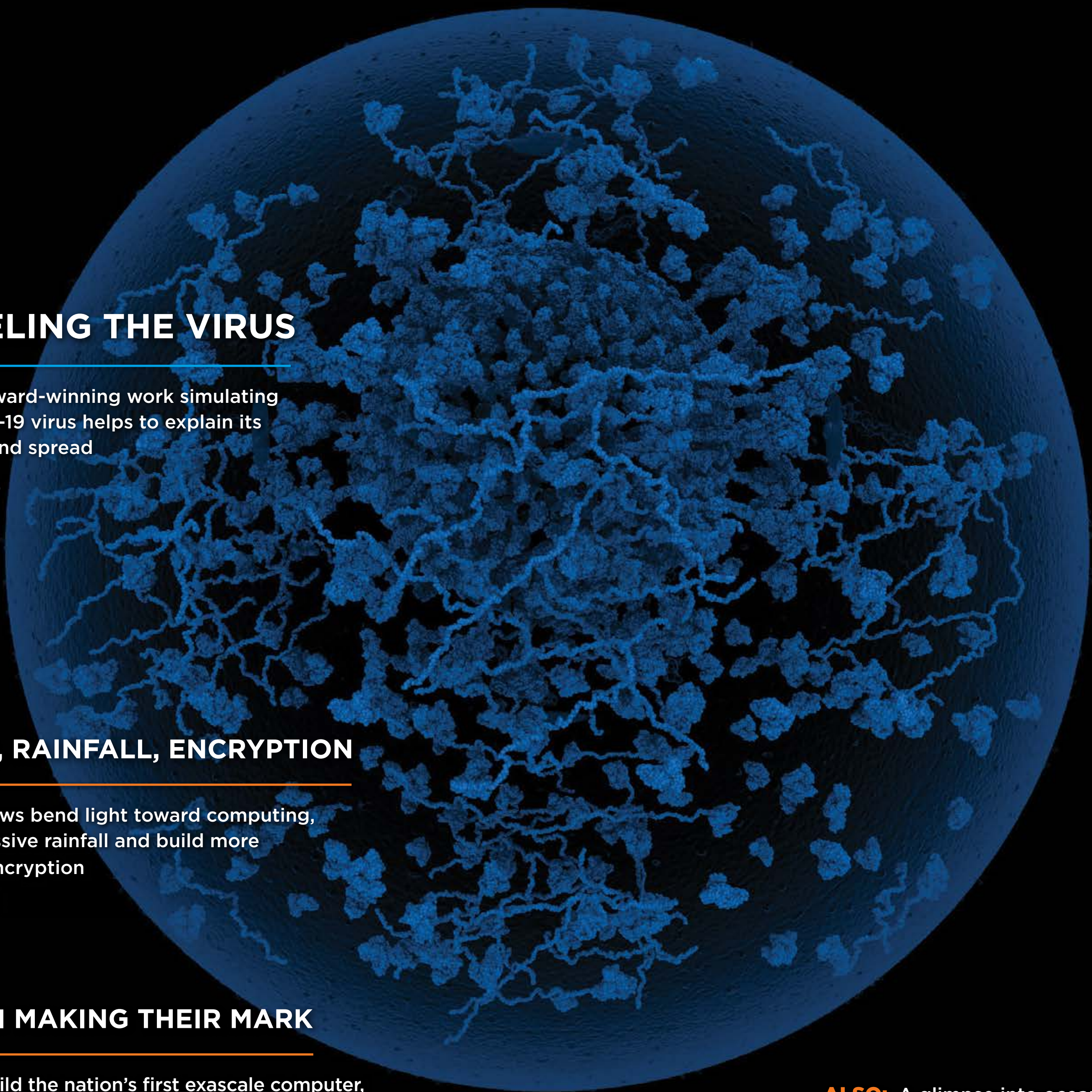
THE DOE CSGF ANNUAL

DEIXIS

2022

DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP



MODELING THE VIRUS

Fellow's award-winning work simulating the COVID-19 virus helps to explain its infection and spread

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LIGHTS, RAINFALL, ENCRYPTION

Other fellows bend light toward computing, model massive rainfall and build more efficient encryption

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ALUMNI MAKING THEIR MARK

Helping build the nation's first exascale computer, modeling and protecting watersheds and showing tissue fiber's build-up and break-down

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ALSO: A glimpse into ocean microbes, dual Howes winners and reflecting on computing's biggest challenges

LARGEST EVER: THE INCOMING DOE CSGF CLASS

In 2022-23, the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) will induct its largest class on record: a total of 33 new fellows studying at 19 different universities from the University of Alabama to Portland State University. Each will learn how to apply high-performance computing to problems of national importance, working in fields such as physical oceanography, neuroscience, polar climates and planetary science.

Daniel Abdulah
Massachusetts Institute of Technology
Planetary Science

Caleb Adams
University of Texas at Austin
Geological Sciences

Christopher Anderson
University of Washington
Ecology

Elizabeth Bennewitz
University of Maryland College Park
Physics

Lucy Brown
Stanford University
Fluid Mechanics

Jackson Burns
Massachusetts Institute of Technology
Computational Science and Engineering

Nina Cao
Massachusetts Institute of Technology
Mechanical Engineering

Ashlynn Crisp
Portland State University
Mathematical Sciences

Max Daniels
Massachusetts Institute of Technology
Mathematics

Zachary Espinosa
University of Washington
Polar Climates and Sea Ice

Jonathan Fajen
Stanford University
Computational Chemistry

Joshua Fernandes
University of California, Berkeley
Chemical Engineering

Nina Filippova
University of Texas at Austin
Computational Astrophysics

Thomas Gade Jr.
University of Minnesota
Plasma Physics

Mary Gerhardinger
University of Pennsylvania
Natural Science

Gil Goldshlager
University of California, Berkeley
Applied Mathematics

McKenzie Hagen
University of Washington
Psychology

Michael Ito
University of Michigan
Computer Science

Alexander Johnson
Harvard University
Gravitational Physics

Katherine Keegan
Emory University
Computational Mathematics

McKenzie Larson
University of Colorado Boulder
Synoptic Meteorology

Jerry Liu
Stanford University
Computational Math

Kerri Lu
Massachusetts Institute of Technology
Computer Science

Storm Mata
Massachusetts Institute of Technology
Wind Energy and Atmospheric Boundary Layer Physics

Tristan Maxson
University of Alabama
Computational Chemistry/Catalysis

Franz O'Meally
California Institute of Technology
Engineering

Miruna Oprescu
Cornell University
Computer Science

Mansi Sakarvadia
The University of Chicago
Computer Science

Carlyn Schmidgall
University of Washington
Physical Oceanography

Michael Tynes
University of Chicago
Computer Science

Grace Wei
University of California, Berkeley
Computational Materials Science

Emily Williams
Massachusetts Institute of Technology
Aeronautics and Astronautics

Joel Ye
Carnegie Mellon University
Computational Neuroscience

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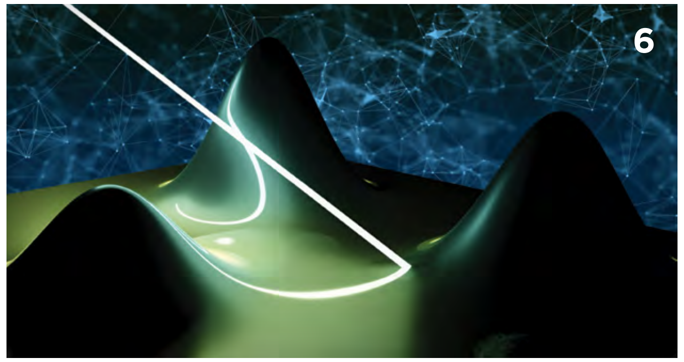

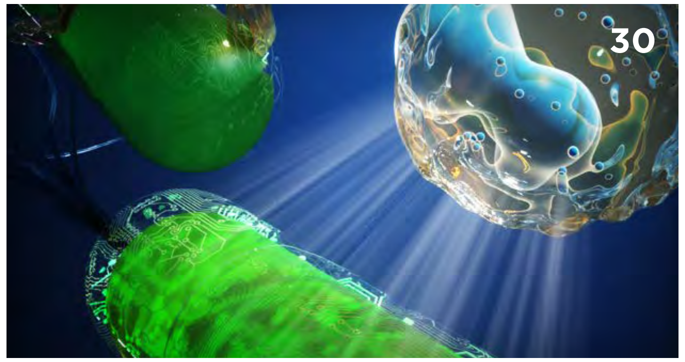

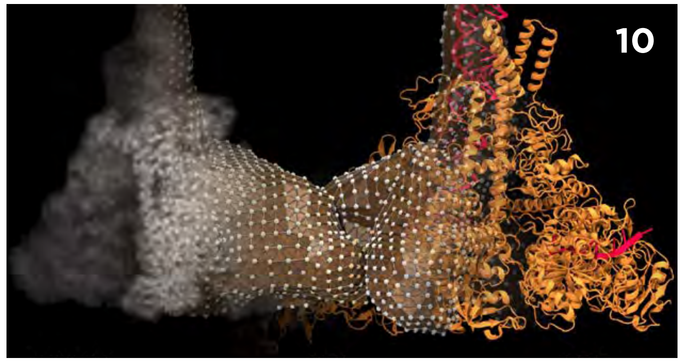

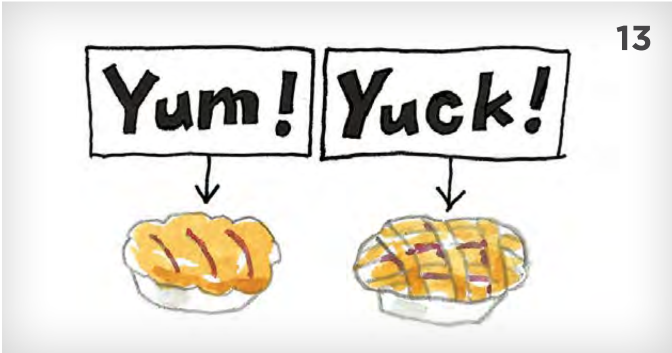

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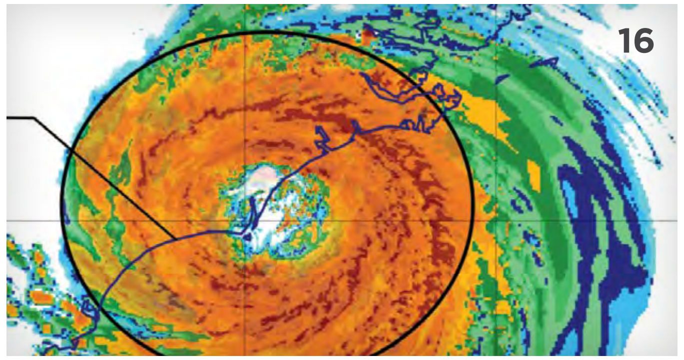

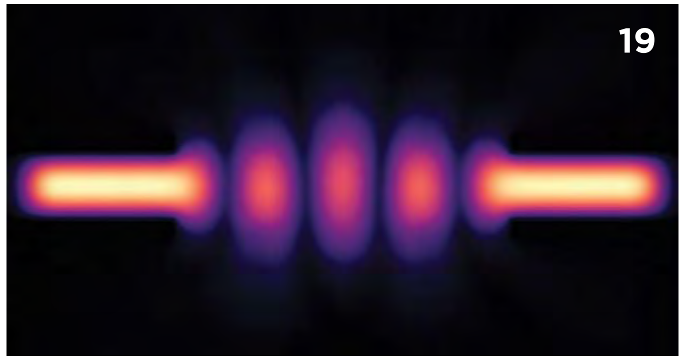

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For additional information about the DOE CSGF program, the Krell Institute or topics covered in this publication, please go to: www.krellinst.org/csgf

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DEIXIS (**ΔΕΙΞΙΣ** — *pronounced dāksis*) *transliterated from classical Greek into the Roman alphabet, means a display, mode or process of proof; the process of showing, proving or demonstrating. DEIXIS can also refer to the workings of an individual's keen intellect, or to the means by which such individuals, e.g. DOE CSGF fellows, are identified.*

DEIXIS, an annual publication of the Department of Energy Computational Science Graduate Fellowship program, highlights the work of fellows and alumni.

DOE CSGF funding is provided by the DOE Office of Advanced Scientific Computing Research (ASCR), within the Office of Science, and the Advanced Simulation and Computing (ASC) program within the National Nuclear Security Administration.

Manager, Science Media — Bill Cannon
Science Media Editor — Thomas R. O'Donnell
Associate Science Media Editor — Sarah Webb
Design — Stilt Studio, Inc.

ON THE COVER: The SARS-CoV-2 virus particle encapsulated in an aerosol droplet that includes proteins from deep-lung fluids. Fourth-year DOE CSGF recipient Anda Trifan was a member of the Gordon Bell Prize finalist team that carried out these simulations. *Credit: John Stone/UIUC and the Amaro Lab/University of California San Diego.*

LIVING SUPERCOMPUTER HISTORY

A longtime DOE CSGF advisor reflects on a life in high-performance computing and how the program has influenced the field.

David Brown retired in 2022 after 37 years with the national laboratories, since 2011 as director of what is now the Applied Mathematics and Computational Research Division in Lawrence Berkeley's Computing Sciences Area. Brown also helped found the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) and has advised the program ever since. This interview has been edited for clarity and length.


David Brown

DEIXIS: WHAT DREW YOU TO A CAREER IN MATHEMATICS AND COMPUTING?

Brown: When I was in high school in the early 1970s, I wasn't sure whether I wanted to become a scientist or a musician. I played viola in a couple of youth orchestras in Palo Alto, and many of my friends at the time ended up choosing music conservatory and careers in orchestras and chamber music. But I also had a passion for science and mathematics, and my high school physics class had access to the district's mainframe computer. I remember writing a simple program to simulate the orbit of a satellite under gravitational pull. This early experience hooked me for life to what later came to be called computational science. Later, as a Stanford undergraduate, I did a summer internship at CERN in Geneva, Switzerland, and ran computer jobs on an IBM mainframe for a physicist designing the beamline for the new accelerator. In a master's program in exploration seismology I learned digital signal processing and, discovering that the mathematics behind the science and engineering was what really interested me, decided to pursue an applied mathematics Ph.D. at Caltech. There, I had my first experience using a CDC (Control Data Corporation) supercomputer, and when I moved to Los Alamos National Laboratory for a postdoc, one of the big draws was access to the latest Cray machines.

YOU COULD HAVE WORKED IN ACADEMIA OR INDUSTRY. WHY THE NATIONAL LABORATORIES?

I thought the Los Alamos postdoc would lead to an academic career. But I soon realized that the labs were just a really exciting place to pursue science. And this was the early days of the lab's Center for Nonlinear Studies and lots of heavily computational research. When the opportunity came up to get a regular staff position, I jumped at it.

HIGH-PERFORMANCE COMPUTING HAS CHANGED A LOT DURING YOUR CAREER. WHAT ARE THE BIGGEST ADVANCES YOU'VE SEEN?

In the 1980s, the early supercomputers were just coming, and big federal labs were buying them – the National Center for Atmospheric Research for long-scale weather predictions, NASA for computational fluid mechanics to design aircraft, and more. On the early Crays, all the compute power was in a few processors. Making computers go faster was all about increasing the speed of individual processors.

The big innovation was massively parallel computers. Physicists studying quantum chromodynamics in the early 1980s realized that their algorithms could be parallelized and computation distributed across many processors to get much faster performance. It wasn't initially clear that this was the right choice for increasing computer performance. The parallel computers were built with lots of relatively slow processors ganged together.

But by the mid-1990s, what is now the ASC (Advanced Simulation and Computing) program started at the DOE Defense Program (now DOE National Nuclear Security Administration, or NNSA) labs and the Department of Energy (Office of Science labs) decided to invest in massively parallel machines. And that has defined the direction of scientific computing since. The exascale machines just coming into service now are the logical extension of those ideas. What is not clear is what the next generation of supercomputing at the national labs will look like. Using accelerators like GPUs is one trend, but supercomputing capability in the commercial world now rivals the labs, and we are seeing innovation in the computer architectures they are creating that may become an important element of how the labs do computing.

More recently, quantum computing has become really interesting. But that's something that is still very far from being practical for general scientific applications.

HOW HAVE THOSE DEVELOPMENTS SHAPED YOUR WORK?

At Los Alamos and after I moved to Lawrence Livermore National Laboratory in 1998, I led a project on programming these massively parallel machines to solve partial differential equations, the mainstay technology for simulation of complex physical processes. We also focused on solving problems in very complicated geometries to understand phenomena like flow over wings and aircraft. Tracking all these different processors changed the programming model for scientific computing, and we were looking for a way to make programming complex scientific applications as easy as it had been on the earlier supercomputers. By the early 2000s, I had moved to Livermore to help manage the recently formed Center for Applied Scientific Computing, and I got much more involved in science management.

WHAT ARE THE MOST EXCITING CHALLENGES IN COMPUTING?

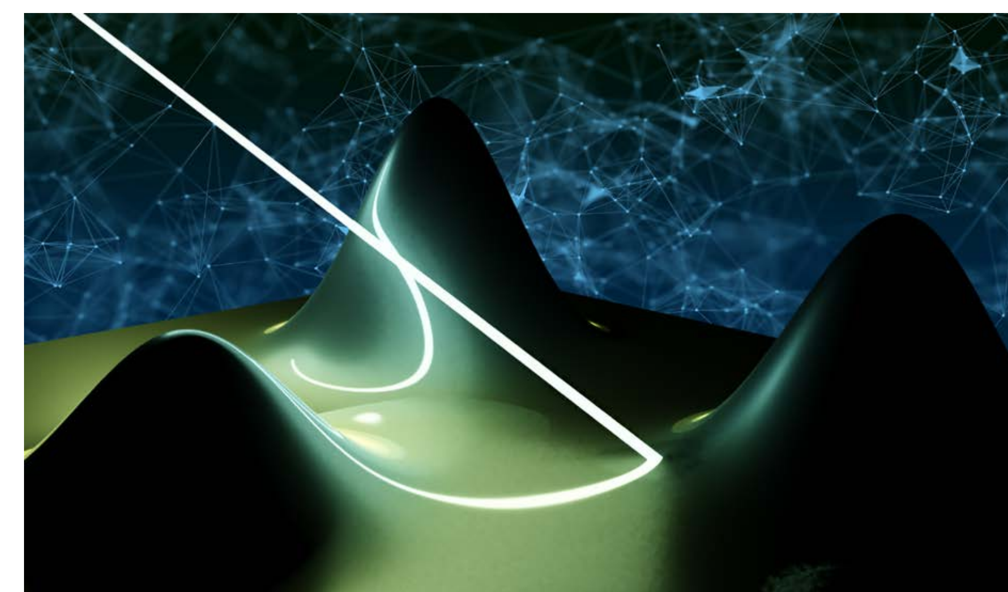
Because the NNSA labs can no longer test nuclear weapons, the simulation of complex physics has dominated supercomputing at those labs. When I came to Berkeley Lab, I discovered that the supercomputing drivers there were much more diverse. Most of the DOE Office of Science labs are focused on science at large facilities such as the Advanced Light Source, the Joint Genome Institute and the Molecular Foundry, which deal with increasingly large amounts of data from experiments. It has become clear that supercomputing and advanced networking have become essential to cope with that – and not only to analyze results. Some of the detectors on the machines produce so much data that it's not possible to move and store it all.

YOU'VE HELPED LEAD THE DOE CSGF SINCE ITS START MORE THAN THREE DECADES AGO. DESCRIBE ITS IMPACT.

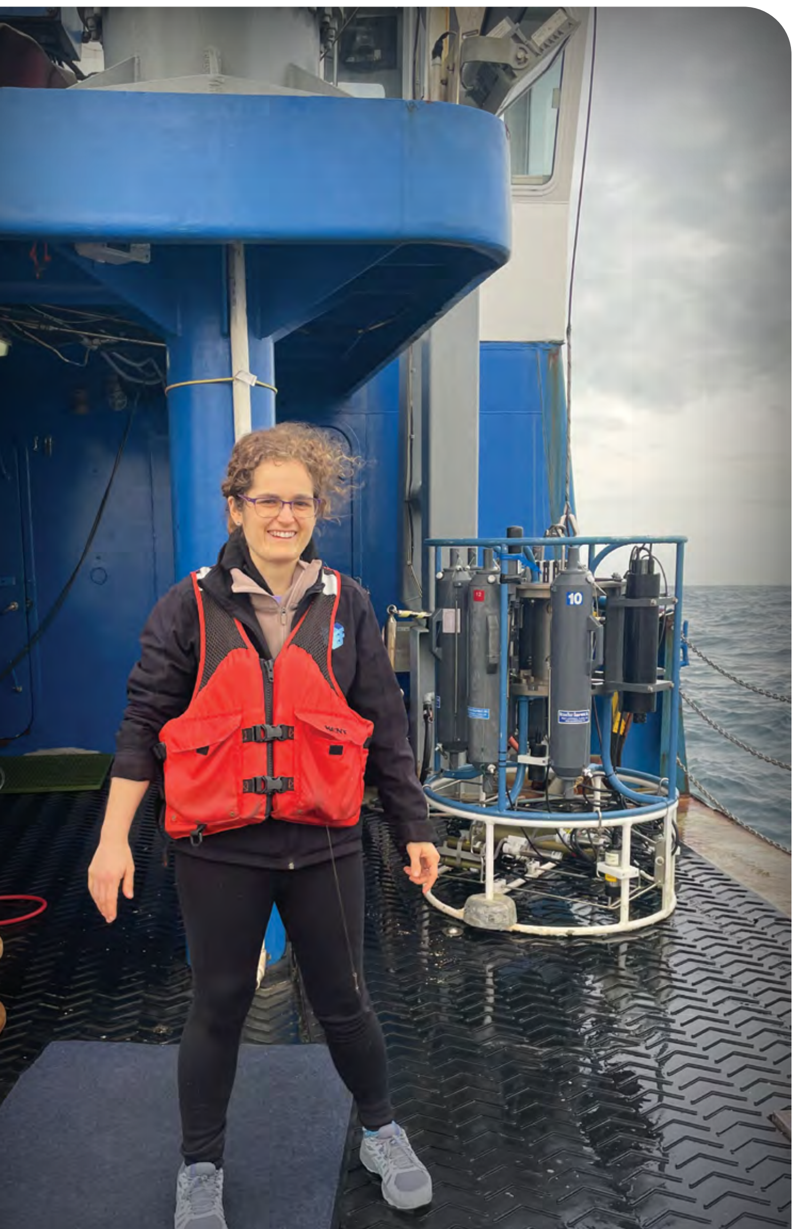
The program was created to attract some of the best and brightest young scientists into computational science. And in 1990 almost nobody knew what computational science was. We needed to train people, but it was an experiment to figure out how best to do that. Clearly, we've consistently attracted very good people into the program. I'm proud we've helped build a community of computational scientists who are, in turn, becoming leaders and sustaining the program. It's a big success.

WHAT'S NEXT FOR YOU?

I'll continue working with the fellowship and small projects at Berkeley Lab. I am hoping to wind down and enjoy retirement and do more traveling with my wife. And I will also be able to spend more time playing my viola in an orchestra and a string quartet.


An artist's concept of the algorithmic processes behind Berkeley Lab's Center for Advanced Mathematics for Energy Research Applications (CAMERA) gpCAM software. David Brown, who recently retired from the lab, helped secure DOE funding for CAMERA. *Credit: Marcus Noack/Berkeley Lab.*

SHELL SCRIPTING: CRACKING THE CODE OF OCEAN MICROBES



Arianna Krinos aboard the R/V Savannah as it cruises the North Atlantic in 2022 during research into algae, a collaboration with Natalie Cohen of the University of Georgia's Skidaway Institute of Oceanography. The crew was preparing to deploy the instrument at right, known as a CTD, for conductivity, temperature and depth. As the device traveled deep into the ocean, it tracked the water's salinity and warmth. The gray bottles trapped ocean water at specific depths for chemical and biological analysis. *Credit: Natalie Cohen.*

The DOE CSGF Communicate Your Science & Engineering Contest gives fellows and alumni the opportunity to write about computation and computational science for a broad, non-technical audience. The author of this year's winning essay studies biological oceanography in the Massachusetts Institute of Technology - Woods Hole Oceanographic Institution Joint Program in Oceanography/Applied Ocean Science and Engineering.

By Arianna Krinos

I grew up in Tampa, where many of my happiest memories were of days spent in and around the water. I was always fascinated by the idea of algal blooms and the deadly red tides of fish and seabird kills that they could cause.

I didn't know it at the time, but the culprits were thousands – even millions – of tiny cells. While they can wreak havoc locally, sometimes closing beaches as they hoard resources and consume oxygen during growth cycle sprints, these organisms are beautiful and important at a global scale. And, luckily for the computational scientist I've become, every drop of ocean water has upwards of a terabyte of data for me to explore, largely thanks to these tiny but mighty plant cells.

I study coccolithophores, algae that are common hundreds of miles from shore in the open ocean. These cells are clever enough to produce their own armor: chalky white pieces, made of the same material as seashells, that they assemble over their bodies. Like a hermit crab, coccolithophores scavenge materials from their environment to protect themselves. Unlike hermit crabs, they're invisible to the human eye, even though they grow so rapidly and in such enormous numbers that masses of them are visible from space. When growth takes off in a bloom, the cells tend to clone themselves more than once a day and the population quickly multiplies.

When the armored algae accumulate in high concentrations over a large swatch of ocean, their simultaneous actions come at a cost. The coordinated coccolithophore cadre pulls a huge amount of carbon from the water. An efficient bloom covering less than 2% of the global ocean's top layer can consume carbon dioxide equivalent to the amount the entire United States emits daily. At one moment, the ocean is a tasty buffet of carbon, nitrogen, and phosphorus – all the ingredients that make life possible. At the next, a busload of ravenous tourists has arrived and consumed much of what's available.

If the bloom comes on quickly enough, no predators in the water have the appetite to eat all the suddenly plentiful coccolithophore supply. Sometimes, many of the cells naturally die and quickly sink to the ocean bottom, like a buried shipwreck that takes much of the dissolved buffet down with it. At other times, a specialized virus takes down the hoard, expediting the downward shipment of goodies. It's an epidemic – but there is no time for a vaccine.

'Algae have been around for millions of years, and they have kept a diary.'

The problem turns out to be an enticing one for a computational scientist. The way algal cells adjust to their environment can be decoded from that terabyte of data in each droplet. In an ocean environment that quickly changes from bright lights to pitch black or from calm to stormy, all while you're a helpless cell forced to go with the flow, it's necessary to adapt quickly to survive. Algal cells have a big advantage in this: Evolution often takes many generations, which fly by for these rapidly dividing cells.

As it happens, this capacity to adapt produces the terabytes of data lurking beneath the ocean waves. The story of many generations of experimentation and adjustment is written in the algae's genetic code. What's more, we can collect the readout of this hereditary playbook via sequencing – identifying and compiling bases, the letters in a cell's DNA. In the lab and field, we can observe acclimation, or slight adjustments that don't involve a permanent DNA change, as well as evolution, more permanent rewrites to the playbook.

By extracting and sequencing the genetic code, we can translate it to huge data troves that we can process on a computer. The task involves taking small data snippets and using algorithms to predict where they came from and their larger context in the cell's genetic playbook.

My work involves writing and adapting computer programs and building databases that can identify and interpret long strings of the bases that make up the genetic code and can gracefully plow through gigabytes and gigabytes of information. For example, I've developed software tools that leverage a custom archive of sequence data from an algal crop we grow in the lab. With this approach, we can use our lab observations to identify microscopic algae in the environment.

Which types of algae are present and what they're doing matters when we try to predict climate change's consequences. It's important to know what survival tools different groups of algae have in their arsenal to respond to rapidly changing ocean conditions. The places we expect to find certain groups of algae today are not written in stone. If a type that is more adept at using nutrients becomes dominant in an ocean basin, more carbon dioxide gas in the air could be taken from the atmosphere down to a final resting place at the ocean's bottom, since algae use carbon dioxide gas to build each new cell.

Algae have been around for millions of years, and they have kept a diary of all the ways they have coped with an ocean that constantly morphs around them. Although they're stunned when things change fast, they can sometimes recuperate and return in full force. By reading their lengthy genetic sequence diaries and using computational tools to process the data, we can begin to understand what coccolithophores already know about adaptability. In doing so, we might also predict what their next move is going to be – and learn to adapt ourselves.

DECODING DISEASE

Fellow Anda Trifan has doggedly applied computational models to COVID-19 and cancer.

By Thomas R. O'Donnell

Anda Trifan, a multilingual Romanian émigré, planned on an international business career and chose DePaul University for its strength in the subject.

But "about a week before school started, I called my counselor and changed all my courses to science courses," thinking she might want to attend medical school, she says. "I just felt like I wouldn't be happy doing business."

The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient completed her degree in chemistry – a subject she hated as a middle schooler in the Chicago suburbs – and fell in love with research, turning her away from medicine. Fortunately, she's still seeking cures while studying theoretical and computational biophysics at the University of Illinois at Urbana-Champaign (UIUC). She's happy she switched majors.

Trifan and her advisor, Emad Tajkhorshid, use computation to penetrate cellular machinery. Experiments are indispensable, but they can only produce static high-resolution images of molecules, which are constantly moving, rotating around their bonds to produce different shapes known as conformations. "For example, if you wanted to see the dynamics of how a drug binds to a protein, you're unable to really do that" via experiments, Trifan says. "The methodology of what we do, for me, is extremely powerful."

Trifan focuses on Ras, a protein that helps regulate how cells divide, grow and eventually die. Mutated forms can lead to persistently multiplying cells, causing cancers in the pancreas, colon, lungs and other organs. Her DOE CSGF practicum, meanwhile, drew Trifan into battle against another health scourge: COVID-19. Her three-month Argonne National Laboratory stay was extended to an internship, producing essential insights and award-winning research.

Tajkhorshid, the J. Woodland Hastings Endowed Chair in Biochemistry, directs the National Institutes of Health Biomedical Technology Resource for Macromolecular Modeling and Bioinformatics. The center develops and uses two main programs: the nanoscale molecular dynamics (NAMD) code, and VMD, or visual molecular dynamics, which generates images from the simulations.

Understanding Ras mutations "is a very important but a very challenging problem," Tajkhorshid says. The protein is part of a signaling cascade in cells and functions at the surface of their plasma membranes. Ras works through multiple pathways, so blocking just one may not disable it. Atom-level "studies like molecular dynamics are perfect for studying Ras because you're able to see how mutations affect behavior" at the membrane's surface, Trifan says.

The Ras subunit governing cell proliferation tethers to the membrane via a flexible linker. Mutations in the protein can keep cells' growth and division signals turned on, spurring cells to become cancerous. Trifan simulated the full Ras protein on Anton 2 at the Pittsburgh Supercomputing Center and showed that this linker helps Ras orient itself on the membrane, optimizing interactions with partner proteins in the signaling pathway. Understanding Ras's functional components could help find cancer treatments.

A mutual interest in Ras prompted Trifan to join Arvind Ramanathan's Argonne group for her practicum in January 2020. The team was developing machine learning (ML) techniques to more efficiently sift data from simulations of protein-membrane interactions. Trifan modified the group's method to distribute time- and memory-consuming model training over multiple graphics processing units (GPUs), which speed calculations in high-performance computing systems.

The practicum was nearly over when dire pandemic forecasts forced business and school closures. Ramanathan's group turned to studying the SARS-CoV-2 virus via simulation, joining with researchers across DOE in a multifaceted consortium. Trifan stayed on, collaborating virtually while pursuing her doctoral research and giving birth to a daughter.

"It was absolutely crazy," with constant meetings and late nights, Trifan says. "I loved it. It was one of the most exciting times of my career, and I appreciate the opportunity."

Trifan's biophysics knowledge complemented the Argonne group's artificial intelligence expertise, but her tenacity also was an asset, Ramanathan says. "Once you give her a problem, she won't rest until it's done."

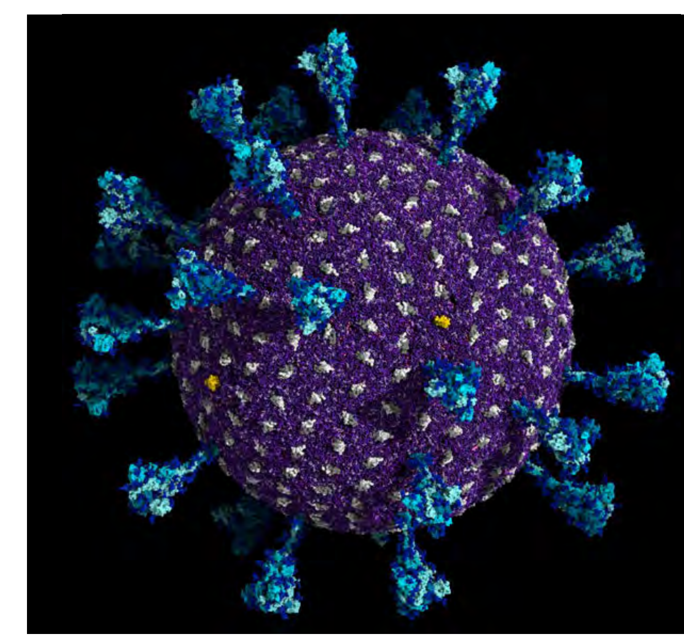
Trifan contributed to many COVID-19 research advances. The biggest success was a collaboration with Rommie Amaro's University of California San Diego (UCSD) biochemistry lab and others to probe the virus's spike protein complex, the main infection mechanism.

The UCSD team ran a 305-million-atom virus model on Oak Ridge National Laboratory's Summit, among the world's most powerful machines. The Argonne group's AI workflow identified rare spike protein conformation changes in the results, accelerating the model by 10 times. Trifan took "a leading role on the biophysics side, trying to explain how the spike binds to the cell surface," Ramanathan says. The project won a COVID-19-focused version of the 2020 Association for Computing Machinery Gordon Bell Prize for outstanding achievement.

Trifan is even prouder of two 2021 Bell Prize finalist papers the collaboration produced. She was first author on one, a simulation of the virus's replication-transcription complex (RTC), which copies genetic instructions enabling viral reproduction. Even cutting-edge experimental techniques such as cryogenic electron microscopy (cryo-EM), which averages multiple two-dimensional pictures, fail to capture RTC structural details or evolution. Researchers also discard terabytes of cryo-EM data. All-atom MD simulations, meanwhile, are precise but often too demanding to track the entire RTC.

The team "tried to do something that hasn't really been done before," Trifan says: augment the discarded experimental data with multiscale simulations that connect all-atom models' detail with less-demanding, larger-scale simulations that track RTC interactions over comparatively longer time spans.

The Argonne team ran an all-atom RTC model, with Trifan coordinating efforts and filling data gaps. The simulations provided input to the larger-scale mesh-based method designed by collaborators at University College London. That method created nodes that blanketed the simulated RTC structure, calculating processes at each to represent the entire complex.



A molecular representation of the delta SARS-CoV-2 all-atom model. Spike proteins are colored in cyan; viral membrane proteins and viral envelope proteins are depicted in gray and yellow, respectively. The viral membrane is in purple. *Credit: Lorenzo Casalino and Abigail Dommer, Amaro Lab at the University of California San Diego.*

Credit: Fred Zwicky/University of Illinois.

QUANTUM PURSUIT

Physicist **Jacob Bringewatt's** doctoral work at the University of Maryland, College Park, focuses on quantum algorithms and quantum sensor networks, in which entanglement and other properties of quantum systems can precisely measure, among other physical properties, electric and magnetic fields. During his 2019 practicum at the Thomas Jefferson National Accelerator Facility, Bringewatt worked with Nobuo Sato on a nuclear theory project designed to understand protons' internal structure, for the first time using high-performance computing to simultaneously fit data from experiments and from recent lattice quantum chromodynamics simulations.

CATCHING THE WAVES

Sarah Greer grew up following her father's geophysics career from Louisiana to Egypt, Norway and Texas and finally into his field, including Ph.D. studies at the Massachusetts Institute of Technology. She researches seismic images created when surface-based sensors record sound waves rebounding from underground rock and soil layers. The pictures are hazy but can help identify oil and gas deposits or useful subterranean structures. Greer researches methods that account for aspects of the rebounding waves so they more closely depict the features that produced them. That includes exploring full waveform inversion, which seeks the optimal solution while avoiding false answers.

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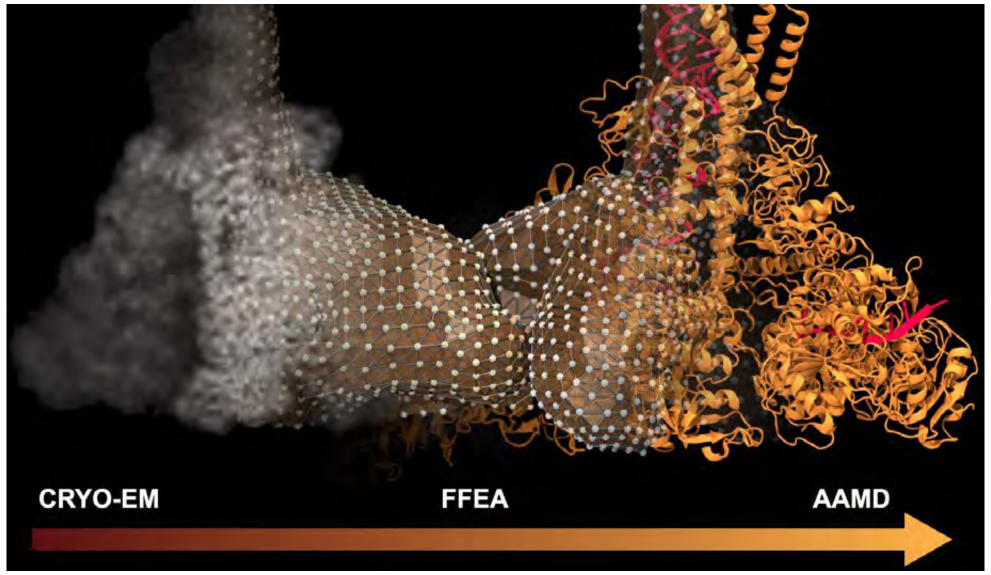


To study how the SARS-CoV-2 replication-transcription complex helps the virus reproduce rapidly within cells, a team that included Anda Trifan and Argonne National Laboratory researchers used AI techniques to bridge static experimental images acquired from cryo-electron microscopy and simulations using all-atom molecular dynamics. Their methods used a fluctuating finite element analysis mesh annotated with the strengths of protein-protein interactions. *Credit: Anda Trifan, University of Illinois at Urbana-Champaign/Argonne National Laboratory; Defne Gorgun, University of Illinois at Urbana-Champaign; and Arvind Ramanathan, Argonne National Laboratory.*

For instance, the MD simulation computed protein-interaction values, which were then plugged into the larger-scale model. "You have completely different behavior" when the mesh-based model "is informed with actual data from all-atom simulations," Trifan says.

The team used AI codes to identify unusual protein conformations and optimized NAMD to run on GPUs. It used Balsam, a workflow manager, to coordinate learning between ThetaGPU at the Argonne Leadership Computing Facility and Perlmutter at DOE's National Energy Research Scientific Computing Center.

"The goal is to give scientists a more complete picture of the protein's behavior, not just one static image," Trifan says. With structures the hybrid code predicts, "we can go back to the 2-D cryo-EM images and put more detail into them."

The project portrayed, perhaps for the first time, an RNA strand unwinding within the RTC – a key step in proofreading transcriptions of the virus's genetic code for replication. "That's important when you want to start treating with drug compounds," Trifan says. "You have to know how the protein behaves in certain conditions."

Ramanathan's group collaborated again with UCSD for the second 2021 Bell Prize finalist paper: portraying a virus-laden aerosol, a breath-emitted droplet millionths of a meter in diameter that can float through rooms and go deep into lungs. The simulations tracked interactions between an unprecedented billion atoms and showed how substances in aerosols help SARS-CoV-2 survive.

The Argonne group steered the macroscopic simulations, using an AI code to find rare protein conformations in weighted ensemble simulations, which increased the odds of identifying such outliers. The simulations found the Delta variant's spike protein opens its shape up dramatically, Trifan says, perhaps explaining its contagious nature.

Trifan is unsure of her post-graduation plans, but Ramanathan is certain she's bound for an exceptional career. After all, she's "one of the few people who can say 'I was involved in three Gordon Bell submissions, all three made it as finalists, and one of them won.'"

SECRETS BEST KEPT

From homeschool direct to a Ph.D. program, this fellow is optimizing cryptographic techniques that let computers work together to solve problems while keeping data safe.

By Jacob Berkowitz

First-year graduate student Lance Roy repeatedly lingered to talk after his fall 2017 Theory of Computation classes at Oregon State University (OSU) in Corvallis. Roy bubbled with follow-up questions that intrigued the lecturer, computer science professor Mike Rosulek. The animated conversations on the walk back to Rosulek's office developed into a personal rapport and a shared research passion.

"I really liked discussing ideas with him," says Roy, a 23-year-old Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient in computer science at OSU. "That was a major factor in my deciding to focus on computational cryptography."

Four years later, with Rosulek as his Ph.D. advisor, Roy has gone from posing questions to a leading researcher to becoming one himself, inventing more efficient techniques for secure multiparty computation (MPC) – the ability for computers to work together without sharing private data.

Roy was a homeschooling high school student in Corvallis in 2015 when he joined a computer visualization research group via the Apprenticeships in Science and Engineering program. Two years later he became the first high school graduate in OSU's 150-year history to be admitted directly to a doctoral program. That's when Roy's longstanding love of logic – and of finding original solutions to vexing mathematical challenges – intersected with cryptography.

"Often in more applied areas of computer science," Roy says, "people don't really care about proving that their methods work. But in cryptography, it's an interesting area where it's both applied and also very theoretical. You need a lot of theory to prove that an attacker cannot break your system."

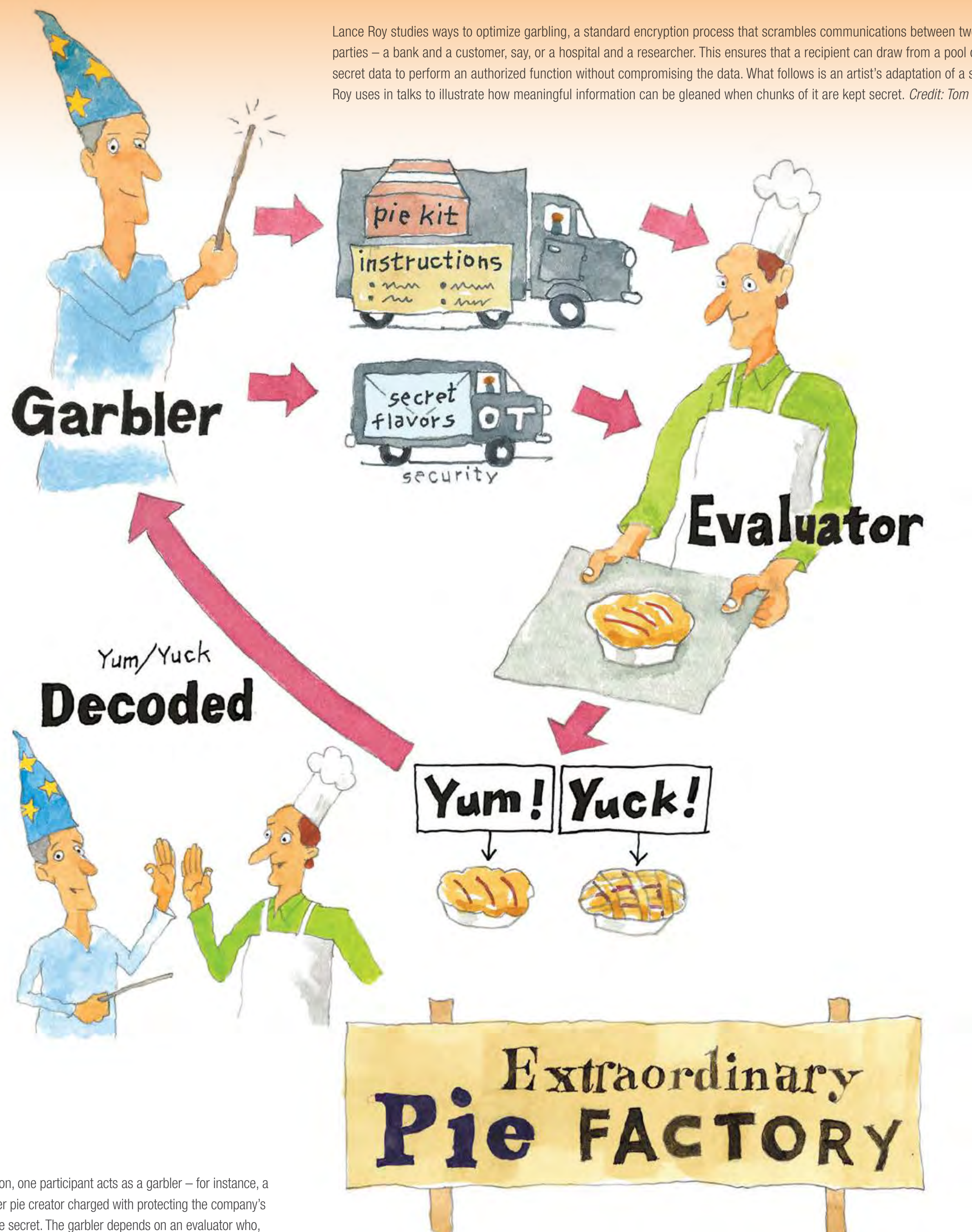
When it comes to digital cryptography, most people think of the tiny lock icon that appears beside the URL in a browser, indicating a secure website. This RSA-type (named after its three inventors) cryptography is a computer-age variant of the ancient Caesar cipher: Data is shared in an encrypted message, and a key is used to decrypt it.

However, in MPC, on which Roy and Rosulek focus, computers solve a common problem that requires data from all machines involved while the information remains private.

Credit: Johanna Carson/Oregon State University.

PERFECTING A SECRET RECIPE

Lance Roy studies ways to optimize garbling, a standard encryption process that scrambles communications between two parties – a bank and a customer, say, or a hospital and a researcher. This ensures that a recipient can draw from a pool of secret data to perform an authorized function without compromising the data. What follows is an artist's adaptation of a slide Roy uses in talks to illustrate how meaningful information can be gleaned when chunks of it are kept secret. *Credit: Tom Dunne.*



In two-party computation, one participant acts as a garbler – for instance, a baking company master pie creator charged with protecting the company's flavors, a valuable trade secret. The garbler depends on an evaluator who, like a line pastry chef on the other side of the plant, must bake a pie with only the information necessary to complete the task.

To pull this off, the pie master sends less sensitive information across the factory lot via truck and top-secret information through OT, which stands for oblivious transfer – a black-box exchange where the evaluator/baker learns the garbled information for the correct inputs, selecting from the secret ingredients and using everything else to produce an output: pie. The evaluator tastes the pie and gets a simple result – "yum or yuck," say – and reports only that result to the garbler. In a complex computation with many inputs, "yum and yuck" is an intermediate step, a starting point for further computation-pie.

"The big picture is that sometimes there are privacy concerns about the data being used in these computations, or just general lack of trust, and nobody's willing to put all the data in one place," explains Rosulek, author of the textbook *The Joy of Cryptography*. Examples include health-care data, proprietary economic data and, increasingly, machine-learning applications whose accuracy benefits from larger datasets.

Thus MPC involves designing protocols, or algorithms, that enable this computational sleight-of-hand. Roy notes that MPC can be viewed as a form of high-performance computing (HPC) in which rules are designed for many interacting processors. With MPC, though, the participants also are distributed over long distances.

"This makes optimizing the communication usage more important than in usual HPC. So a major theme of my research is improving the efficiency of these protocols. I'm trying to make them as fast as possible."

Roy has already succeeded in devising a surprising, major improvement in the speed of a garbled circuit, a key MPC protocol. The circuit is a computation consisting of gates to combine bits through operations such as *and, or, not*. Each gate's operation is garbled, or encrypted, so it's unknown to the participants. Thus, all participants receive the computational output but not other participants' inputs or any intermediate values.

In 2020, the most efficient garbled circuit construction was one Rosulek had published five years earlier. After reflection – and having handed the problem to successive graduate students – he'd come to believe that his formulation was theoretically optimized and couldn't be improved.

Roy got wind of this sense of the impossible. He considered the garbled circuit problem and said to himself, "Oh, that sounds interesting." After a year of persistent trial-and-error, a process he likens to debugging a computer program, Roy thought he'd made a better garbled circuit. He shared the idea with his advisor.

"I said we can definitely talk about it," recounts Rosulek, who tweets as @GarbledCircus. "And then I'll explain to you why you're wrong because I've thought about this for much longer than you."

Instead, Roy's discovery, co-published with Rosulek, received honorable mention for best paper when he presented it at the 42nd annual International Cryptology conference held virtually in August 2021. The new garbled circuit technique uses a process dubbed "slicing and dicing," in which "if the way the garbled circuits is built is randomized, as in rolling some dice, the circuit is made secure," Roy explains. The technique is 25% more efficient than the one described in Rosulek's 2015 paper, meaning significant energy and time savings for secure MPC projects using it.

Meanwhile, Roy also has spent two years honing his cryptographer's mind by helping author the OSU Security Club's international cybersecurity Capture the Flag competition, a digital version of the summer camp game.

Inspired by the garbled circuit research, Roy turned to improving the efficiency of the IKNP (named after its inventors) oblivious transfer (OT) extension protocol, a building block of MPC techniques, including garbled circuits. Communicating OT information between computers is usually the bottleneck in MPC efficiency, Roy says. Besides his OT research, he contributed to improving the usability of Regent, an HPC parallel programming language, during his summer 2019 practicum at the SLAC National Accelerator Laboratory.

In a paper posted online as a preprint, Roy proposes a new SoftSpokenOT technique that he believes could quadruple OT communication speed. "We'll see if the reviewers like it as much as I do." Roy's advisor Rosulek is already impressed: "This is another breakthrough that I didn't think was possible."

The research also is Roy's first solo-authored paper. Says Rosulek: "I encouraged him to make it a single author to make sure he can exercise his independence, seeing a project all the way through, from the ideas, to the writeup, to the publication. Because that's one of the fundamental skills that an academic researcher needs – the ability to write and explain what they're doing."

Motivating Roy's solo writing pace: his previous experience in the vagaries of competitive research. Recalling a co-written theory paper on a way to improve the computational cost for a technique called homomorphic sharing, he says "our main result was scooped in the time between submission and review, but it turned out that the technique was still a few times more efficient than the scoop."

When he graduates this year, Roy hopes to pursue an academic research career in computational cryptography. If so, there's a good chance he'll continue his ardent conversations, perhaps in conference hallways, with his former advisor. "Lance's ideas have a simplicity and elegance and are something people can actually implement," Rosulek says. "It's been a total pleasure getting to work with him."

STORM CHASER

An interest in severe weather and improving warnings fueled a fellow's journey from television photojournalist to hurricane modeler.

Credit: Andrea Starr/PNNL.

By Sarah Webb

For nearly a decade, Ryder Fox captured footage of floods, tornadoes and blizzards for local television stations from Texas to Minnesota. "That developed my passion for being in the field and for access to information and warnings," Fox says. "Rural areas are often those that are most impacted and have the least services or even access to warnings or support."

Today the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient models hurricanes and other storms at extreme resolution – a task that leads to many challenges. In a key project, studying 2018's Hurricane Florence, it took nearly a year to get the model to follow the storm's track, a direct hit on the Carolina coastline and a slow churn inland. Fox jokes, "I just kept sending hurricanes up the eastern coast or down the eastern coast, wherever they wanted to go!"

The goal is to understand rainfall accumulation enough to help weather researchers predict storms and their impacts. An unusually large and lengthy hurricane such as Florence, which dumped more than 30 inches of rain over three days, offers troves of data, but Fox also is interested in common systems such as large weather fronts and severe thunderstorms.

Fox, who uses they/them/theirs pronouns, has made a dramatic shift to science over the past decade. They grew up in an ultra-religious community without a traditional K-12 education system. Fox left as a teenager and worked in fast food restaurants and volunteered for television work until they landed a paid position.

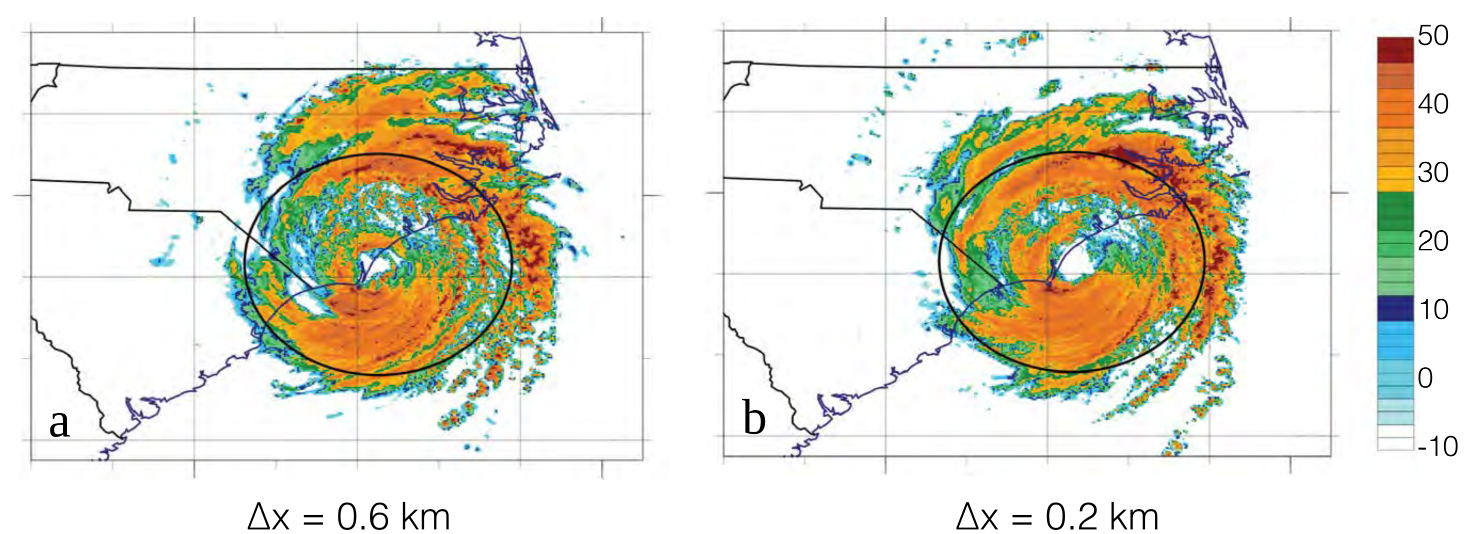
In 2007, Fox left that career and started a corrective exercise business. Much of that work involved helping clients with physical limitations find ways to expand and optimize their capabilities. Curious by nature, Fox completed numerous training certifications and wondered whether it was time to test personal boundaries by pursuing a college degree.

"I went to community college and was just taking basic science, basic math classes," Fox recalls. "Can I do this? Yeah, I can. It's very different in a community college setting where there are adult learners than in a more traditional educational environment."

Earth science courses brought Fox back to meteorology. They pursued an undergraduate degree in atmospheric physics at the New Mexico Institute of Mining and Technology and focused on getting practical experience through research. Then Fox learned about a diversity-related internship, the Significant Opportunities in Atmospheric Research and Science (SOARS) program, through the University Corporation for Atmospheric Research in Boulder, Colorado. They spent two summers there working on high-resolution hurricane models. The program supplied mentors who helped with research, writing, coding and even life check-ins.

"From the beginning, they treat you 100% like you are a scientist," Fox says, in contrast with most other academic environments, and alumni have a bonded, familial connection. "I guide people into that program when I know that they aren't having the best experiences in academia but do belong in STEM and need opportunities." Fox later completed an internship with NASA at the Marshall Space Flight Center, where they used machine-learning methods to assess tropical cyclone models.

That led to DOE CSGF-supported Ph.D. research in meteorology and physical oceanography at the University of Miami. A typical weather model resolves systems in 20-kilometer chunks. In the initial study of Hurricane Florence, Fox used the Weather Research and Forecasting model to zoom in to a 200-meter resolution near the eye. Brian McNoldy, a senior research associate at the school, helped Fox with the model and its many features. Fox learned quickly and was both independent and resourceful, McNoldy says, particularly when adjusting for cloud microphysics – the inner workings of rain, ice, snow and more.



Hurricane Florence's simulated radar reflectivity during landfall near Wilmington, N.C., on Sept. 14, 2018, at two different resolutions (0.6 kilometers, left, and 0.2 km, right). Fox used the Weather Research and Forecasting model's WDM6 microphysics scheme to calculate the storm's precipitation and focused on the 150 km surrounding the storm's center (black circle). *Credit: Ryder Fox.*

Continued from page 12

GOOD REACTIONS

In high school, **Olivia Hull** took calculus because she wanted to challenge her disdain for math. That led to mathematics, biology and chemistry majors in college and to physical chemistry doctoral studies at Kansas State University. There she has modeled plasmonic nanoparticles, clumps of atoms whose electrons oscillate in unison when a specific frequency of light shines on them. The nanoparticles can assist with difficult chemical reactions without using high heat or other extreme inputs. Her computational work explores how the particles cleave these strong molecular bonds. She's also applied lessons from her 2019 National Renewable Energy Laboratory practicum to develop approximations and other tools that can speed computation with minimal accuracy loss.

OPEN-SOURCE SUPERNOVAE

University of Hawaii astronomy doctoral candidate **Michael Tucker** concentrates on fleeting celestial events called transients, which include supernovae – exploding stars – and flares. Transients provide a glimpse into astrophysical processes governing black holes, the creation of heavy elements and more. But scientists must observe the objects quickly before they disappear. To find transients, astronomers painstakingly compare new images to those from previous nights. It's a big-data problem that demands high-performance computing. Tucker has updated data-analysis tools, converting them from demanding languages such as FORTRAN to open-source code. The algorithms cross-correlate observed spectra with an archive of template spectra for known objects, identifying the handful of significant transients out of thousands found each night.

COMPILING ACCOMPLISHMENTS

William Moses' milieu is compilers, software that converts code into executable computer instructions and can boost programs' efficiency, perhaps by changing them from a serial approach to a parallel processing scheme. At MIT, he's helped optimize the compiler technology LLVM to run faster on multicore processors. With Enzyme, an LLVM plug-in, Moses and his collaborators tackled an issue related to machine learning (ML) and automatic differentiation (AD), in which code robotically calculates derivatives. Developers often must rewrite their AD code into ML-specific languages. Enzyme can automatically differentiate code from a range of languages so developers can optimize programs before executing AD, boosting speed by as much as four times.

Continued on page 21

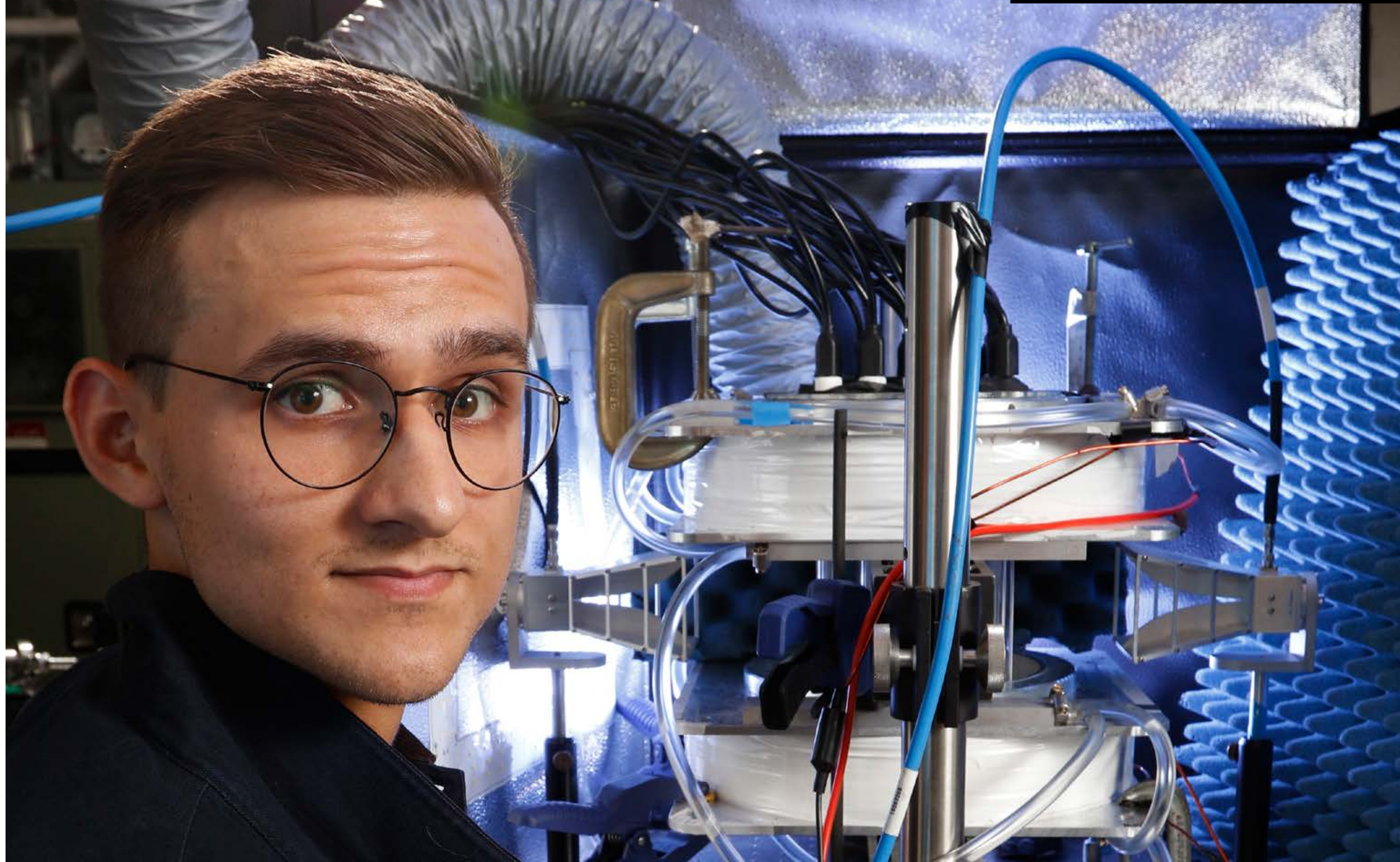
In summer 2021, Fox extended that work through a Pacific Northwest National Laboratory (PNNL) practicum with Adam Varble, where they worked on shorter-lived storm systems. Varble studies how clouds form and interact with the atmosphere around them and had led Cloud, Aerosol and Complex Terrain Interactions (CACTI), a 2018 DOE-supported project. The CACTI team measured cloud dynamics, microphysics and aerosols in north-central Argentina, a key agricultural region that produces dramatic and long-lived storms. The goal was to gather large amounts of data and improve cloud-based microphysics models. Fox and Varble identified two high-rainfall events of interest, and Fox has been modeling those storms at varying scales to understand cloud processes such as ice growth and melt and their impact on rainfall.

Because of the DOE CSGF, "Ryder knows a lot more about computing, (system) architecture, distributing memory and competing load and all these things," Varble says. "And Ryder's been good at basically wrapping their head around a big project and breaking it into individual, achievable chunks that get constructed together along the way."

Although the official practicum has ended, Fox will continue to work with Varble's team and expects to remain at PNNL through their Ph.D. defense in spring 2023. The access to DOE scientists and computing resources – including a yearly allocation on the Cori supercomputer at Lawrence Berkeley National Laboratory's National Energy Research Scientific Computing Center – have been vital to Fox's Ph.D. research. "The biggest reason for choosing the CSGF was that it had these practicums and deeper connections to the labs," Fox says. And they hope to continue at a national lab after graduation.

Besides research work and maintaining some corrective exercise clients, Fox actively supports scientists from marginalized backgrounds and has served in leadership roles with Out in Science, Technology, Engineering and Medicine (oSTEM), a professional organization for LGBTQ+ people working in the STEM community. "There's a diversity push that's really about checking boxes," Fox says, an emphasis that sidesteps "asking what actually makes somebody want to stay working where they are." Not only do people need to see a more diverse workforce, but they also need to see inclusive values in their workplaces, they say.

More recently, Fox's service work pivoted to leading and volunteering with THRIVE Lifeline, a 24-hour crisis line that grew out of oSTEM's activities and expanded dramatically during the COVID-19 pandemic. The team, with volunteers worldwide, has served more than 3,000 people in 30 countries since June 2018. "Thirty percent of the people that reach out to us tell us they have nobody else to talk to who understands," Fox says. "That's an easy thing to fix. We are another person you can talk to. At the base human level, we're trying to help people thrive."



FUSING OPTICS AND COMPUTING

A passion for math, computing and plasma physics converges to build optical computing devices and fusion models.

By Sarah Webb

Jesse Rodriguez isn't big on relaxing. He thrives on challenges – plasma physics, machine learning, snowboarding, rock climbing and complex cuisine, from Asian American to his family's Mexican recipes. He has a favorite quote, from climber Alex Honnold in the documentary *Free Solo:* "Nothing good happens in the world by being happy and cozy."

Rodriguez, a Stanford University mechanical engineering Ph.D. student, manipulates electromagnetic waves using plasma, a hot, charged, gaslike state of matter. He and others hope to exploit the plasma principle to make processors that compute via light rather than electricity. Advisor Mark Cappelli calls Rodriguez, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient, "a triple threat," equally at home with complex instruments, theoretical equations and computational analyses.

Credit: Paul Sakuma.

Rodriguez grew up in Salem, Oregon, with interests in dinosaurs, local flora and the stars. A high school physics teacher, Michael Lampert, recognized Rodriguez's talent for translating mathematics to real-world phenomena and encouraged him to stick with physics. Lampert also had financing from the Intel Science and Engineering Fair, which, Rodriguez recalls, "gave me that first taste of how fun it can be to try to find out something new." For an Intel fair cosmic rays project, he built particle-detecting cloud chambers that he attached to a weather balloon to collect stratospheric data.

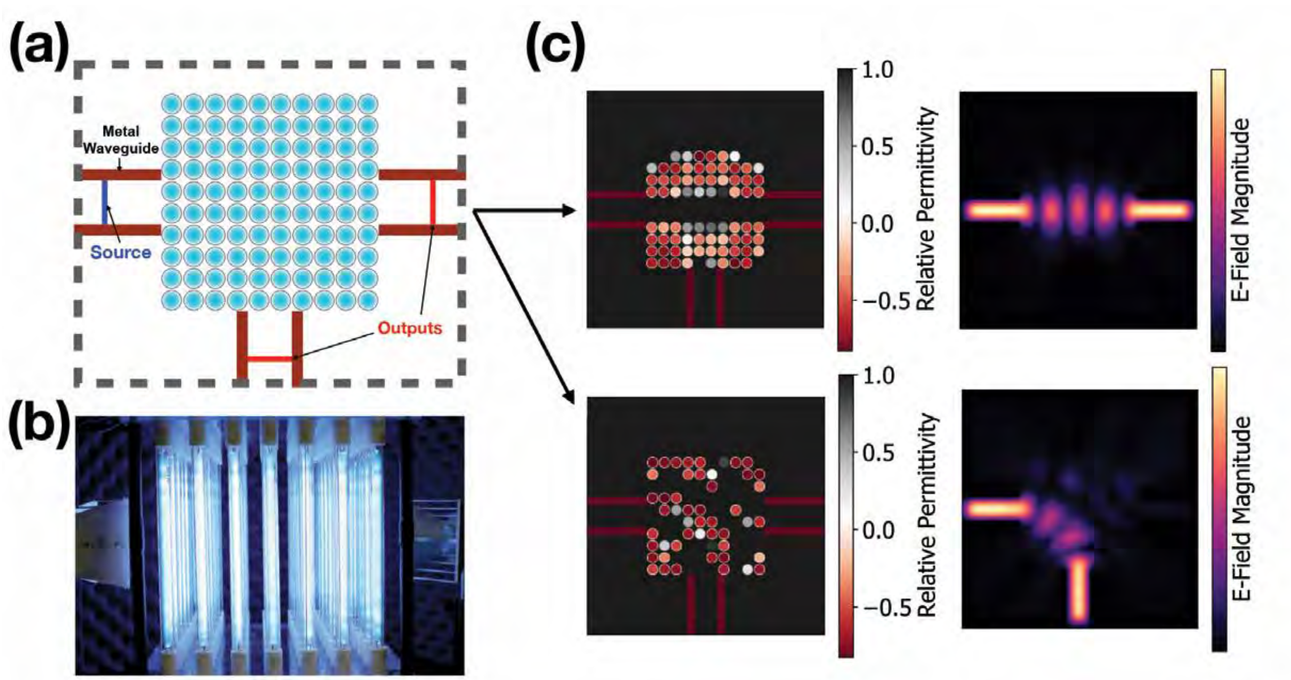
His undergraduate studies began at the University of California San Diego with structural engineering, as Rodriguez aimed to join his father's construction business. But a growing interest in fusion energy soon drew him back to the Northwest, to Oregon State University and nuclear engineering. He added majors in physics and mathematics.

After a vector calculus course as a freshman, his professor, Juan Restrepo, invited Rodriguez to work on research that explored how beach sand dries when you step on it. Rodriguez presented that work at a 2015 engineering conference hosted by the Society for the Advancement of Chicanos and Native Americans in Science. There he met graduate students from Cappelli's plasma physics group who encouraged him to pursue summer research internships through the NSF Research Experience for Undergraduates program. The following summer Rodriguez went to the University of Chicago to study diffuse interstellar bands, then, in 2017 and just before his senior year, to Cappelli's Stanford lab to probe plasma jets' velocity.

Despite his wide-ranging science and math interests, Rodriguez had done little computational work. When he applied for the DOE CSGF, he recognized high-performance computing could be useful for tackling complex plasma physics problems. He was surprised to be selected, he says, and is happy he was. "I've learned way more about computer science, particularly machine learning and software development, than I ever would have otherwise."

That broad training has let him peer into the plasma physics-computation interface in an emerging field called optical computing. Rodriguez has examined how a device made from many plasma elements can alter light's propagation through its interior. Because the electrons within a plasma move freely, highly dense plasma can behave like a conducting metal, reflecting light like shiny copper. Light can pass through low-density plasma, but the plasma stretches it to a longer wavelength. Magnetized plasma produces other exotic effects.

By developing optical devices composed of tunable plasma elements, Rodriguez hopes to design systems and algorithms that can accomplish various tasks, such as identifying handwritten digits. Traditional neural networks, algorithms that process inputs based on training data rather than programming, often require layers of time-consuming calculations. When carried out via electrical signals on today's computer chips, that process can lead to significant energy loss as heat. An all-optical neural network could be faster and more efficient.



A top-down diagram of a 10-by-10 array of plasma rods (panel a) and an experimental version with a 7-by-7 array pictured in panel b. By altering these plasma parameters, source waves can be directed to move in a straight line (top images, c) or to bend 90 degrees (lower images, c). Manipulating light in new ways could lead to optical computing devices. *Credit: Jesse Rodriguez.*

Optical neural networks would operate at light-speed without resistance, immediately directing a light signal to a detector that recognizes a specific digit. Other researchers are already working on light-based systems that can perform calculations using static, non-tunable materials, Rodriguez says. "I imagine a future where we have very application-specific components like this in computing systems."

During his 2021 Princeton Plasma Physics Laboratory practicum with William Tang, Rodriguez returned to his longstanding nuclear fusion interest, using machine learning approaches to predict plasma turbulence that can produce potentially catastrophic disruptions in tokamaks, devices that use strong magnetic fields to contain fusion reactions. "It's still a totally open problem," Rodriguez says. "We don't understand the physics. And it's just very difficult to write software that that operates on time scales fast enough to mitigate these disruptions."

Tang's team, working remotely during the pandemic, includes DOE CSGF alumni Julian Kates-Harbeck and Kyle Felker and current fellow Ian DesJardin. They've used experimental electron-cyclotron emission imaging from the DIII-D fusion research facility in San Diego to train machine-learning algorithms and fine-tune physics predictions. Rodriguez has worked on extending the methods from one-dimensional data to two. From his Stanford base, he continues to log in on weekends, setting up new training data for a machine-learning model, and he checks back later to analyze the software's performance. He's carried out much of this work on Traverse, a PPPL HPC cluster with a combination of central processing units and graphics processing units that resembles the Summit supercomputer at Oak Ridge National Laboratory.

Rodriguez expects to complete his Ph.D. in 2023 and to pursue postdoctoral research that uses machine learning to understand complex physical phenomena. "Now I'm much more confident that I can make contributions in a team that is, at its basis, a deep-learning team."

Rodriguez doesn't rule out a career in industry, but he's aiming for an academic position. Thinking back to his early influences made him realize he'd like to mentor others. "It really was just having somebody who knew a lot more than me saying, 'Hey, man, you're good at this. You should keep going down that road.' And because of that, I'm here."

Continued from page 18

BACK FROM THE PAST

Samuel Olivier reached into the past for improved solutions to the radiation transport equation, which calculates heat release and absorption as atoms split in nuclear reactors or merge in fusion experiments. Techniques to accelerate these calculations call for precise discretization, which casts a mesh of points through the modeled region and calculates the physics at each. At the University of California, Berkeley, Olivier helped revive the variable Eddington factor, a 1960s-vintage algorithm that separates meshes for radiation transport and for equations that accelerate the computations.

GENETIC CODE

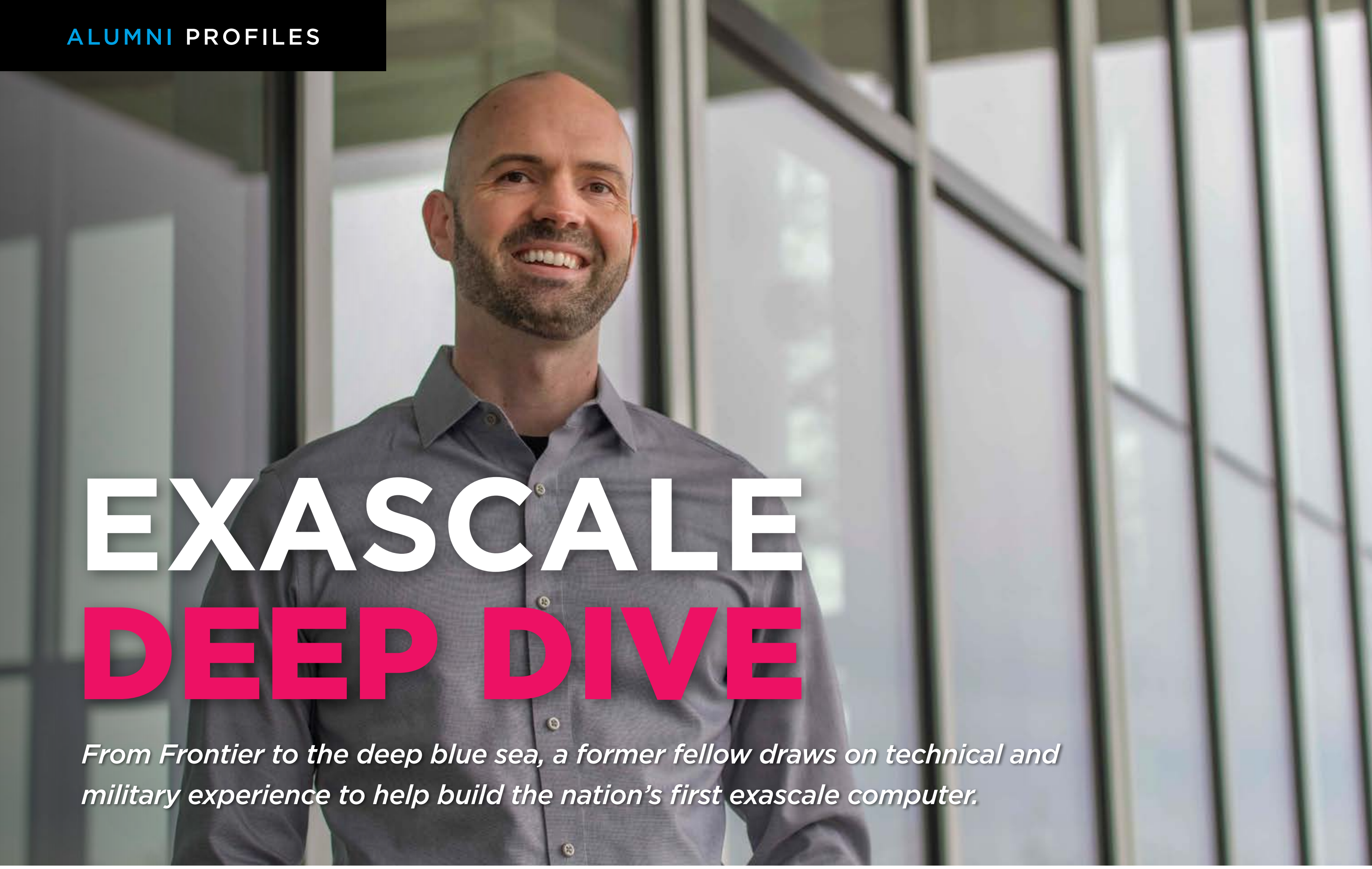
Melissa Queen's research aims to shrink computing far beyond transistors by encoding equations and calculations in molecular arrangements. She uses computer science to analyze data from her University of Washington wet lab colleagues, tackling such problems as measuring and comparing energy consumption of traditional processors versus molecular systems. Many molecular computation systems use DNA, which stores and encodes biological instructions. But interactions between DNA strands tend to release rather than store energy, so Queen must account for factors such as the energy required to synthesize the molecules.

LIGHT DUTY

Grace Johnson could have followed her mother, grandmother and aunt into medicine but found math and physics more engrossing. Now the Stanford University Ph.D. candidate uses demanding quantum mechanical methods to grasp atom-level processes, such as how plants' light-harvesting proteins convert photons into chemical energy during photosynthesis. She and her colleagues use graphics processing units to accelerate the most expensive part of these calculations. Johnson also has focused on electron repulsion integrals, computations of interactions between paired electrons that help drive these reactions. Her lab team is scaling these operations so that fully quantum-mechanical simulations can run on the largest supercomputers.

Longer profiles are available:

krellinst.org/csgf/fellows/fellow-reflections



EXASCALE DEEP DIVE

From Frontier to the deep blue sea, a former fellow draws on technical and military experience to help build the nation's first exascale computer.

By Steve Koppes

Noah Reddell's path from the U.S. Naval Academy to Hewlett Packard Enterprise (HPE) and beyond included a voyage under the North Pole in a fast-attack nuclear submarine.

His doctoral dissertation at the University of Washington was similarly exotic: simulations of plasma physics for fusion energy – the nuclear reactions that power the sun – which ran continuously for more than a month on hundreds of computer nodes.

Reddell, who completed his doctorate in 2016 and recently left HPE to join the fusion startup Zap Energy as principal computational scientist, needed supercomputer power to solve the most complete models of plasma physics – the physics of electrically charged gas. At Zap, he works on kinetic plasma models.

"You can come up with all kinds of different models," says Reddell, a 2009-2013 Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient. "Some are narrowly focused or narrowly applicable. Or you can come up with more complex models for plasma that work in wider scenarios or might be more accurate. But those tend to take more computational power to calculate."

As HPE's manager of the Frontier Center of Excellence, Reddell led a team that helped develop the Frontier supercomputer at the Oak Ridge Leadership Computing Facility. It is the nation's first exascale machine, able to perform more than 1.5 quintillion calculations per second.

"The talent of the people that I get to work with is unmatched. The teams that the DOE has selected for us to work with are top-notch. They're very seasoned in the computational science community."

Reddell, a commander in the U.S. Navy Reserve, brings a blend of military and civilian leadership and technical skills to his work.

He earned a bachelor's degree in electrical engineering from the academy in 2002, then served as a submarine officer for six years. U.S. nuclear submarines are powered by fission, a process much less powerful than fusion, which engineers strive to attain. "I learned a lot of foundational knowledge as a Navy submarine officer that made me interested in fusion energy when I was thinking about what next."

Reddell received a master's degree in electrical engineering from Stanford University during his Navy service. His DOE CSGF fellowship trained him to develop software and run it on supercomputers and to master the underlying mathematics and numerical methods behind simulations.

What's more, he says, the program let him "interact with fellows from all kinds of different fields. You work with a wide variety of very talented people."

At HPE, Reddell worked with teams developing software for simulations that lead to otherwise impossible scientific advances, from fields that included plasma physics and cosmology, meteorology and materials science.

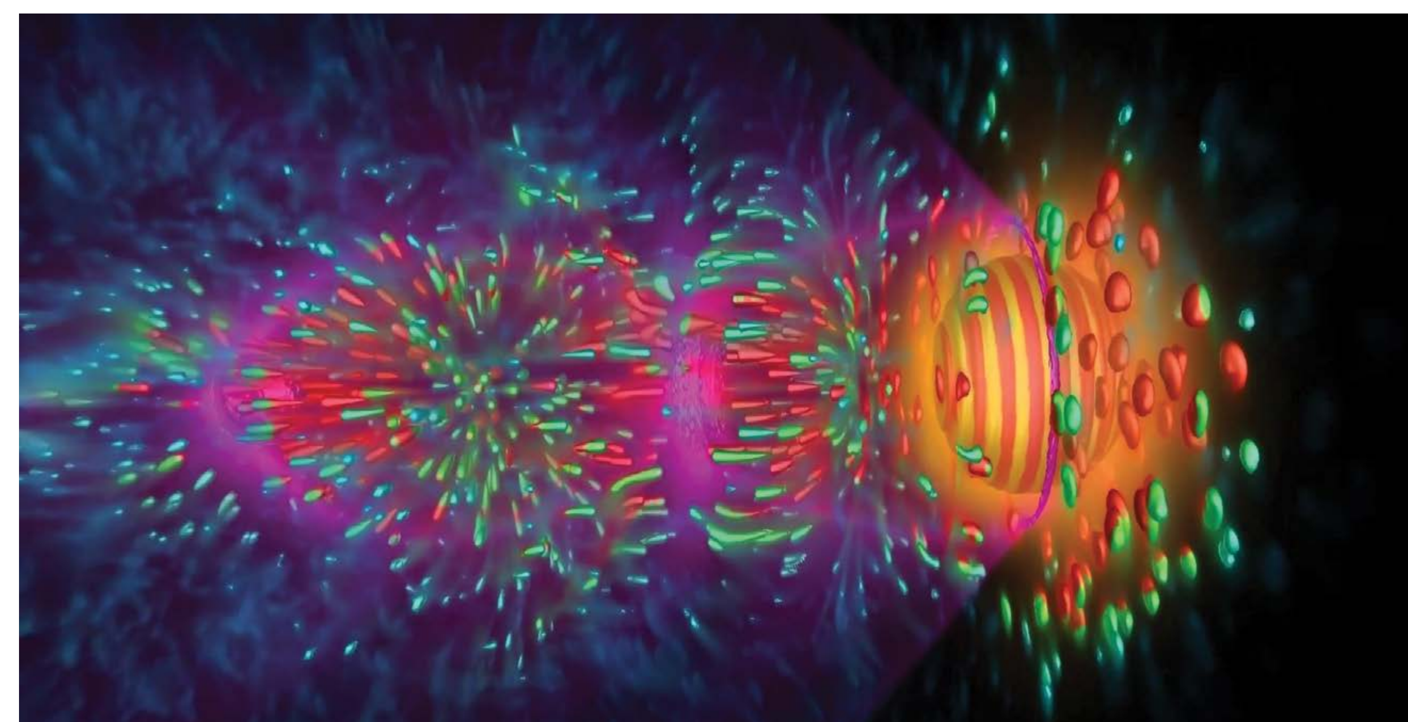
Reddell's team excelled at "knowing how to make the math of their models work well on the supercomputer." His colleagues also tested compilers, which translate source code into a language that Frontier can understand. "Compilers may look like they're working, but in the end you find out that they're calculating the wrong answer or creating code that calculates the wrong answer."

One benefit of the Frontier work: early access to graphics processing units and other components that are still under development. "But that comes with a challenge in that often they don't work as you want or think that they should."

'The talent of the people that I get to work with is unmatched.'

Reddell's team spent the past four years helping to develop Frontier and a second exascale system, Lawrence Livermore National Laboratory's El Capitan. In late 2021, the team entered a final, critical stage of testing the Livermore system, whose architecture is the same as Frontier's but a fraction as large.

"The anticipation is very high," he says. "The machines will be record-breakers in their compute performance. They truly will have the capacity to do science simulations for humanity that hasn't existed before."



Noah Reddell has helped build software to support future science on the Oak Ridge Leadership Computing Facility (OLCF) Frontier supercomputer. An example: a snapshot from a simulation of high-intensity laser pulses (orange-striped sphere) driving a plasma wave in ionized helium gas. Purple areas denote the electron density. Streams depict stronger (red) and weaker (green and blue) electric fields. This was generated in a test on OLCF's Summit using ISAAC, a tool for visualizing simulations in real time. *Credit: Felix Meyer/Helmholtz-Zentrum Dresden-Rossendorf. Previous page: Malcolm Smith.*

DAMAGE CONTROL

A program graduate applies computational power to grasp the pathology of fibrosis and other tissue diseases

By Thomas R. O'Donnell

Ashlee Ford Versypt's research is like a hike through the human body. "We have projects in the bone, the lung, the kidney, the eye and tumors," particularly those tied to breast cancer, says Ford Versypt, a chemical and biological engineering professor at New York's University at Buffalo. "We take a computational approach to try to bring systematic understanding to how these parts interact."

Chemical and physical forces in these tissues, plus the biology of infection and immune response "are complex systems that one can do experiments on, but they're hard to unravel," says Ford Versypt, a 2006-2010 Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient.

Many of her group's projects examine fiber formation and degradation. When this process is balanced, proteins and other molecules knit together to form vital support structures in tissues such as bone. But in some lung and kidney diseases, excess fiber can accumulate, thickening and scarring tissues.

Fibrosis can happen when molecules introduced through diet, infection, drugs and more mingle in organs. Ford Versypt wants to know "which things happen negatively that we might reverse, slow or stop and which things are positive that we want to reinforce or use therapeutically."

Her early work as a doctoral candidate and postdoctoral researcher focused on controlled release of drugs – how biomaterials exposed to bodily fluids dissolve. These compounds respond over time to a chemical stimulus. As she moved into academia, Ford Versypt considered tissues comprised of heterogeneous biomaterials – and the entire body is biomaterials – where processes also are subject to chemical stimuli. That led to her fibrosis research.

In 2017 the American Institute of Chemical Engineers named Ford Versypt one of 35 researchers under 35 who have made significant contributions. In 2019 she received a prestigious National Science Foundation Faculty Early Career Development Program (CAREER) grant providing $550,000 over five years to simulate a diabetic kidney.

Ford Versypt also has a five-year National Institutes of Health Maximizing Investigators' Research Award. She's used it to collaborate with experimentalist Brenda Smith, a nutritional sciences professor at the Indiana University School of Medicine, on interactions between digestive bacteria, the immune system and bone. A paper on the research, with Ford Versypt lab postdoctoral researcher Mohammad Aminul Islam as lead author, was chosen for a special issue of *Industrial & Engineering Chemistry Research* recognizing influential researchers.

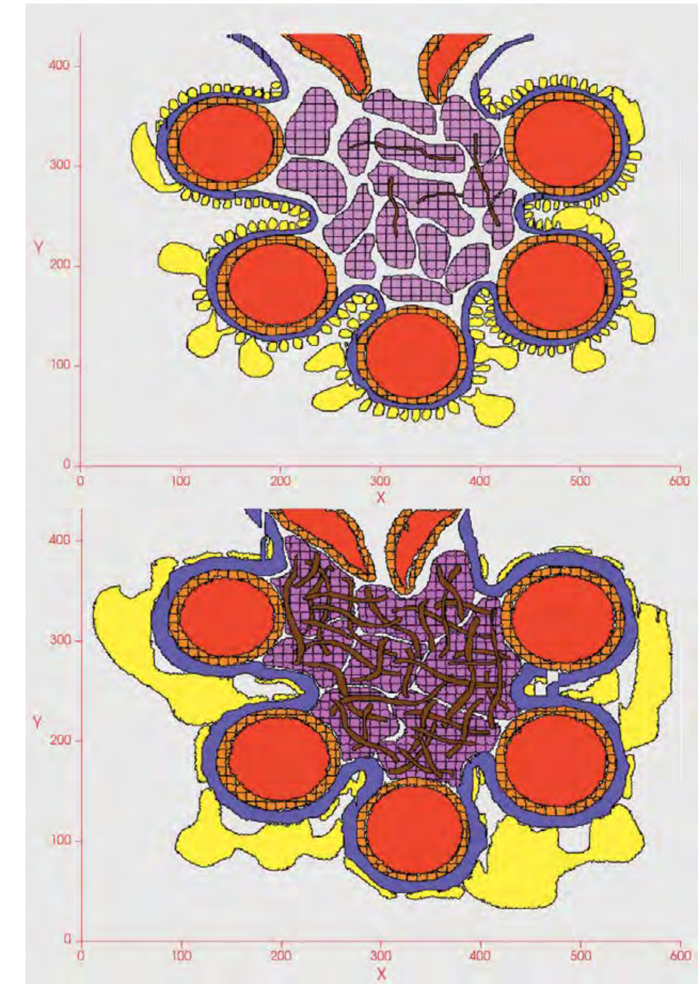
They wanted to understand why butyrate, a fatty acid produced by human gut bacteria during digestion, appeared to suppress chronic inflammation that can lead to osteoporosis, or bone loss, Ford Versypt says. That's "three systems interacting but playing a nice, orchestrated role in promoting health."

In a cascade of interactions, butyrate triggers immune cells to differentiate into regulatory T cells. These migrate to the bone and produce transforming growth factor beta, which suppresses inflammation and triggers production of Wnt-10b, a protein that promotes bone cell production.

The researchers investigated this network with a computational model connecting the three body compartments involved. They expected that butyrate's only function was to trigger the process, like tipping the first domino, with Wnt-10b as the main bone growth promoter. But the model found Wnt-10b is only partly responsible. Further modeling suggested butyrate also moves to the bones, where it has a direct role in fostering growth. The models suggested three explanations for this phenomenon that Smith's lab is testing.

"The model let us probe mechanistic questions that hadn't been considered experimentally," Ford Versypt says. The collaborators narrowed the possible causes, helping guide Smith's experiments.

Ford Versypt also is dedicated to fostering the next generation of chemical engineers. Among several leadership roles, she's chaired the Chemical Engineering Division of the American Society for Engineering Education (ASEE), where she created initiatives to promote racial diversity, including weekly conversations for division members on inclusion and thriving and a panel discussion at the society's annual meeting. She's also an academic trustee of Computer Aids for Chemical Engineering, which unites research faculty with industry and government laboratory computational modeling experts to promote development of computer and technological educational aids for chemical engineering.



Two cross-section views of the glomerulus, a blood-filtering kidney tissue, from a simulation performed in Ashlee Ford Versypt's lab that shows how healthy tissue (top) changes after major damage from diabetes (bottom). Capillaries (red) are surrounded by the glomerular basement membrane (blue), and mesangial cells (purple) that connect adjacent capillaries. Specialized cells called podocytes (yellow) encircle the glomerulus and aid filtration. As diabetes progresses, fibers (tangled brown structures) form in the glomerulus' center, membranes thicken and podocytes enlarge. *Credit: Ashlee Ford Versypt. Previous page: Douglas Levere/University at Buffalo.*

Classes, research and service are a lot to carry, but Ford Versypt also allots time to exercise. She and husband Joel signed onto a hiking challenge to explore western New York's trails and waterfalls. She documents their adventures via social media so "people have a more positive, non-snowy impression of Buffalo."

'Forces in these tissues plus the biology of infection and immune response are complex systems that are hard to unravel.'

A RIVER OF DATA RUNS THROUGH IT

A former fellow's open-source software is helping model watersheds and related climate issues the world over.

By Jacob Berkowitz

When Oak Ridge National Laboratory scientist Ethan Coon takes his three kids into Tennessee's wild areas, he's sharing a lifelong passion for the outdoors. And in the process, Coon, a computational hydrologist, observes the flow of creeks and topography of hollows, informing his research to model, understand and ultimately protect watersheds.

"I went into grad school wanting to find a place where math could be applied to science problems that were relevant to societal concerns," says Coon, a Columbia University graduate and a 2005-2009 Department of Energy Computational Science Graduate Fellowship (DOE CGSF) recipient. "I've been chasing that since then and the DOE labs have really allowed me to do that."

The primary result of this personal mission is the Advanced Terrestrial Simulator (ATS), world-leading open-source software for the multiscale modeling of environmental issues in watersheds and related climate applications. A decade in the making – with a 14-person multidisciplinary core team across four DOE national laboratories – today ATS is used by research groups internationally, as well as for a variety of core-mission DOE research projects, and was awarded an R&D 100 award in 2020.

While leading ATS development, Coon has co-shepherded his career.

His Ph.D. research focused on using finite element methods for earthquake simulation. On reflection, he's amazed at how the multiscale models he developed then – ones that excelled at integrating granular, subgrid-scale detail into computable approximations – have informed his ATS research. "It's still math applied to earth sciences, just now water and climate," says Coon, a scientist in ORNL's Climate Change Science Institute and Earth Sciences Division.

As a postdoc and then research scientist at Los Alamos National Laboratory until joining ORNL in 2017, Coon was introduced to the code Amanzi ("water" in Zulu). It was developed as a multilab project beginning in the early 2000s to model how reactive contaminants move through groundwater in support DOE environmental site remediation. Coon harnessed Amanzi for another growing environmental concern: climate change.

"We took the math and code guts of Amanzi and used it to start to build up this capability around carbon released by melting Arctic permafrost, and it became the ATS," Coon explains. The "A" in ATS wasn't always for "advanced." It originally stood for "Arctic." As ATS applications were extended to temperate and even tropical environments, the A morphed with it.

"What makes ATS unique is its ability to scale the complexity up and down to meet the need" and for researchers to add or remove soil conditions or evapotranspiration and other physical properties, Coon says. Now researchers use ATS to model everything from post-fire hydrology to algal blooms and how climate change-related warming of water affects power plant cooling. "As rivers warm, that might become a limitation on energy production," he says.

A decade ago Coon mostly worked alone, writing the ATS code and thinking about the model physics. "Now the majority of my time is supporting scientists to use the ATS code and shape the conceptualization of that research into something that's answerable with the code and the data." Writing code, he notes, is largely relegated to his "pristine me time," a couple of hours at night after the kids have been put to bed.

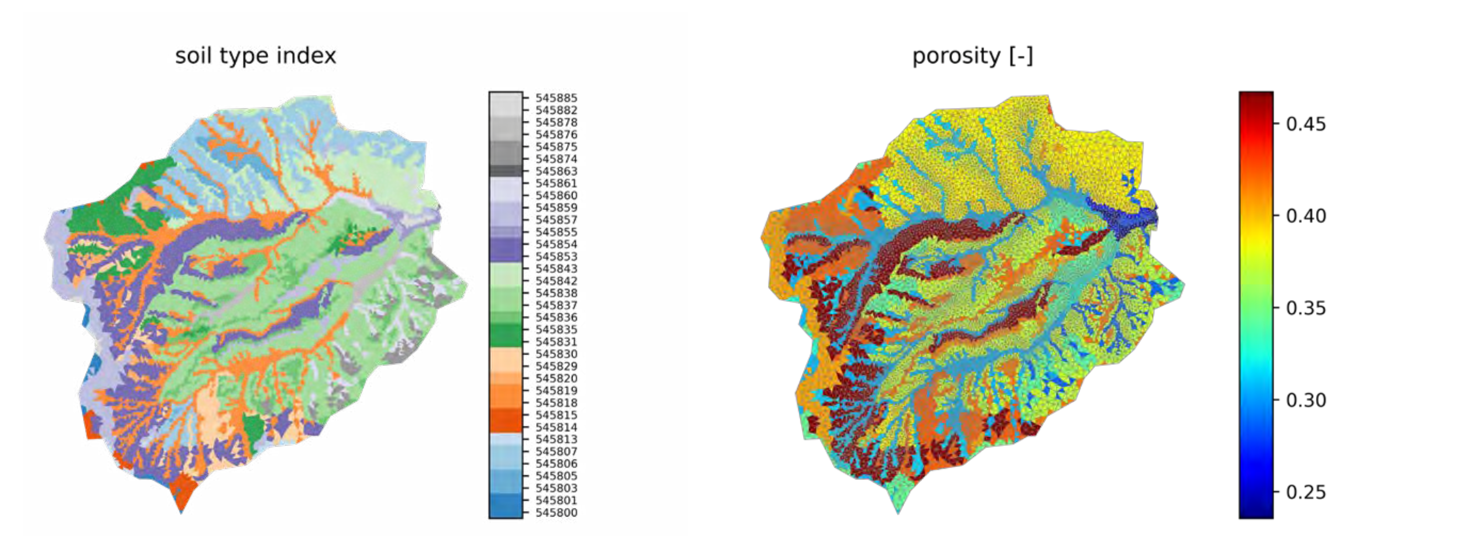
In 2021, Coon ran the first ATS user short course, a virtual event that attracted researchers from seven countries. This close collaboration with science users has benefitted ATS, guiding its development to focus on elements that are of concern to users, who create everything from simple one-dimensional models run on a researcher's laptop to full 3-D models using thousands of nodes on DOE supercomputers, including ORNL's Summit. The result is that Coon is co-author with scientists from diverse disciplines on papers in journals ranging from *Computational Geoscience* to *Water Resources Research* and *Environmental Research Letters*.

'I wanted to find a place where math could be applied to science problems that were relevant to societal concerns.'

The challenge of optimizing ATS for a range of computational platforms will grow increasingly important as Coon prepares it for the exascale era in his role as project integration lead in ExaSheds, a multi-institutional effort to model watersheds.

He'll also continue to push the edge of ATS physics, including the long-standing challenge of "what humans mean in an earth systems model," he says. In 2020, he and Christa Brelsford, his spouse and an ORNL colleague who specializes in social data for climate applications, characterized patterns of changes in impervious urban surfaces – asphalt and concrete. It's a key issue with climate change-related urban flooding and was their first project together.

"There's a lot of really important climate and water research and modeling that needs to happen to understand the impacts on society," Coon says, "and especially to focus on adaptation and limiting the impact on the most vulnerable."



Ethan Coon uses the Advanced Terrestrial Simulation code to model soil and water conditions in high resolution. These show various soil types (left) and porosities (right) mapped within the model's mesh for the Coweeta Hydrologic Laboratory, a U.S. Forest Service research site in western North Carolina. *Credit: Ethan Coon. Previous page: Carlos Jones/ORNL.*

FINESSING FUSION AND ELECTRICITY DEMAND

Kelley and Mandell are honored for producing energy advances and mentoring future researchers.

By Jacob Berkowitz

Morgan Kelley

Noah Mandell

A process engineer and a fusion scientist, both of whom apply numerical modeling to address pivotal 21st-century energy challenges, are the Frederick A. Howes Scholars in Computational Science for 2022.

A committee of alumni and friends of the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) chose Morgan Kelley and Noah Mandell for the annual award, named for the DOE's leading applied mathematics research official at his death in 1999. The award recognizes recent fellowship alumni for excellent research and outstanding leadership, integrity and character.

Mandell, a 2015-2019 fellow, completed his plasma physics Ph.D. at Princeton University in 2021. He's now a DOE Fusion Energy Sciences postdoctoral fellow at the Massachusetts Institute of Technology. Kelley, a 2017-2021 fellow, earned a process systems engineering Ph.D. from the University of Texas at Austin in 2021 and now is a data scientist at Dell Technologies.

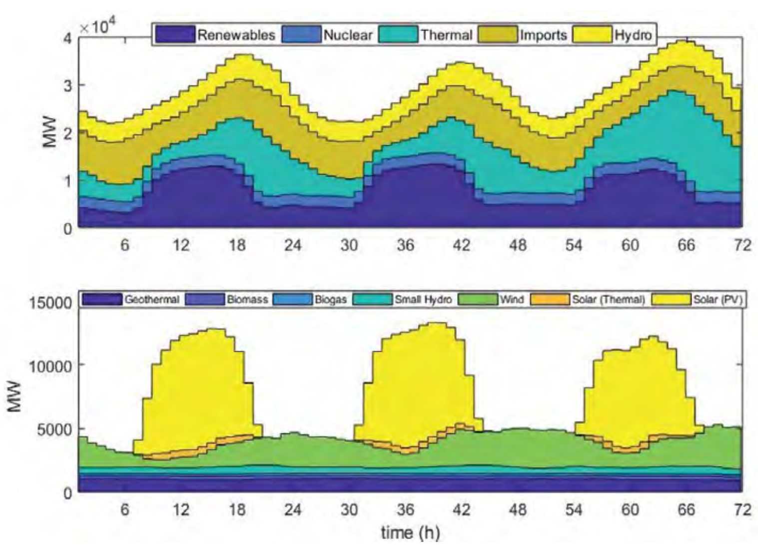
In her doctoral research, Kelley developed a unique mathematical model that lets industrial chemical companies optimize production when electricity rates are lowest. Industrial demand response scheduling, as it's called, helps both the company's bottom line and the environment. "By doing this, companies reduce emissions by using energy during peak solar times when electricity is cheaper," Kelley says.

She developed her code on supercomputers at UT Austin's Texas Advanced Computing Center and then reduced the optimization solver to run on a desktop machine in minutes, making it commercially viable.

In her last project before graduation, Kelley applied her model to a year's worth of operating data from Linde Plc, the world's largest industrial gas company, developing a demand response regime that cuts electricity costs by nearly 10%.

At Dell, Kelley uses her process modeling skills to help the computer company forecast demand and optimize placement of new warehouses around the world. "It's not chemical process engineering, but the problems are similar."

In his doctoral work with the DOE's Princeton Plasma Physics Laboratory (PPPL), Mandell developed a breakthrough computational simulation of plasma turbulence in the outer edge of a tokamak, a donut-shaped fusion reactor. The tokamak heats a gas of neutral hydrogen isotopes to create a plasma

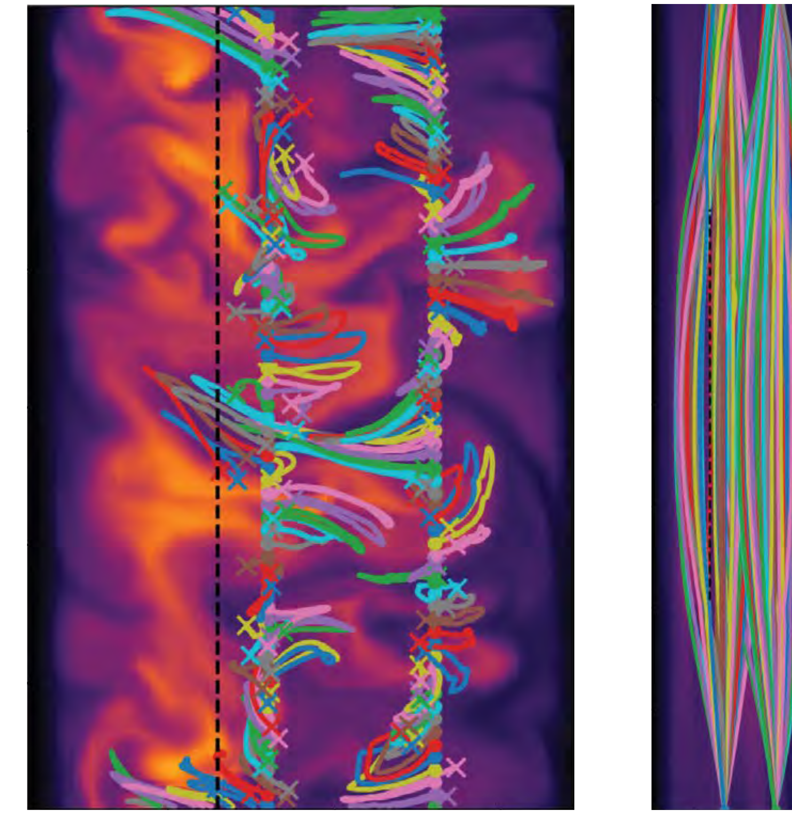


Industrial demand response scheduling uses electricity price and grid-side emissions data, enabling load-shifting and reductions in emissions, operating costs and stress on the grid. *Credit: Morgan Kelley.*

of charged particles that it confines with strong magnetic fields. With further heating, the plasma reaches starlike temperatures, sparking nuclear fusion and releasing energy. A key challenge, Mandell says, is ensuring even heat distribution in the tokamak, particularly at the outer edge. "You have to make sure that the heat exhaust is not going to melt the walls of the reactor."

Mandell joined the Gkeyll (pronounced Jekyll) code-development team and created the first kinetic plasma turbulence algorithm capable of modeling electromagnetic interactions between the plasma and the confining magnetic field in the outermost tokamak region, where the field lines intersect the walls. Mandell's code enables the simulation and design of reactors with improved heat distribution.

Mandell continues working on Gkeyll at MIT while also developing a new code, called GX, to model plasma turbulence in a tokamak's hot core. He plans to stitch the results together with his thesis work. "Then we'd have a whole-device model of turbulence in the fusion plasma." Notably, GX runs exclusively on GPUs, the ultra-fast graphics processors imported from gaming that underpin exascale supercomputers.



A snapshot of turbulent electron density fluctuations in a Gkeyll simulation that models plasma dynamics in the edge of the National Spherical Torus Experiment at the Princeton Plasma Physics Laboratory. *Credit: Noah Mandell.*

Mandell already is sharing his love of plasma physics and scientific discovery with the next generation of researchers. As part of MIT's Summer Research Program, which draws students from underrepresented groups, he mentored a College of William and Mary undergraduate in fusion science. Earlier, in the PPPL Science Undergraduate Laboratory Internship program, he mentored an Oxford University student who's now pursuing a physics Ph.D. at the California Institute of Technology. Mandell finds it "rewarding to train the next generation similar to the opportunities I was given as an undergrad, and it's been fun to see the success they've had."

He's also an accomplished jazz saxophonist and keeps his instrument standing in the corner of his home office. "There's a lot of overlap between the kind of thinking that you have to do in jazz and in scientific problems. You have to be creative in your approaches and think on the fly."

Kelley rose as a dynamic mentor and leader in her chemical engineering department, overcoming the onset of an autoimmune disease that left her unable to stand for more than a few minutes at a time. She developed a marriage algorithm that matches new graduate students in the department with advisors to optimize happiness. "Making that was super fun."

Kelley also organized and ran the department's graduate Friday seminar series, providing an important growth opportunity for third-year students to present their research to first years. And she introduced middle-school students, many from disadvantaged backgrounds, to the joys of chemical engineering as part of the NSF-sponsored Raising Future Scientists program.

Both Kelley and Mandell say their mix of science and service is partly payback for mentors and DOE predecessors who've nurtured their love of science.

Kelley's grandfather, Al Baye, 99, was an engineer on the Manhattan Project. "He was always fixing stuff in his garage, and I would go help him. We would build things. He really shaped my curiosity."

Mandell credits his high school physics teacher and undergraduate advisor for igniting his love of, and path in, physics. Now, he works to achieve the long-held goal of commercial fusion energy. "It's a really exciting time to be in fusion because we have a few major efforts that are based in the knowledge we've developed over the past 60 years and really have a very good chance of succeeding."

A PIECE OF THE SUN AND OTHER PRIZES

Former fellows shine, garnering honors and contributing to discovery, policy, training and communication.

In April 2022, Massachusetts Institute of Technology mechanical engineering professor **Asegun Henry** (2005-2009) and MIT and National Renewable Energy Laboratory colleagues published a *Nature* article about what they call the "sun in a box," a super-efficient thermophotovoltaic cell. In 2021, Henry received the Bell Labs Prize for the device, a low-cost energy storage technology that could help decarbonize the energy grid and reduce emissions by up to 40%. The $100,000 prize recognizes game-changing innovations in science, technology, engineering and mathematics.

Alicia Magann (2017-2021) was named a Sandia National Laboratories' 2022 President Harry S. Truman Fellow in National Security Science and Engineering. She explores the possibilities of quantum control in computing, an extension of her Princeton University doctoral research. Magann works with Sandia's Mohan Sarovar, who advised her DOE CSGF practicums.

The Breakthrough Prize Initiative chose **Norman Yao** (2009-2013) for a 2022 New Horizons in Physics Prize, recognizing his pioneering theoretical work on non-equilibrium matter, including a quantum system of particles called time crystals. The $100,000 award goes to early-career scientists and mathematicians who are making substantial impacts in their fields. Yao is a Lawrence Berkeley National Laboratory scientist and University of California, Berkeley, professor.

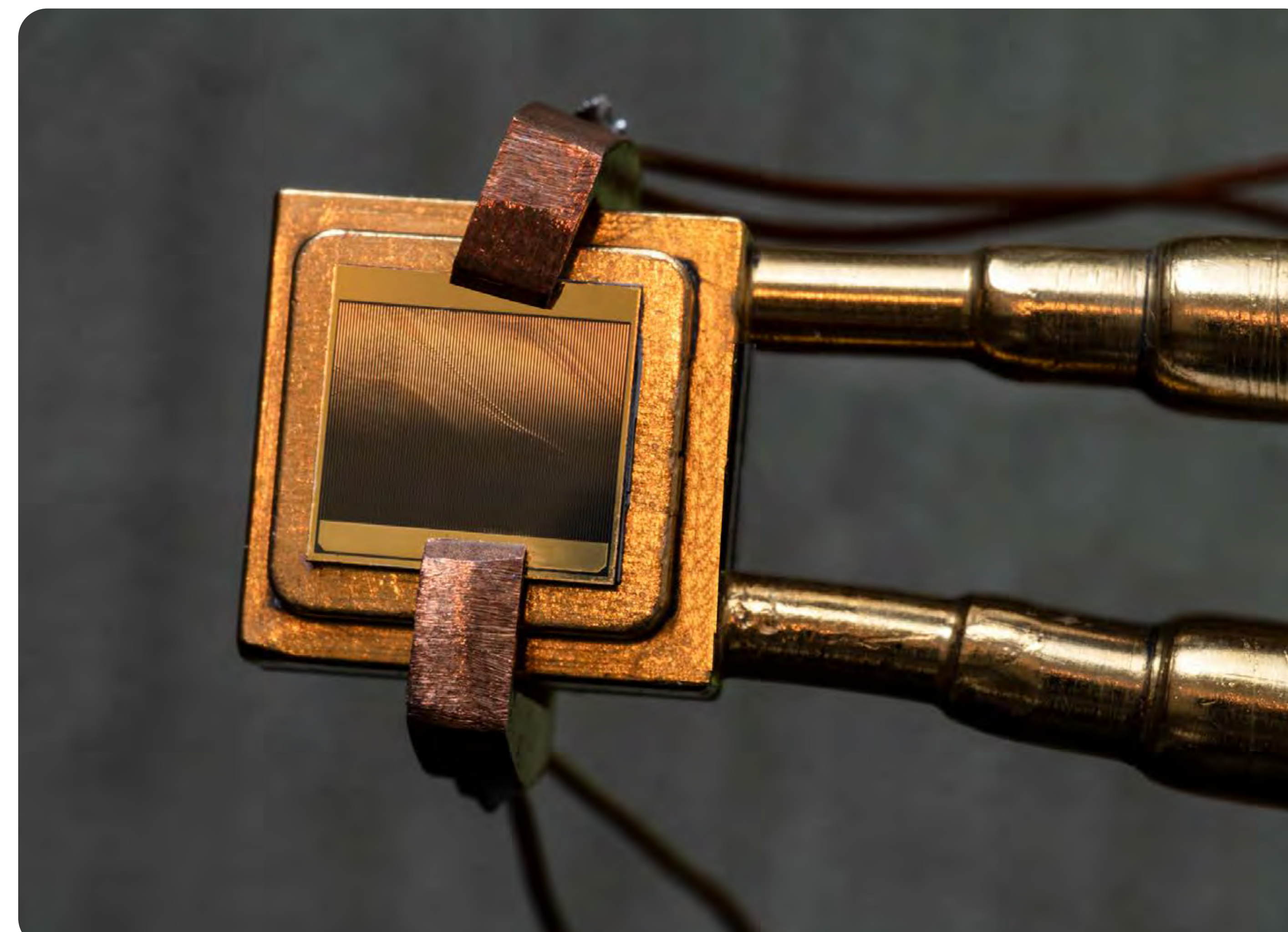
DOE CSGF alumnus Tal Danino of Columbia University co-led a study in which the team engineered bacteria (green objects) with a temporary "cloak" (transparent coating around bacteria) that helps them evade immune cells (larger objects). *Credit: Ella Marushchenko, Alex Tokarev, Danino Lab/Columbia University.*

Richard Barnes (2015-2019) joined the National Energy Research Scientific Computing Center in November as Berkeley Lab's newest Admiral Grace M. Hopper Postdoctoral Fellow. His projects include applying high-performance computing and novel algorithms and methods in new science areas.

Berkeley Lab recognized **Anubhav Jain** (2008-2011) with a 2021 early scientific career achievement award. Jain studies materials informatics and develops software tools and techniques that help research groups use computational screening to design materials.

Duke University professor **Amanda Randles** (2010-2013) was named a 2021 National Academy of Inventors Fellow. The program highlights academics who have demonstrated a spirit of innovation in creating or facilitating inventions that have made a tangible impact on quality of life, economic development and society's welfare.

Fellowship alumni served as guest editors and authors for the November/December 2021 issue of the journal *Computing in Science & Engineering* to recognize the DOE CSGF's 30th anniversary. **Jaydeep Bardhan** (2002-2006), **Mary Ann Leung** (2001-2005), **Eileen Martin** (2012-2016) and **Randles** were guest editors and wrote an introduction. Longtime DOE CSGF supporters and steering committee members David Brown of Berkeley Lab, James Hack of Oak Ridge National Laboratory and Robert Voigt of research company Leidos described the fellowship's founding and early years. **Allison Baker** (1999-2003), **Julianne Chung** (2006-2009), **Mala Radhakrishnan** (2004-2007), **Eric Chi** (2008-2011) and **Jarrod McClean** (2011-2015) contributed articles about the fellowship's impact on their work and careers.



Asegun Henry's team at MIT and NREL designed a thermophotovoltaic cell that converts heat to electricity and could reduce emissions by up to 40%. The team is working to integrate these cells into larger devices to produce a thermal battery that could absorb and store renewable energy. *Credit: Felice Frankel.*

Biomedical engineering professor **Tal Danino**'s Columbia University team reported on a "bacterial cloaking" system that temporarily hides therapeutic bacteria from the immune system, letting the microbes deliver cancer-killing drugs to tumor cells in mice. The work was published in the March 2022 *Nature Biotechnology*. Danino was a 2006-2010 fellow.

Priya Donti (2017-2021) was a lead author on a November 2021 report entitled *Climate Change and AI: Recommendations for Government*. It makes 48 recommendations for how governments can support AI's application in climate challenges and address AI's climate-related risks. Donti is a co-chair of Climate Change AI and a Ph.D. student at Carnegie Mellon University.

Brian Cornille (2016-2020) and **Ian Ochs** (2016-2020) gave invited talks at the American Physical Society's Division of Plasma Physics meeting in November 2021. Cornille completed his Ph.D. at the University of Wisconsin-Madison and is now a software system design engineer for AMD. Ochs is a Ph.D. student at Princeton University.

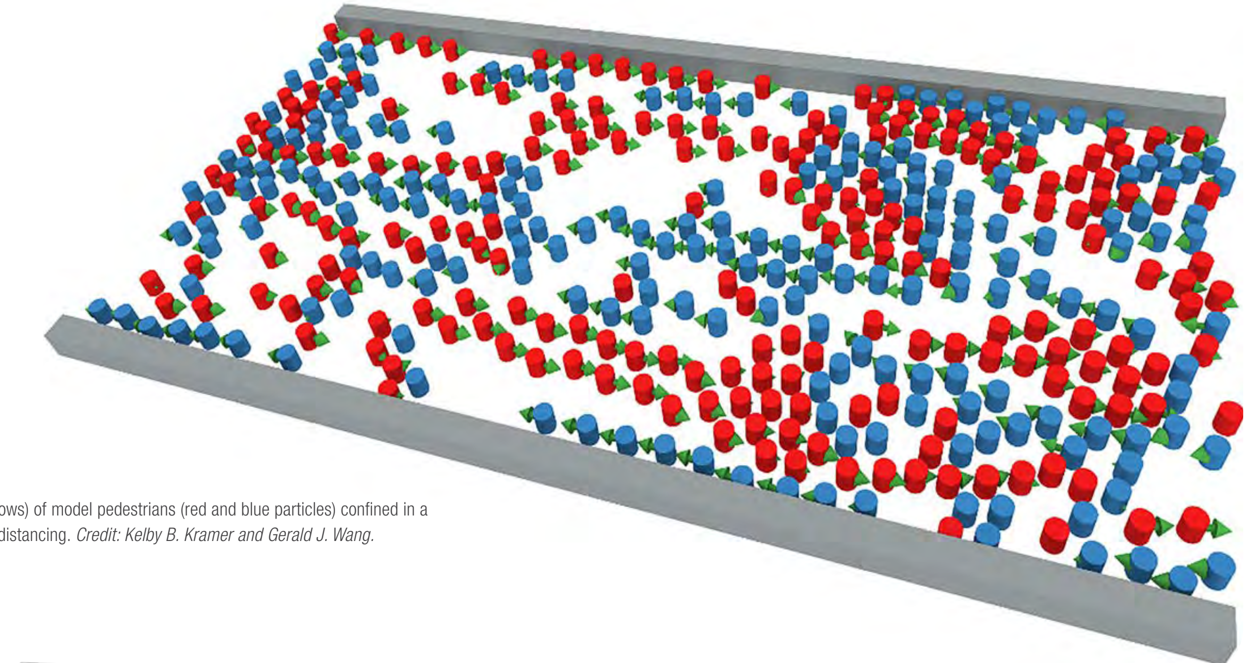
The University of Notre Dame recognized biological sciences professor **Alex Perkins** (2007-2011) with a 2021 College of Science Research Award. He uses modeling to study the ecology and epidemiology of infectious diseases, especially those mosquitoes carry. Perkins' team published a *Nature Communications* paper in September 2021 evaluating forecasting models for the Zika epidemic.

The *Philadelphia Inquirer* covered research published by **Gerald J. Wang** (2014-2018) investigating the effects of social distancing in enclosed spaces such as hallways. The study modeled pedestrians as particles moving through a pipe and showed that increasing distance significantly slows foot speed, which can increase congestion in these areas. Wang is a professor of civil and environmental engineering at Carnegie Mellon University.

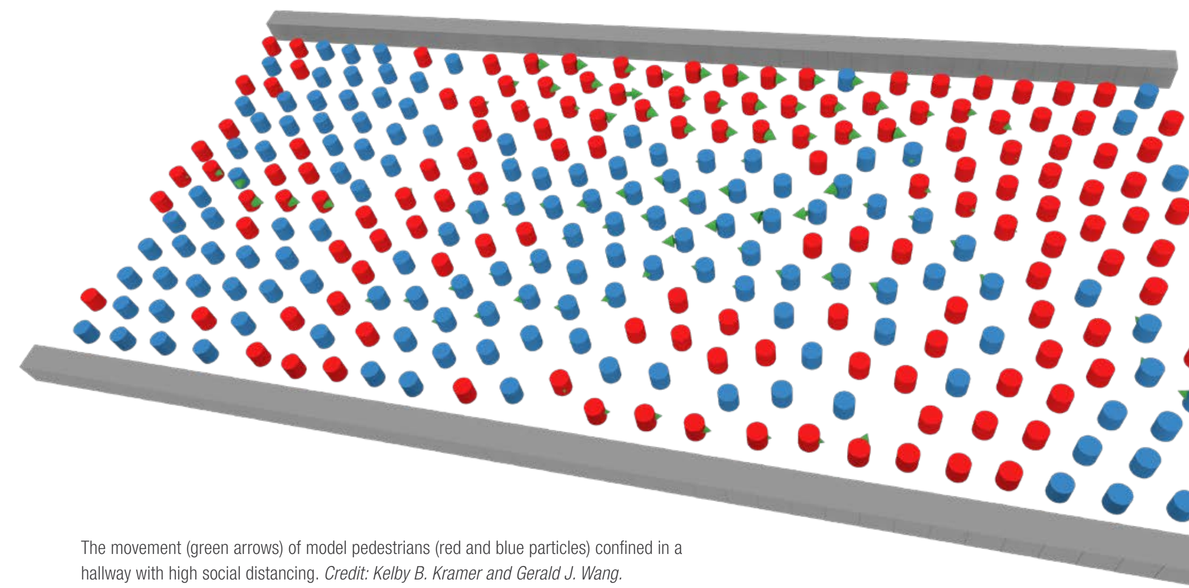
William Barry (1994-1998) was named dean of the Allen School of Engineering and Computing at Trine University in Angola, Indiana. He has been a civil and environmental engineering professor there since 2008.

Sommer Gentry (2001-2005), previously a United States Naval Academy mathematics professor, has joined the New York University Grossman School of Medicine to co-direct its Center for Surgery and Transplant Applied Research.

Corones Award winner Paul Sutter hosts the *ArsTechnica* web series *Edge of Knowledge*.



The movement (green arrows) of model pedestrians (red and blue particles) confined in a hallway with weak social distancing. *Credit: Kelby B. Kramer and Gerald J. Wang.*



The movement (green arrows) of model pedestrians (red and blue particles) confined in a hallway with high social distancing. *Credit: Kelby B. Kramer and Gerald J. Wang.*

Argonne National Laboratory computational scientist **Kyle Felker** (2014-2018) has led the effort to port FusionDL FRNN, a collection of machine-learning models and implementations for fusion energy science, to Aurora, the lab's upcoming exascale computer. The work is part of the Aurora Early Science Program project "Accelerated Deep Learning Discovery in Fusion Energy Science" led by William Tang at Princeton Plasma Physics Laboratory.

Paul Sutter (2007-2011) received the Krell Institute's 2022 James Corones Award in Leadership, Community Building and Communication. The award is named in honor of Krell's late founder; Krell manages the DOE CSGF. Sutter hosts *Edge of Knowledge*, an eight-episode series on the science website *Ars Technica*, covering topics that include dark matter and colonizing Mars. Sutter also is the author of *How to Die in Space* and *Your Place in the Universe* and hosts the *Ask a Spaceman!* podcast and YouTube series. He is a research professor at SUNY Stony Brook and a guest researcher at the Flatiron Institute.

Sanjeeb Bose (2009-2013) of Cascade Technologies Inc. received 100,000 node hours on the Oak Ridge Leadership Computing Facility's Summit supercomputer for the project "Achieving Higher Efficiency Turbomachinery Design via Large Eddy Simulation."

CLASS OF 2022

Christiane Adcock
Computational and Mathematical Engineering
Stanford University
Advisor: Gianluca Iaccarino
Practicum: National Renewable Energy Laboratory (2021, 2022)

Kaley Brauer
Astrophysics
Massachusetts Institute of Technology
Advisor: Anna Frebel
Practicum: Lawrence Berkeley National Laboratory

Jacob Bringewatt
Physics
University of Maryland, College Park
Advisor: Alexey Gorshkov
Practicum: Thomas Jefferson National Accelerator Facility

Kimberly Cushman
Physics
Yale University
Advisor: George Fleming
Practicum: Thomas Jefferson National Accelerator Facility and National Renewable Energy Laboratory (both 2020)

Justin Finkel
Computational and Applied Mathematics
University of Chicago
Advisor: Jonathan Weare
Practicum: Los Alamos National Laboratory

Ryder Fox
Meteorology and Physical Oceanography
University of Miami
Advisor: David Nolan
Practicum: Brookhaven National Laboratory and Pacific Northwest National Laboratory (both 2021)

Steven Fromm
Physics
Michigan State University
Advisor: Sean Couch
Practicum: Los Alamos National Laboratory

Sarah Greer
Mathematics and Computational Science
Massachusetts Institute of Technology
Advisor: Laurent Demanet
Practicum: Los Alamos National Laboratory (2019, 2020, 2021)

Olivia Hull
Physical Chemistry
Kansas State University
Advisor: Christine Aikens
Practicum: National Renewable Energy Laboratory

Edward Hutter
Computer Science
University of Illinois at Urbana-Champaign
Advisor: Edgar Solomonik
Practicum: Oak Ridge National Laboratory

Dipti Jasrasaria
Chemistry (Physical - Theory)
University of California, Berkeley
Advisor: Eran Rabani
Practicum: Lawrence Livermore National Laboratory

K. Grace Johnson
Chemical Physics
Stanford University
Advisor: Todd Martinez
Practicum: National Renewable Energy Laboratory

Margaret Lawson
Computer Science
University of Illinois at Urbana-Champaign
Advisor: William Gropp
Practicum: Lawrence Livermore National Laboratory

William Moses
Computer Science
Massachusetts Institute of Technology
Advisor: Charles Leiserson
Practicum: Lawrence Berkeley National Laboratory (2019) and Argonne National Laboratory (2021)

Samuel Olivier
Nuclear Engineering
University of California, Berkeley
Advisor: Rachel Slaybaugh
Practicum: Los Alamos National Laboratory (2019) and Lawrence Livermore National Laboratory (2020, 2021)

Melissa Queen
Information Theory
University of Washington
Advisor: Luis Ceze
Practicum: National Renewable Energy Laboratory

Jesse Rodriguez
Plasma Physics/Optics
Stanford University
Advisor: Mark Cappelli
Practicum: Princeton Plasma Physics Laboratory

Lawrence Roy
Cybersecurity
Oregon State University
Advisor: Mike Rosulek
Practicum: SLAC National Accelerator Laboratory

Steven Stetzler
Astronomy
University of Washington
Advisor: Mario Juric
Practicum: Los Alamos National Laboratory (2021, 2022)

James Sullivan
Astrophysics
University of California, Berkeley
Advisor: Uros Seljak
Practicum: Argonne National Laboratory

Anda Trifan
Theoretical and Computational Biophysics
University of Illinois at Urbana-Champaign
Advisor: Emad Tajkhorshid
Practicum: Argonne National Laboratory (2020, 2021, 2022)

Michael Tucker
Astronomy
University of Hawaii
Advisor: Benjamin Shappee
Practicum: Lawrence Berkeley National Laboratory

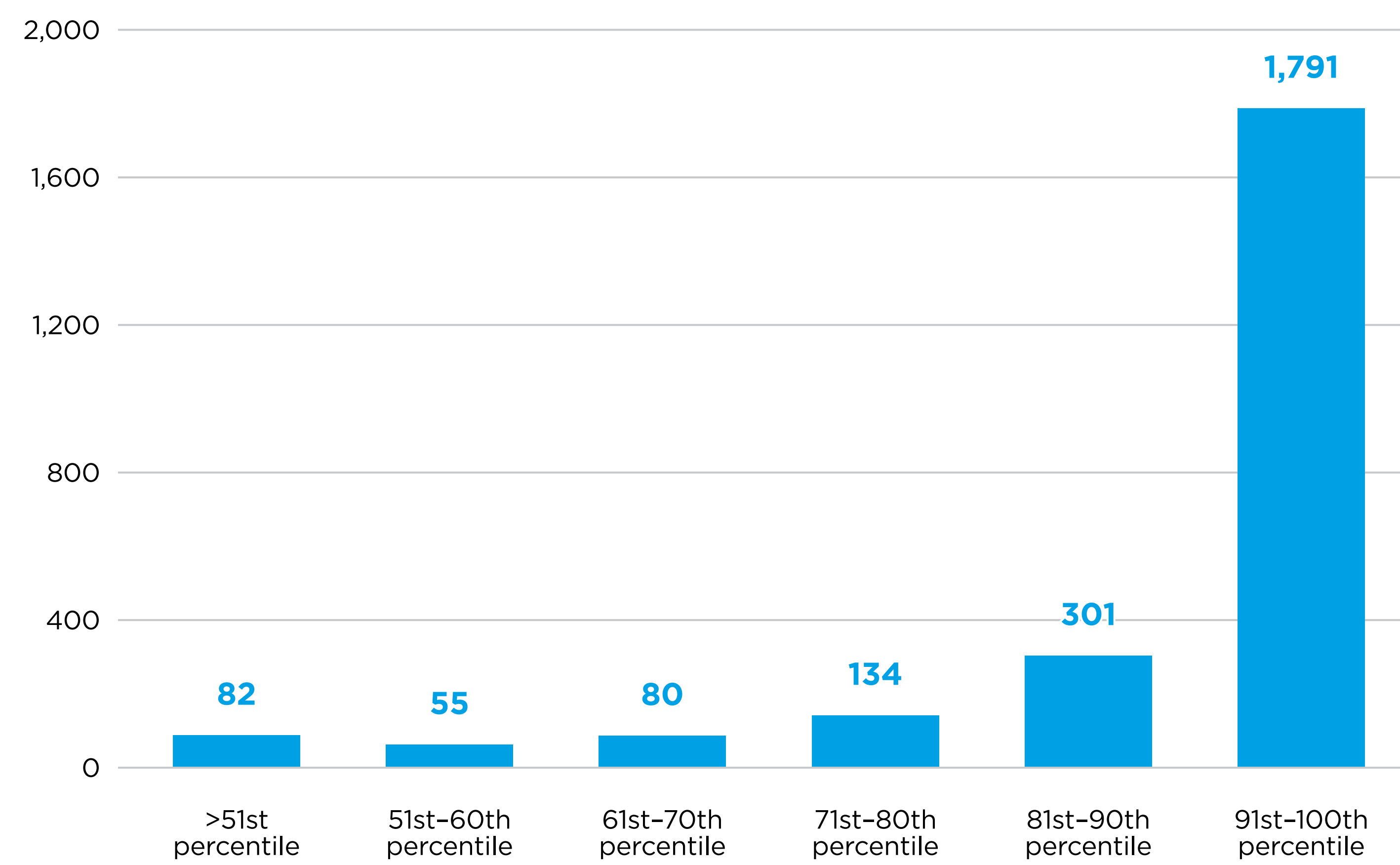
Caitlin Whitter
Computer Science
Purdue University
Advisor: Alex Pothen
Practicum: Lawrence Berkeley National Laboratory (2019, 2021)

Paul Zhang
Geometric Data Processing
Massachusetts Institute of Technology
Advisor: Justin Solomon
Practicum: Sandia National Laboratories, New Mexico

DOE CSGF: RESEARCH WITH IMPACT

The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) trains top researchers who generate results that shape their fields. An analysis of 2,443 program alumni publications indicates that the overwhelming majority appeared in highly influential journals. The Eigenfactor (EF) score quantifies a journal's influence in a particular year by weighing how frequently other researchers cite its articles. The Eigenfactor Project ranks journals by percentile based on their score, placing the influential journals in the upper brackets. The study found nearly three quarters of alumni articles published between 1997 and 2015 appeared in journals with EF scores in the top 10%. Another 12% were in journals with EF scores between the 81st and 90th percentile. *Source: U.S. Department of Energy Computational Science Graduate Fellowship 1991–2021: A Follow-up Study of Recipients and Programmatic Outcomes.*

Eigenfactor (EF) score percentile rankings of journal articles published by DOE CSGF alumni



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