on the impact of the CSGF on my professional paths and experiences. After completing my Ph.D. in 2009, which was supported by the DOE CSGF program from 2006 to 2009, I held a National Science Foundation (NSF) Mathematical Sciences Postdoctoral Research Fellowship in the Department of Computer Science, University of Maryland, College Park, from 2009 to 2011, a faculty position at the University of Texas at Arlington, from 2011 to 2012, and a faculty position at Virginia Tech, where I am currently an Associate Professor in the Department of Mathematics.

When I reflect on the biggest impact of the CSGF, it is the establishment of *community*—the vibrant research community, the opportunities, the role models, the personal connections, and the friendships. Navigating the world of academia is rife with challenges, from the application process to the tenure process. We are expected to establish an internationally renowned research program, develop innovative teaching materials, engage students in research, secure funding, and strike a delicate balance of professional service (all while many of us are also starting families!)—so it is important not only to have established mentors as role models but also to have friends who are in similar career stages, also known as "near-to-peer" colleagues, for empathy and support. The CSGF program has been pivotal in creating and sustaining such a community, and I believe it is what truly sets this program apart.

My goal for this article is to provide a retrospective since my time as a CSGF fellow, looking back at various highlights from my research contributions in the field of large-scale inverse problems to educational and outreach endeavors that have been particularly meaningful to me. I also hope to provide some inspiration and ideas about what we can do to create and nurture the next generation of computational scientists.

RESEARCH EXPERIENCES

My research is on the development of computational methods for large-scale *inverse problems*. Inverse problems arise naturally and are of core importance in many scientific fields, such as astronomy, biology, and

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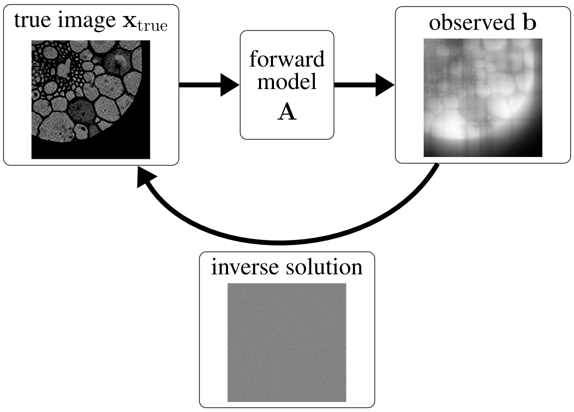

FIGURE 1. Image deblurring is an inverse problem, where the goal is to reconstruct the true image, $\mathbf{x}_{\text{true}}$, given the observed image, $\mathbf{b}$, and knowledge of the forward blurring process, $\mathbf{A}$. The problem is ill-posed, so the inverse solution computed as $\mathbf{A}^{-1}\mathbf{b}$ is severely corrupted with noise and errors.

medicine.[1] A classic example of an inverse problem is image deconvolution (or deblurring), where signals measured by machines (e.g., cameras) are distorted, and the aim is to recover the original input signal. See Figure 1 for an example of a deblurring problem. Another example of an inverse problem arises in atmospheric inverse modeling where the primary goal is to estimate greenhouse gas fluxes or air pollution emissions at the Earth's surface using satellite observations of these gases collected in the atmosphere. See Figure 2 for three-hourly reconstructed fluxes from Orbiting Carbon Observatory 2 satellite observations.[2]

More precisely, most inverse problems have an underlying mathematical model, where the measurements in $\mathbf{b}$ can be represented as

$$\mathbf{b} = F(\mathbf{x}_{\text{true}}) + \delta \quad (1)$$

where $\mathbf{x}_{\text{true}} \in \mathbb{R}^n$ represents the desired solution or unknown parameters, the functional $F(\cdot) : \mathbb{R}^n \to \mathbb{R}^m$ models the forward data acquisition process, and $\delta \in \mathbb{R}^m$ represents inevitable noise or errors that arise from measurement error, discretization error, or round-off error. For the image deblurring example, the forward model is defined by the kernel or point spread function that describes the blur, and for the atmospheric inverse modeling problem, F is defined by an atmospheric transport model. Although errors in the forward model may be incorporated in the definition of F, we assume that we have near-perfect knowledge of the forward model. Then, the inverse problem can be stated as follows.

Inverse problem
Given measured data, $\mathbf{b}$, and forward model, $F(\cdot)$, the **goal of the inverse problem** *is to compute an approximation of $\mathbf{x}_{\text{true}}$.*

State-of-the-art inverse problems that we target present enormous computational challenges, and tackling these challenges requires sophisticated tools from mathematics, statistics, and computer science as well as synergistic collaborations with engineers. For example, in atmospheric inverse modeling, the fast and accurate estimation of greenhouse gasses and air pollution emissions is important because of the threats they pose to energy security (i.e., the availability of natural resources for energy consumption), public health, and safety. However, due to the massive amounts of satellite data that need to be processed and the fine-scale resolution at which the reconstructions are needed, the sheer size of the inverse problem poses many computational challenges especially in the context of threat detection. Solving these inverse problems requires recovering unknown parameters in $\mathbf{x}_{\text{true}}$ which number in hundreds of millions from observed data in $\mathbf{b}$ which number on the order of several millions. High-performance computing resources have proved to be invaluable for handling these large datasets, but this alone is not enough. Like most inverse problems, reconstructing greenhouse gas fluxes from satellite data is both an underdetermined and an *ill-posed* problem.[a] By using a Bayesian approach, we can incorporate prior information about the parameters of interest, in a process that is commonly referred to as *regularization*, and provide a natural framework for uncertainty quantification (UQ). Unfortunately, for very large inverse problems, computing the maximum a posteriori or "most likely" estimate and quantifying the uncertainty associated with the reconstructions can be prohibitively expensive.

Furthermore, there are enormous statistical challenges. It is well known that the quality of the reconstruction depends crucially on the statistical model for the prior and the noise distributions as well as on the appropriate choice of hyperparameters that govern these distributions. For capturing abnormally large, disproportionate atmospheric emissions, so-called "super-emitters," that are surrounded by spatially diffuse emissions sources, new computational

[a]A problem is ill-posed if a solution does not exist, or is not unique, or does not depend continuously on the data.

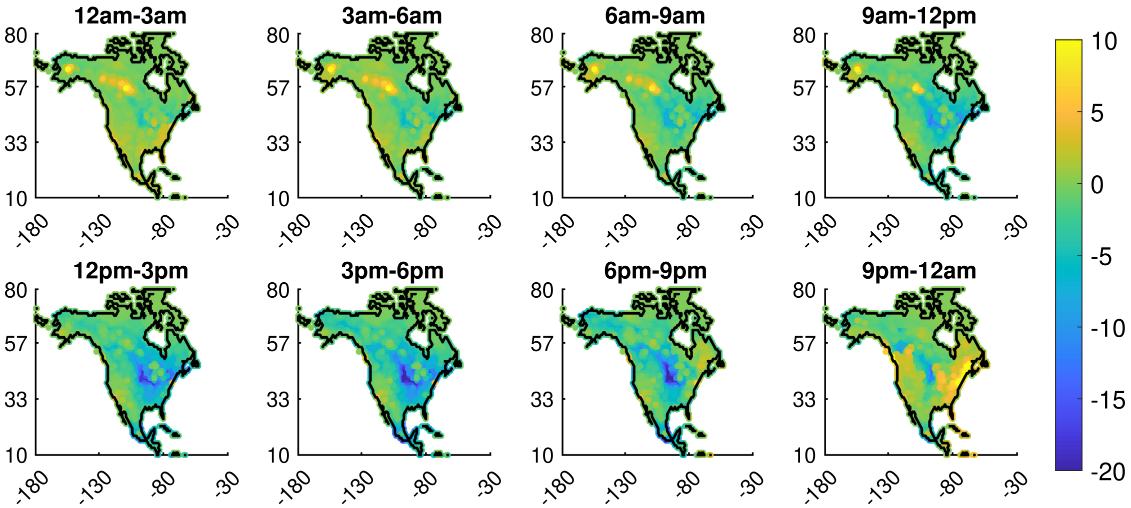

FIGURE 2. In atmospheric inverse modeling, the goal is to reconstruct spatio-temporal greenhouse gas emissions, $\mathbf{x}_{\text{true}}$, given satellite observations, $\mathbf{b}$, and atmospheric transport model, F. Shown above are three-hourly reconstructed gas fluxes from Orbiting Carbon Observatory 2 satellite observations. A video demonstrating the measurement acquisition is available.[b]

methods are needed to be able to incorporate nontraditional regularization terms. Moreover, many of the existing regularization methods can be implemented efficiently if regularization parameter(s) are known *a priori* but fall short of clear strategies for simultaneous parameter selection.

In a world with a growing abundance of data, we have great interest in both learning from data (e.g., extracting relevant information from data) and handling massive amounts of data. Machine learning techniques, in particular, supervised learning, have had transformative impacts on computer vision applications. Open problems remain, however, regarding how to combine data-driven and traditional knowledge-driven approaches for the solution of inverse problems. A key question is how to find the right balance in treating bias on the training data, statistical accuracy and robustness, stability, and interpretability.[3] Furthermore for extreme-scale scientific computing, randomized or sampling algorithms are transforming the way in which we handle massive or streaming data.

Many of these computational and statistical challenges are common to a broad range of scientific applications, and addressing these challenges requires a careful integration of advanced tools from numerical linear algebra, numerical optimization, statistical analysis, and high-performance computing. In the following sections, I highlight some of my key research contributions in the area of computational inversion and analysis.

[b]https://ocov2.jpl.nasa.gov/science/

Computational Methods for Inverse Problems

For many inverse problems, an important task is to solve an optimization problem of the form

$$\min_{\mathbf{x}\in\mathcal{C}} \mathcal{J}(\mathbf{b} - F(\mathbf{x})) + \lambda\mathcal{R}(\mathbf{x}) \qquad (2)$$

where $\mathcal{J}$ is a loss (or fit-to-data) function, $\mathcal{R}$ is a regularization operator, $\lambda > 0$ is a regularization parameter that controls the amount of regularization, thereby determining how faithful the modified problem is to the original problem, and $\mathcal{C}$ denotes the set of feasible solutions (e.g., those that satisfy some constraints).

Using tools from numerical linear algebra and numerical optimization, we have developed efficient and robust solution methods for solving inverse problems. For the case where $\mathcal{J}$ and $\mathcal{R}$ are expressed in the 2-norm, forward models are linear $F(\mathbf{x}) = \mathbf{A}\mathbf{x}$ where $\mathbf{A} \in \mathbb{R}^{m\times n}$, and $\mathcal{C} = \mathbb{R}^n$, we get the so-called standard-form Tikhonov problem

$$\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda\|\mathbf{x}\|^2. \qquad (3)$$

This problem arises in many scientific applications and has been widely studied in both the mathematics and statistics communities. Nevertheless, computing Tikhonov-

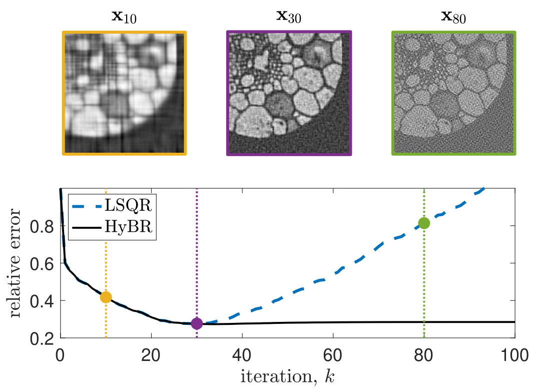

FIGURE 3. "Semiconvergence" of iterative methods for ill-posed problems is often revealed in the "U-shaped" plot of the relative errors, $\frac{\|\mathbf{x}_{\text{true}}-\mathbf{x}_k\|_2}{\|\mathbf{x}_{\text{true}}\|_2}$, where $\mathbf{x}_k$ is the solution at the kth iteration (here, the true image is known). Reconstructions correspond to dots on the LSQR plot. HyBR corresponds to a hybrid Tikhonov method.[4]

regularized solutions can still be challenging if the size of $\mathbf{x}$ is very large or if λ is not known *a priori*.

Hybrid projection methods combine iterative projection methods with variational regularization techniques in a synergistic way, providing researchers with a powerful computational framework for solving very large inverse problems. These methods are computationally efficient since the main costs per iteration are matrix–vector multiplications or forward operator evaluations. The significant benefits of hybrid projection methods include avoiding semiconvergence, whereby later reconstructions are no longer dominated by noise (see Figure 3 for an illustration) and adaptive selection of regularization parameters.

However, realizing these benefits in practice is nontrivial. As a DOE CSGF fellow, I developed a weighted generalized cross-validation method for hybrid methods[4] in collaboration with my Ph.D. advisor James Nagy (Emory University) and my postdoctoral mentor Dianne O'Leary (University of Maryland, College Park). During my CSGF practicum at the Lawrence Berkeley National Laboratory under the supervision of Chao Yang, we developed a high-performance implementation of hybrid methods and applied it to cryo-electron microscopy reconstruction.[5] These works formed the foundation for extending hybrid methods to solve a larger scope of problems and to impact more scientific applications. For example, Arvind Saibaba (North Carolina State University) and I developed generalized hybrid methods for problems where explicit computation of the square root and/or inverse of the prior covariance matrix are not possible,[6] and Silvia Gazzola (University of Bath) and I developed flexible hybrid methods for ℓ_p-regularized problems.[7] We have developed various extensions of hybrid projection methods for nonlinear inverse problems and streaming inverse problems, with new applications in mining engineering (e.g., for making mines safer using passive seismic tomography) and computational biology (e.g., for obtaining real-time endogenous and exogenous signals in living organisms using respirometry). I point the interested reader to a recent survey on hybrid projection methods.[8]

Computational Methods for UQ

Once computed, a solution to an inverse problem can help experts to make difficult decisions, but an informed decision will rely on knowledge of model assumptions, as well as an error analysis and quantifiable measures of confidence in the solution. We have enabled sophisticated UQ tools for realistic, large linear models by exploiting tools from numerical linear algebra, thereby paving the way for extensions to nonlinear models. For solving dynamic inverse problems, where the underlying parameters of interest change in time, such that the total number of unknowns is on the order of millions, we showed that incorporating prior information regarding temporal smoothness in algorithms can lead to better reconstructions.[9] Furthermore, we showed that low-rank approximations obtained using the generalized Golub–Kahan bidiagonalization can be used to estimate pixel- and voxel-wise solution variances and can be used to efficiently generate samples from the posterior distribution.

With Arvind Saibaba and Scot Miller (Johns Hopkins University) who is also a fellow DOE CSGF alum, we are further extending these tools and developing new computational tools for large-scale atmospheric inverse problems for the specific purpose of quickly and efficiently identifying superemitters for threat detection. These computational tools can take advantage of new observing capabilities, handle the large amount of data collected by satellites, and distinguish anomalous emissions at high spatiotemporal resolution.

Learning Approaches for Inverse Problems

Learning has been used in various contexts for solving inverse problems. In many real-life applications, training or calibration data are readily available and can be used to inform the selection of regularization parameters and to improve the prior. In my research, I have developed computational and statistical tools for designing optimal regularization. In collaboration with

Matthias Chung (Virginia Tech) and Dianne O'Leary, we proposed an optimal approach to select regularization parameters using methods from optimal experimental design.[10] By utilizing an (empirical) Bayes risk formulation, we introduced the selection of regularization parameters in an offline stage by minimizing the associated risk. The inversion can then be computed efficiently online in a fraction of the time it takes for standard methods and without requiring the user to tune parameters. Our work on using training data to design optimal filters quickly led to our consideration of the more challenging problem of designing an optimal regularized inverse matrix. We developed efficient rank-update approaches for computing optimal regularized inverse matrices, even for problems where the forward model is not known. Using these approaches, computed parameters are expected to be optimal *on average* or with respect to other design criteria. These approaches work well in many scenarios but may fail if the observation is very different than the training set.

OUR WORK ON USING TRAINING DATA TO DESIGN OPTIMAL FILTERS QUICKLY LED TO OUR CONSIDERATION OF THE MORE CHALLENGING PROBLEM OF DESIGNING AN OPTIMAL REGULARIZED INVERSE MATRIX.

To remedy this, another class of supervised learning methods that has gained increased attention in recent years is based on deep neural networks (DNNs) such as convolutional neural networks or residual neural networks. Initially, these machine learning techniques were used for postprocessing solutions, e.g., to improve solution quality or to perform tasks such as image classification. However, deep learning techniques have also been used for solving inverse problems. The prevalent approach, especially in image processing, is to take an end-to-end approach or to use deep learning methods to replace a specific task (e.g., image denoising or deblurring). For example, neural networks have been used to learn the entire mapping from the data space to the inverse solution, and DNNs have been used to learn the entire regularization functional. Note that these approaches do not include domain-specific knowledge, but rather replace the inversion of a physical system with a black-box forward propagating process also referred to as surrogate modeling. Hence, the limitations of these approaches appear in the sensitivity of the network (e.g., to large dimensional input–output maps as they appear in imaging applications). In newer work with Babak Maboudi Afkham (Technical University of Denmark) and Matthias Chung, we are developing approaches that combine DNNs and inverse problems so that we can exploit advantages of the learning process, while still maintaining the underlying physics of the problem.[11] We assume that there exists a nonlinear *target function* $\boldsymbol{\Phi} : \mathbb{R}^m \to \mathbb{R}^p$ that maps an input vector $\mathbf{b} \in \mathbb{R}^m$ to a vector of parameters defining the regularization strategy, $\boldsymbol{\lambda} \in \mathbb{R}^p$,

$$\boldsymbol{\lambda} = \boldsymbol{\Phi}(\mathbf{b}). \tag{4}$$

The function $\boldsymbol{\Phi}$ is a nonlinear mapping that takes any vector in $\mathbb{R}^m$ (e.g., the observations) to a set of parameters in $\boldsymbol{\lambda}$ (e.g., the regularization parameters). By approximating the *observation-to-regularization* mapping $\boldsymbol{\Phi}$ with a neural network and using training data to learn the parameters of the network, we learn a mapping from observation to regularization parameters that exhibits better generalizability since the computed regularization parameters are tailored to the specific data.

Era of Big Data

In the "Learning Approaches for Inverse Problems" section, we described various computational approaches for solving inverse problems that learn important information (e.g., hyperparameters) from data, but another question is how do we handle massive amounts of data or data that are being streamed. With data being generated at ever-increasing rates, sophisticated mathematical and statistical tools are needed to extract relevant information from these large datasets. The size of the forward model matrix may exceed the storage capabilities of computer memory, or the observational dataset may be enormous and not available all at once. Row-action methods that iterate over samples of rows can be used to approximate the solution while avoiding memory and data availability constraints. However, their overall convergence can be slow. We introduced a family of sampled iterative methods for computing Tikhonov-regularized solutions that uses an approximation of the global curvature of the underlying least-squares problem to speed up the initial convergence and to improve the accuracy of iterates.[12] We developed adaptive approaches to update the regularization parameter that are based on sampled residuals, provided a limited-memory variant for larger problems, and proved that the sampled Tikhonov method converges asymptotically to a Tikhonov-regularized solution.

Currently, we are extending these stochastic approximation methods for nonlinear problems, e.g., for the training of DNN architectures where the neural network can be separated into a nonlinear feature extractor followed by a linear model. This is a joint work with Matthias Chung, Elizabeth Newman (Emory University), and Lars Ruthotto (Emory University).

My Research Community

Many of these research advancements were achieved in collaboration with talented scientists from different fields and required the integration of tools from computational mathematics, statistics, and scientific computing. The DOE CSGF program was pivotal in helping me to establish a foundation for interdisciplinary research and collaboration. The academic breadth afforded by the CSGF program of study ensured that I would have knowledge in mathematics, computer science, and biomedical engineering, which has not only been critical for my research developments but also provided me the agility to jump into new research topics. Also, my CSGF practicum experience at the Lawrence Berkeley National Laboratory provided me with hands-on experience with parallel computing and forced me to think outside of my core discipline. Perhaps the most valuable lesson that I learned from the CSGF is the importance, and often great challenge, of *communicating across fields*. With patience and hard work (sprinkled with some lighthearted laughter), I have found that these interdisciplinary collaborations can make great impacts and can be very rewarding.

Although I am able to present only a subset of my research projects, I would like to take this opportunity to thank *all* of the research collaborators and students who have contributed to my research program. My research community includes many people: my collaborators in mathematics and statistics who work with me to develop new methodologies and theoretical developments, my collaborators in computer science who provide the computational know-how for efficient implementations, my collaborators in medicine and engineering, my students who bring great enthusiasm, dedication, and hard work to projects, and my friends and colleagues in the research community who provide support, conversation, and feedback.

EDUCATIONAL EXPERIENCES

Many of my research activities are closely integrated with my educational goals, which include course development, mentoring of students and early career researchers, and scientific outreach. Building a supportive and diverse community is core to all of these goals.

Teaching and Coursework

At Virginia Tech, I have taught a range of courses (from linear algebra and programming to numerical analysis and mathematical optimization) and at various levels (from first-year undergraduates to advanced graduate students). In all of my courses, I challenge myself to incorporate real-life examples from my research and to use active-learning, group-based projects. For example, I motivate methods for solving linear systems with examples from image deblurring, and I provide MATLAB projects on image compression for students to experience the utility of the SVD.

CMDA MAJORS OBTAIN A BROAD YET TECHNICAL EDUCATION IN QUANTITATIVE SCIENCE, WITH ELEMENTS FROM MATHEMATICS, STATISTICS, AND COMPUTER SCIENCE.

As part of an interdisciplinary team of faculty, I have also been active in the development of the Computational Modeling and Data Analytics (CMDA) undergraduate program at Virginia Tech. Similar to the interdisciplinary nature of the CSGF, CMDA majors obtain a broad yet technical education in quantitative science, with elements from mathematics, statistics, and computer science. Newly developed integrated courses emphasize techniques at the forefront of applied computation and provide quantitative and programming skills for tackling today's massive data-based problems. Students from this program have gone on to various careers from industry to elite graduate programs in computational science, some even with the support of the DOE CGSF.

Mentoring and Networking

Each academic year, like the waves of the sea, we observe the predictable ebb and flow of students—from the surge of incoming first-year students who are eager to begin their journey to the graduation of accomplished students who expectantly move forward to their next challenge. And as professors, we are honored to have the time and opportunity to interact with these students, to serve as their educators and mentors, and to help them find their way. Sometimes we make an impression on these students. Sometimes the students make an impression on us. But what is important throughout all of these interactions is the community that we build, that we nurture, and that we leave behind.

Mentorship is an investment of time and resources, but it is core to building a positive and nurturing community.

I have had the great pleasure to advise and interact with many undergraduate students, graduate students, and postdoctoral researchers. From advising student research projects to helping students prepare for their first conference presentation, it is inspiring to work with impressive, motivated, and determined students. When I think about all of the people who mentored and invested in me, helping others (especially students and early career researchers) is my way of paying it forward. The hope is that these students in turn inspire others, creating a cascade of broader impact.

AS PROFESSORS, WE ARE HONORED TO HAVE THE TIME AND OPPORTUNITY TO INTERACT WITH THESE STUDENTS, TO SERVE AS THEIR EDUCATORS AND MENTORS, AND TO HELP THEM FIND THEIR WAY.

The importance of networking and personal interactions in the scientific community cannot be emphasized enough, and community building often occurs at workshops and conferences. Beyond the CSGF program, there are various initiatives that encourage these mentoring relationships that can be pivotal in helping to create a diverse and inclusive scientific community. For example, the Sustainable Horizons Institute runs the Broader Engagement program at the Society for Industrial and Applied Mathematics (SIAM) Conference on Computational Science and Engineering, which is designed to make conferences more accessible for students from underrepresented and underprivileged backgrounds. These activities make students feel welcome and provide opportunities for connecting and sharing experiences. Although everyone's experience is different, there are common struggles, and connecting with others to share strategies can have a major effect.

In addition to the Broader Engagement program, I have been involved in programs such as the MIT Path of Professorship that supports graduate students and postdocs interested in academia. With support from NSF and NSA, I am part of a group of faculty from Clemson University and Virginia Tech who are organizing Mathematics - Opportunities in Research and Education (MORE) workshops for undergraduate students to learn about opportunities in research and education. Other programs such as the Association for Women in Mathematics (AWM) mentor network and the SIAM Workshop Celebrating Diversity provide opportunities for finding mentors and highlighting diversity.

Mentoring and networking have become more critical than ever, especially during the COVID-19 pandemic. With conferences and workshops being canceled or moved online, we had to rethink how we can support each other and how to build community virtually. As children and pets became part of our zoom meetings, the line between our work life and our personal life became very blurry or even indistinguishable. Nevertheless, some things became easier as we connected across time zones and cultures to commiserate over how we juggle becoming elementary school tutors, while engaging students in online learning, on top of our already packed agenda of research projects, students, and service.

Finding Your Community

Throughout undergraduate and graduate schools, I never had a female math professor, but I did not let that deter me—instead, I had strong advocates in the department who helped me to find strong female mentors and role models in the community. The AWM has played a big role in my professional development. In graduate school there was a small group of female graduate students, and together we established an AWM student chapter. I have also served as a faculty mentor to AWM student chapters. It has been wonderful to see the Virginia Tech AWM student chapter provide programs to encourage women and individuals from underrepresented backgrounds to pursue careers in mathematical sciences, to expose students to various research areas, and to provide students with mentorship and role models. These events provide community and leadership positions for female students but are open to anyone who supports women in mathematics.

I have also led and been involved in outreach activities through the Science Museum of Western Virginia, Career Days for middle-school girls, and multiple Sonia Kovalevsky Days for middle-school and high-school girls. The challenge (but fun!) in planning these activities is finding creative ways to share the essence of research projects using hands-on and age-appropriate activities. For example, in one activity I take a glass jar, put a toy object inside, and cover the jar with translucent paper to mimic skin (see Figure 4). Then, I give the students a flashlight and challenge them to determine the object. Students are not allowed to open the jar but can shine the flashlight into the jar at different angles. This is a fun activity that mimics the inverse problem that radiologists face when locating cancers inside the body.

Then, to emphasize the mathematical challenges and to drive home the need for computational algorithms for tomographic reconstruction, we do another activity

FIGURE 4. Goal is to determine the hidden object, using only a flashlight to illuminate the object from different angles.

where students use black and white plates to fill a 3×3 grid, given the row and column sums (see Figure 5). Students enjoy rearranging the plates to solve the "puzzle," especially for the more challenging 4×4 grid. We explore various concepts from linear algebra (e.g., existence and nonuniqueness of solutions). Many are in awe to realize that radiologists use mathematics to solve similar problems for 500×500 grids, or even larger.

It is hard to quantify the impact of these outreach activities, but if we can touch or inspire just one student, then I believe it is worth it.

> *"One student expressed disinterest in any topic even verging on math, but after your activity, she spent much of the rest of the week asking for more puzzles like the one you presented and seeking out other math activities."* – Mrs. Weiss, *Science Museum of Western Virginia.*

FIGURE 5. Activity to discover underlying mathematical challenges of tomographic reconstruction. Given row and column sums, students need to place the black and white plates that count for 0 and 1, respectively, to match the sums.

CONCLUSION

Some people know early on that a scientific research career is what they want—that was never me. Instead, it was a series of people and experiences that have helped me to discover what I love and have helped me along the way. Looking forward, I hope to encourage more students to get involved in computational science and to help them find their passions.

Sometimes it is our love and enthusiasm for our work that can be inspiring to students; but as a community, there is more that we can do.

- We can encourage love of mathematics at every educational stage—through outreach and in the courses we teach.
- We can value mentoring and networking activities, whether that is advising a research project for a driven, hard-working student or engaging in a one-on-one conversation with a mentee.
- We can make conferences and workshops more welcoming by participating in programs such as Broader Engagement or offering an encouraging word to a student who just gave their first conference talk.
- We can put a little extra effort to make our research talks accessible for a wider audience.

Of course, these suggestions are based on my experiences. Nonetheless, each of us can do our part toward building a welcoming scientific community, as this can have a significant impact on the recruitment and retention of a diverse next generation of computational scientists. The question that remains is: *What will you do?*

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