THE DOE CSGF ANNUAL
1991-2021 Celebrating 30 Years

DEIXIS

2021

DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP

TOUR DE FORCE

Final-year fellow Quentarius Moore looks at how mechanical stress alters chemical reactions.

PAGE 16

STARS ARE BORN

Of galaxies, quantum control and climate change – other fellows share their stories.

PAGE 10

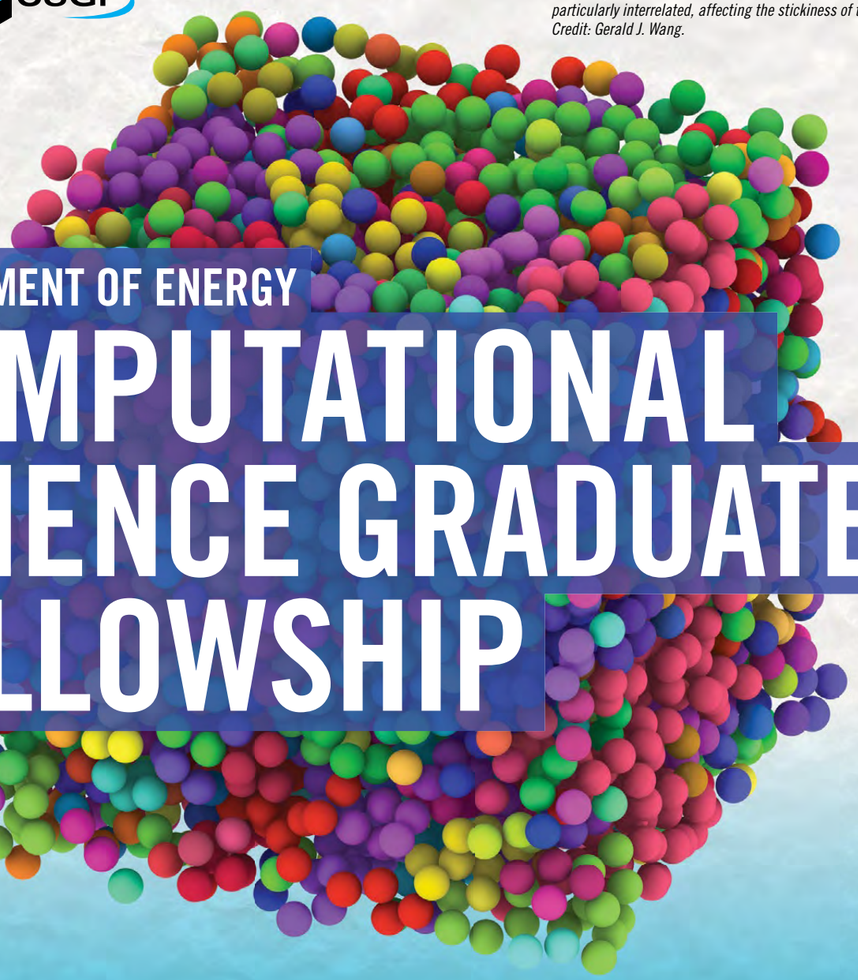
WHAT THEY'RE DOING NOW

Program alumni search for ways to put germs to work, store renewable energy and optimize simulations.

PAGE 22

PLUS: A conversation about NERSC's next big machine, dual Howes winners and more.

DOE CSGF 1991-2021 Celebrating 30 Years



Closely packed particles in a colloidal suspension with friction, from a simulation by DOE CSGF alumnus Gerald J. Wang of Carnegie Mellon University. The colors differentiate particle groups whose motions are particularly interrelated, affecting the stickiness of the whole material. Credit: Gerald J. Wang.

DEPARTMENT OF ENERGY

COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP

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

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

BENEFITS

+ $38,000 yearly stipend
+ Payment of full tuition and required fees
+ Yearly program review participation
+ Annual professional development allowance
+ 12-week research practicum experience
+ Renewable up to four years

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

www.krellinst.org/csgf

This equal opportunity program is open to all qualified persons without regard to race, gender, religion, age, physical disability or national origin.

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RECORD-SETTING: THE INCOMING DOE CSGF CLASS

For 2021-22, the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) will induct a record-setting class of 32 new fellows attending institutions across the country, from the University of California, San Diego, to the University at Buffalo. Each will learn how to apply high-performance computing to problems of national importance, working in fields that include atmospheric science, condensed matter physics and quantum information.

Jezrielle Annis
Texas A&M University
Physical Chemistry

Olivia Asher
University of Georgia
Bioinformatics

Lucas Attia
Massachusetts Institute of Technology
Chemical Engineering

Alexandra Ballow
Montana State University
Algebra and Quantum Mechanics

Zoe Barbeau
Stanford University
Engineering

Bryn Barker
University of North Carolina at Chapel Hill
Applied Mathematics

Paul Beckman
New York University
Mathematics

Vivek Bharadwaj
University of California, Berkeley
HPC/Scientific Computing

Marianne Cowherd
University of California, Berkeley
Ecosystem Sciences

Ishani Ganguly
Columbia University
Theoretical Neuroscience

Krystian Ganko
Massachusetts Institute of Technology
Chemical Engineering

Souradip Ghosh
Carnegie Mellon University
Computer Science

Juan (Felipe) Gomez
Harvard University
Condensed Matter Theory

Jalen Harris
Cornell University
Materials Science and Engineeing

Bowen Jing
Massachusetts Institute of Technology
Computer Science

Gabrielle Jones
University of Michigan
Engineering

Caleb Ju
Georgia Institute of Technology
Computational Science and Engineering

Olorundamilola (Dami) Kazeem
Johns Hopkins University
Computational Linguistics

Madeleine Kerr
University of California, San Diego
Geophysics

Joy Kitson
University of Maryland, College Park
Computer Science

Nicole Pagane
Massachusetts Institute of Technology
Computational and Systems Biology

Shehan Parmar
University of California, Los Angeles
Aerospace Engineering

Abigail Poteshman
University of Chicago
Computational and Applied Mathematics

Sonia Reilly
New York University
Mathematics

Paulina Rodriguez
The George Washington University
Mechanical Engineering

Rahul Sahay
Harvard University
Physics

Courtney Shafer
University at Buffalo
Geological Sciences

Timothy Taylor
University of Colorado at Boulder
Atmospheric Science

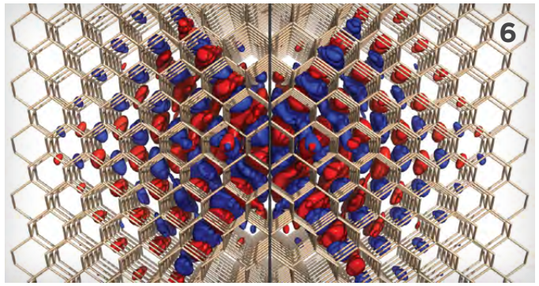
Samuel Varner
California Institute of Technology
Chemical Engineering

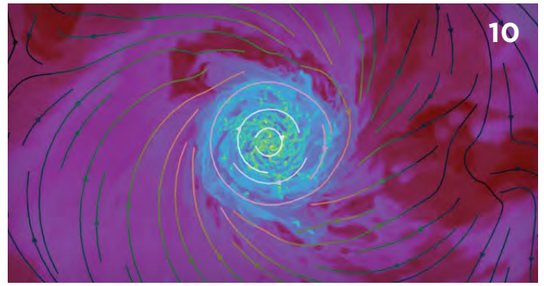
Julia Wei
University of California, Berkeley
Condensed Matter Physics, Quantum Information

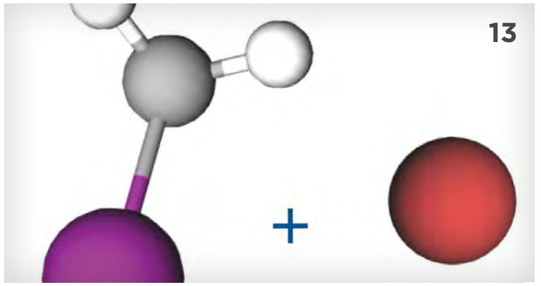
Steven Wilson
Arizona State University
Chemical Engineering

Victor Zendejas Lopez
California Institute of Technology
Mechanical Engineering

IN THIS ISSUE

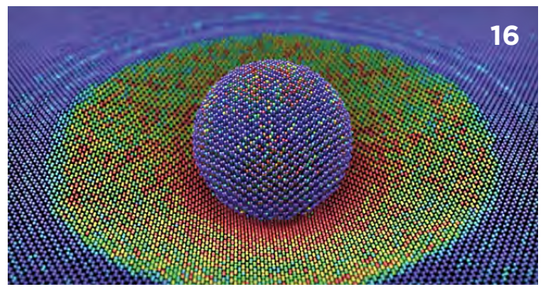


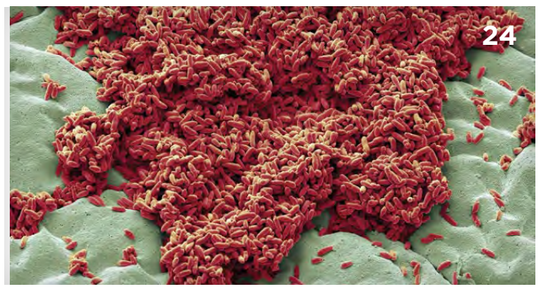




Departments

Features





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For additional information about the DOE CSGF, 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 is an annual publication of the Department of Energy Computational Science Graduate Fellowship that 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: Final-year fellow Quentarius Moore simulates how mechanical forces shape chemical reactions. The Mississippi native hopes to show children in his home state the range of available career options in science. Read more about his work on page 16.
Credit: Chris Jarvis/TAMU

DOE CSGF
Celebrating 30 Years

BIGGER COMPUTING CHALLENGES

A DOE CSGF alumnus reflects on how Perlmutter and other new supercomputers will help researchers tackle larger science problems.

Jack Deslippe leads the Application Performance Group at the National Energy Research Scientific Computing Center (NERSC) and chemistry and materials applications portion of the Department of Energy's (DOE's) Exascale Computing Project (ECP). He was a DOE Computational Science Graduate Fellowship (CSGF) recipient from 2006 to 2010.

Jack Deslippe

DEIXIS: CAN YOU TELL ME ABOUT YOUR EARLY SCIENCE INTERESTS?

Deslippe: As a kid, I dreamed of being an astronaut, and during high school, I became interested in physics – all the cool and weird things that happen at really big scales and really small ones. While majoring in physics at Clemson University, I fell in love with the idea that you could try to discover things as a career. For my Ph.D. I worked in a computational theory group at the University of California, Berkeley, trying to understand how materials work or how to design new ones from the ground up with unique properties for batteries, photovoltaics, energy conversion devices and more.

WHAT ABOUT COMPUTING?

I've always been a gadget guy. I fondly remember programming Texas Instruments TI-82 calculators in middle school and high school. I did web development in high school and became passionate about open-source software and Linux as a young adult.

But my current position is largely because of the CSGF. The scientific problems in my Ph.D. presented a serious computational challenge that requires high-performance computing (HPC) systems with tens to thousands of nodes and hours to days of calculation time. I discovered that I really loved algorithmic development and parallel programming. I wanted to tackle the HPC application development challenge within the scientific community.

HOW DID YOUR GRADUATE RESEARCH LEAD INTO YOUR WORK AT NERSC?

I was calculating the nanoscale properties of materials such as graphene sheets, some of the largest calculations ever with these methods. The codes that I needed just didn't exist or weren't meant to scale to very large systems. So I started developing the codes that could solve the problem. I led a team that produced our public release of a massively parallel HPC code, BerkeleyGW, that could take advantage of the country's biggest HPC systems. When I applied for my original position at NERSC in 2011, as a materials science consultant, I kept one foot in the science domain and had one foot in the computational science and HPC space.

WHAT DOES THAT WORK LOOK LIKE?

We're focused on the delivery and successful deployment of the Perlmutter system, the biggest, most powerful system ever at NERSC, up to four times that of Cori (previously NERSC's most powerful system). Much of its capability comes from graphics processing unit (GPU) accelerators that are embedded within a significant fraction of the system's nodes. We're partnering with different research teams around the country to prepare their applications for those GPU accelerators. We communicate regularly as a team, but we also have hackathon events, where we sit together and look at code, optimizing it and then recompiling it to see the difference. We want teams to be able to execute more challenging science problems on this system ones that take advantage of both the added computational power and our applications work.

WHAT ARE SOME RESEARCH PROJECTS THAT YOU'VE WORKED ON?

Recently I collaborated with my UC Berkeley research group on simulating a prototype qubit-type system with more than 10,000 electrons, the largest-ever calculations done on a material system using this level of fidelity. The work was a finalist for the Gordon Bell prize last year. Two years ago, I was part of a team that won the Gordon Bell prize for work that involved training an artificial intelligence model to automatically detect extreme weather events like hurricanes and atmospheric rivers in climate datasets.

WHAT ABOUT THIS INTERSECTION OF AI AND HPC? HOW DO YOU SEE THEM COMING TOGETHER?

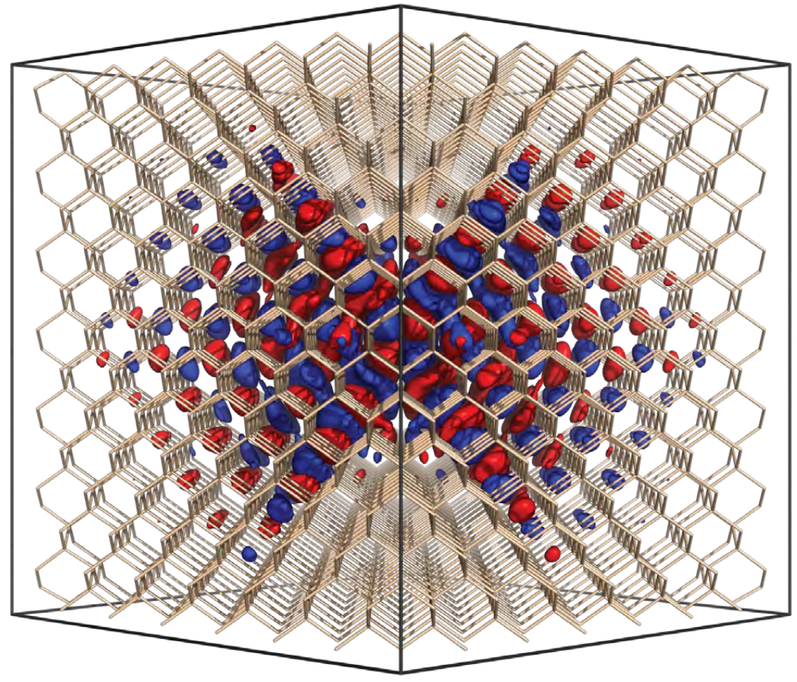
Coupling AI with HPC is really exciting. It can help us interpret the data from experiments or simulations accurately and efficiently, such as in our project on climate simulations. In addition, coupling AI directly with simulation could replace some computationally expensive, high-fidelity models with AI-based inference models. We're already seeing this in molecular dynamics, where we simulate atoms or molecules interacting with each other in response to heat, cooling or other extreme conditions. These calculations are computationally expensive because you have to model the forces atoms experience from all the others in the neighborhood.

Today researchers are developing AI-based forcefield models and training them on results from these expensive calculations, leading to new methods with similar accuracy but much lower computational cost. That allows you to study a much larger system for a longer time to answer questions that might not have been possible before.

EXASCALE COMPUTING IS ALMOST HERE. WHAT WILL THAT MEAN GOING FORWARD?

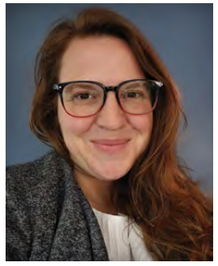
One grand challenge in materials science is to solve the Schrödinger equation directly for an interacting materials system. You can't do it because it's an exponentially growing problem as you add more and more electrons to your system. But we can do a randomly sampled approach called quantum Monte Carlo. One ECP application will allow us to extend quantum Monte Carlo from smaller systems with up to one hundred atoms to those with thousands of atoms using QMCPACK. With a high-fidelity method on a system this size, you can now tackle things like defects and interfaces between materials. These more complex systems' properties drive functional materials' behavior and are the bases for devices like batteries and photovoltaics.

Clever scientists have been working around these limitations for years, but it's exciting to think about having enough computing power to perform the highest fidelity calculations directly on materials of interest.



Jack Deslippe and his colleagues have improved BerkeleyGW code to perform the largest-ever high-fidelity calculations of materials such as this representation of more than 2,700 silicon atoms and nearly 11,000 electrons. Their research paper was a 2020 Gordon Bell Prize finalist. *Credit: Berkeley Lab/University of California, Berkeley/Stanford University.*

SEX ISN'T EVERYTHING



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 is a first-year fellow studying environmental health science at the University of North Carolina, Greensboro.

By Ellis L. Torrance

If you're reading this article, you're probably well aware of the nuances of the birds and the bees: that humans and other animal species engage in sex to pass their genetic material to their offspring.* Through sexual reproduction, both parents are able to contribute some mixture of their DNA to create a genetically unique individual.

This genetic uniqueness is instrumental for evolution and adaptation through survival of the fittest. Each population of individuals contains a mosaic of traits and, ideally, only the most favorable ones are passed down to offspring, letting them survive long enough to reproduce.

Bacteria, however, don't play by these rules. When they procreate, they simply divide, creating clones of themselves. Despite their reproductive simplicity, bacteria proudly claim the title of the most abundant group of organisms on this planet. Through their approximately 3.5-billion-year existence, they've adapted to and are found in nearly every environment where we've sought them, from volcanic lakes of sulfuric acid to Arctic permafrost and, of course, coating nearly every square inch of our bodies.

This magnificent and unrivaled ability to survive is due in part to their extensive catalog of genetic diversity. However, bacteria's clonal nature presents quite an evolutionary quandary: If these organisms are only genetic copies of their parents, how are bacteria so diverse and how can they adapt and evolve so quickly?

My research focuses on this key question wherein I use genetic data and high-performance computing (HPC) to understand the genealogy of these ubiquitous organisms. What I learn could help us predict and perhaps control bacterial evolution to improve human health.

Scientists have found that bacteria have a kind of superpower: They can pass pieces of DNA between each other. That's like your cousin, Usain Bolt, handing you a bag of genes that lets you run as fast as humanly possible after a family dinner. As a bonus, you get to pass these traits down to your children, enabling your whole family to sweep the next Olympics.

This capacity to share genetic material allows an incredibly vast range of genetic diversity within a single bacterial species and means different populations could have disparate capabilities. A great example is *E. coli*, which often harmlessly cohabitate in our intestines — while genetic variants of the same species can cause a lettuce recall (and potentially explosive diarrhea).

That's like your cousin, Usain Bolt, handing you a bag of genes that lets you run as fast as humanly possible after a family dinner.

Researchers understand that, at least for bacteria, sex isn't everything. However, it's burdensome to determine how often these organisms transfer genetic material in real time. As you're aware, they're pretty small, and we don't know what they're up to most of the time in their literal microcosm. Detecting how often they change would require growing and maintaining a species of bacteria for years and stopping to sequence its DNA every so often to seek genetic transfer episodes. Because there are more than 30,000 named bacterial species (so far) this would require time, labor and resources that we, as scientists, simply lack.

Luckily, since the sequencing of the first bacterial genome – decoding a microbe's DNA to record its entire genetic instructions – in 1995, scientists across the globe have steadily published genomic data to digital repositories for thousands more species. This means that even though we aren't able to fully observe DNA transfers in real time, there is abundant informative DNA data we can use to analyze bacteria's genetic diversity.

For my research, I use thousands of whole-genome sequences to predict the frequency of DNA exchange for many bacterial species. To do this, I begin by generating phylogenetic trees. Much like a family tree, they follow bacteria's descent from a hypothetical last common ancestor and record the genetic changes that led species to diverge within the lineage.

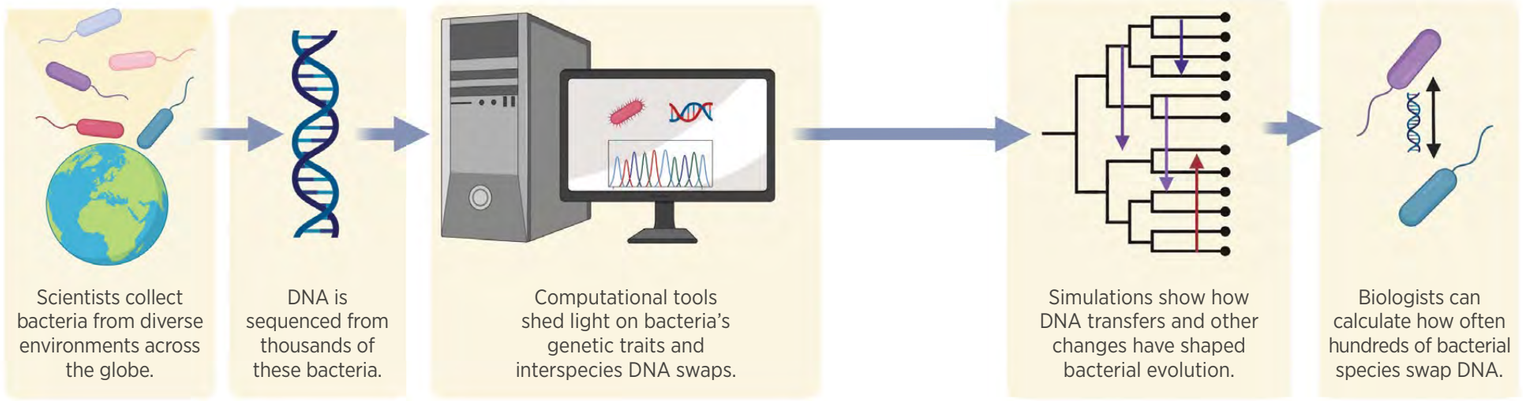
Phylogenetic trees are widely used to model evolution of all species, but they don't implicitly consider bacteria's unique ability to transfer DNA. The trees instead assume that any genetic differences in an individual were due to random mutation over the course of their evolutionary descent. However, they do provide rough frameworks for bacterial diversification without DNA transfer and thus give us an indication of what the ancestral bacterial sequence might have looked like.

Simply put, I can use the predicted ancestral sequence of a species to simulate forward-in-time evolution across a phylogenetic tree while using HPC to specifically apply different rates of DNA transfer in hundreds of thousands of simulations. Each of these simulations generates a population of bacterial genomes that should look identical to the real things – assuming the chosen DNA transfer rate was close to the one the bacteria experienced as they evolved.

Ultimately, by simulating life itself – or at least the bacterial evolution part – I can reconstruct how often genetic transfer events occur and have occurred over eons of bacterial evolution. This will enable me to answer questions about how this process contributes to these organisms' advancement through time, as well as their adaptive abilities in modern day.

What I learn will update evolutionary models, such as the phylogenetic tree, that assume bacteria are truly clonal. What's more, and important for our continued evolution as a species, I and other scientists can use this information to help explain how bacteria develop into organisms that cause disease, spread rapidly and resist antibiotics. In time, this knowledge will prepare researchers to combat these dangerous qualities – making a little *E. coli* in your lettuce not such a big deal.

*Among other reasons.



Scientists analyze massive amounts of bacterial genomes to enable computational simulation of the frequency of DNA exchange, illuminating the microbes' evolution and shedding light on how some become dangerous. *Credit: Ellis Torrance. Generated with BioRender.*

STAR POWER

Fellow Claire Kopenhafer grapples with galaxies and faces off in sword duels.

By Thomas R. O'Donnell

Whether gigantic things or small, Claire Kopenhafer perceives the physics that surround us – sometimes painfully so.

The Michigan State University (MSU) doctoral candidate is a historical European martial arts enthusiast. She and "a bunch of nerds," Kopenhafer says, battle with longswords and other weaponry from the late Middle Ages and Renaissance.

The swords have blunt edges, and the fighters wear safety gear. Nonetheless, accidents happen.

Early in 2020, Kopenhafer was dueling with a partner whose sword had no rubber tip. It slipped under her glove and stabbed her in the hand.

Kopenhafer, who has recovered, views the episode with a physicist's eye. "The design of a sword is to focus all the force onto a point, and if you don't have anything to redistribute that" it can harm competitors. Fortunately, such incidents are rare, and she usually leaves matches with only bruises.

In her studies, Kopenhafer moves from fine points to vast astronomical bodies. With advisor Brian O'Shea, she creates high-performance computing simulations to better understand star formation, a key source of matter throughout the universe.

O'Shea describes Kopenhafer as "really interested in both the astrophysics and the computational aspects. That's fairly rare." In fact, Kopenhafer is seeking dual doctorates in astrophysics and in computational mathematics, science and engineering.

Growing up near MSU's East Lansing campus gave Kopenhafer opportunities to satisfy her science interests. She leaned toward engineering until a nuclear science summer camp introduced her to the fascinating world of physics.

Fast forward to her freshman year. At a meet-your-professors event, Kopenhafer reintroduced herself to O'Shea, a camp instructor. She later joined his group as an undergraduate research assistant and never left.

Credit: Derrick Turner/Michigan State University.

Her project then revolved around data from an instrument that captures the visible light spectra from multiple locations on astronomical objects. She devised a computational tool to produce mock observations – datasets that show what a simulated object would look like if seen with real-life astronomical instruments.

Until then, Kopenhafer hadn't considered astrophysics research. "I always thought it was just telescopes and observations. But there was this whole other side that was computers and simulations. I thought that was really cool."

Now the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient studies the circumgalactic medium (CGM) – a gas halo that surrounds a galaxy, along with invisible dark matter whose gravity helps hold it all together. Recent observations have made the CGM accessible to researchers, Kopenhafer says, providing "a wealth of opportunities to potentially address some of the issues we've always known."

One of them: what controls star formation. Calculations say galaxies should convert gas in and around them into stars more efficiently than observations indicate. "There's some sort of self-regulation," O'Shea says. If there wasn't, star formation "would be all over the place."

Gravity pulls gas from the hot CGM into the galaxy, where it condenses and binds into potential star nurseries. Researchers think negative feedback, energy that pushes against cooling, slows this cycle. It may come from supernovae – exploding stars – or from the black hole at the galaxy's center, which emits radiation that energizes the CGM.

Researchers think feedback pushes gas into the CGM. Much as rising clouds produce rain, the gas cools and falls back into the galaxy in what astrophysicists call the precipitation theory of star-formation regulation.

"You keep this cycle going of droplets falling in, fueling star formation," Kopenhafer says, while feedback pushes material out. At some point, the energy drives matter too far away to precipitate, and star formation slows.

The theory is well developed analytically, but Kopenhafer plans to modify a cosmological code to model star-formation physics in an evolving galaxy.

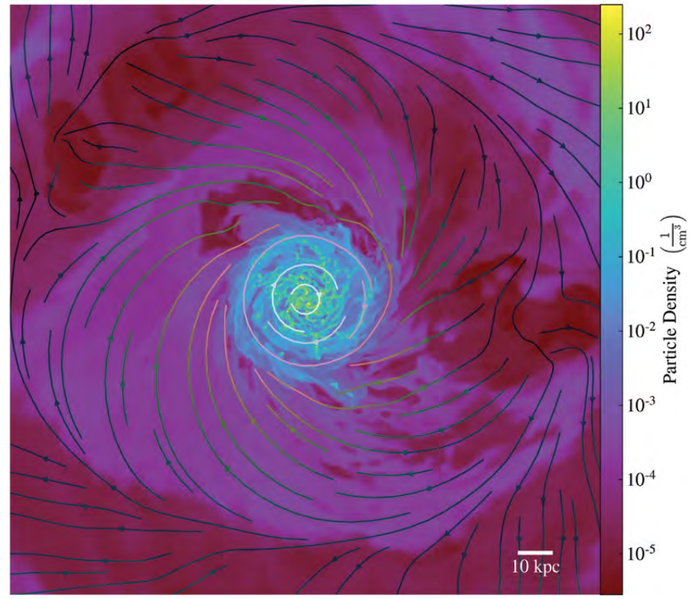
Simulating an idealized galaxy lets Kopenhafer perform numerical laboratory experiments, O'Shea says. "She can tweak the parameters. She can change how the feedback occurs, how the CGM is distributed," helping explain the process and improve the physics in large cosmology simulations.

Kopenhafer also hopes to make galaxy-evolution and star-formation models more accurate. Feedback happens on scales too small to capture in full galaxy simulations, but it still affects their output. Researchers tune models to match statistics from observations instead of calculating the fundamental physics.

But the model may miss turbulence, cosmic rays, magnetic fields and possibly plasma effects, Kopenhafer says. She adds individual elements to the code to improve its physics and reduce parameter tuning – a process that will stretch beyond her Ph.D.

Tuning parameters also makes the model's output less precise. Kopenhafer plans to use uncertainty quantification (UQ) calculations to characterize how much astrophysicists can trust the results. Working with an undergraduate researcher, she'll adjust selected parameters and calculate the impact on uncertainty.

Kopenhafer aimed to dig into UQ during her 2019 practicum at Sandia National Laboratories in New Mexico. The lab houses the Z machine, a giant device that produces massive, brief electric jolts that generate intense magnetic fields, pressures and radiation.



A slice through the midplane of a simulated galaxy with colors representing gas density, increasing from less in deep purple to more in yellow, and lines tracking gas flow velocity. Brighter colors indicate higher speeds. The scale bar signifies size in thousands of parsecs. Each parsec is about 3.26 light years, or more than 19 trillion miles. *Credit: Claire Kopenhafer.*

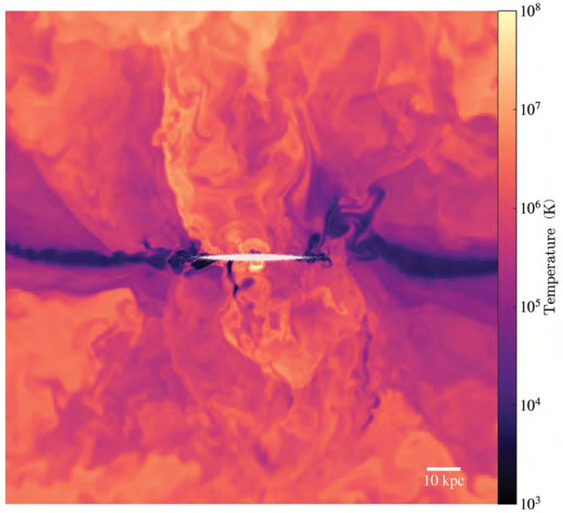
ALGORITHMS GO DEEP

University of Washington fellow **Robert Baraldi** loves exploring math, so, with Aleksandr Aravkin, he dug into geophysics, a field with interesting issues requiring novel algorithms. Baraldi often deals with inverse problems, which start with observations such as images and seek the conditions that produced them. In one project, Aravkin's group works with earthquake sensor data and other information from UW geophysicists who map molten rock flow beneath Mount St. Helens. Baraldi helped develop an algorithm that combines readings from multiple instruments with physics knowledge to boost accuracy from a particular sensor.

TWOFOLD FOCUS

Matthew Carbone works on condensed matter physics theory at Columbia University while maintaining machine-learning projects from his 2018 Brookhaven National Laboratory practicum. With David Reichman at Columbia, Carbone examines the theory behind excitations in transition metal dichalcogenides, semiconducting materials that form atomically thin layers and could be used in many applications. At Brookhaven, Carbone and Shinjae Yoo worked with colleagues to train a machine-learning algorithm on X-ray absorption spectroscopy (XAS) data. The method then was able to predict geometries of absorbing sites from new XAS data, giving researchers a tool to quickly translate results into information about an absorbing molecule and how its geometry changes, for example, during a chemical reaction.

In one Z experiment, researchers convert combinations of materials into plasmas of different densities and take X-ray images of how they mix. "Our models of how that works are highly incomplete," says Kris Beckwith, a Sandia physicist who worked with Kopenhafer. As Z's energy knocks electrons from the materials' atoms, the plasmas become coupled. Simulations "break down, and so we're in the dark as to how the physics for that works."



A simulated galaxy cut in half, showing hot outflowing and cold inflowing gas. Colors represent increasing temperature in degrees Kelvin. Darker colors are cooler. The galaxy disk is seen edge-on at the center, with each star marked as a pale dot. The scale bar signifies size in thousands of parsecs. *Credit: Claire Kopenhafer.*

Researchers took two X-ray radiographs of the experiment at different times to track how the plasmas diffuse into each other. Simulations suggested the interface would take on a dip shape that would broaden and become shallower. Physicists were surprised when the dip in the interface narrowed and deepened.

Kopenhafer translated simulation data into synthetic radiographs – mockups of the ones captured in live experiments – by adapting an analytical tool called yt. With Beckwith, she chose parameters focusing on electric fields and ionization states.

The synthetic radiographs indicated that the researchers needed to probe the plasmas in new ways and at different times to better understand how they mix. Kopenhafer's results "forced us to take a step back and think more deeply about how we were conducting the experiments," Beckwith says. "We learned things from her work that we weren't expecting."

The practicum ended before Kopenhafer could perform UQ calculations, and the pandemic blocked plans for her to return. Nonetheless, Beckwith says, "what we did get was really influential."

The experience gave Kopenhafer a deeper understanding of plasma physics, which she hopes to work into her star-formation model. "That sort of desire would not have happened if I hadn't done my practicum."

Kopenhafer plans to join academia after graduation. Besides mentoring an undergraduate, she's joined an MSU version of the American Physical Society's IDEA (Inclusion, Diversity and Equity Alliance), which fosters acceptance of underrepresented populations in physics departments.

And she still swings a blade. "Swords are cool," Kopenhafer says, but she also appreciates the hobby's physical nature. "I've grown a lot of awareness of how my body moves," especially sword fighting's "dancer-esque" aspects. "They remind me of ballet, but very grounded and practical."

TAKING QUANTUM CONTROL

Theoretical research is revealing new ways to simulate the quantum mechanical control of chemical systems – and contributing to the first DOE quantum computers.

By Jacob Berkowitz

As a senior chemical engineering major at Arizona State University, Alicia Magann methodically searched the internet for just the right graduate program. She'd come to love control engineering, finding ways to create desired behaviors in a system by applying the right regulators. The Phoenix native also became fascinated with quantum mechanics, the strange ways matter and energy act at the scale of atoms and molecules.

Quantum mechanics is famous for Heisenberg's uncertainty principle, so the two fields hardly seemed like a good mix. That is until Magann's search led her to Princeton University's Herschel Rabitz, a pioneer in the field of quantum control theory. "It was really the perfect combination," says Magann, who contacted Rabitz and arranged a visit to New Jersey. "I remember being pretty nervous before the meeting, but he really welcomed my enthusiasm, and we had this great conversation."

Now, four years on in the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) with Rabitz as her advisor, she's working to push the frontier in simulating quantum control. The research has led Magann to an unexpected destination: advancing DOE's leadership in the current grand challenge of quantum control, the decades-long dream of building and using quantum computers.

Since his landmark 1992 paper "Teaching Lasers to Control Molecules," Rabitz's lab has been a world leader in developing the theory, algorithms and experiments to control the quantum dynamics of chemical reactions. He uses ultra-fast laser pulses to create specific quantum states in molecules and thus function as so-called photonic reagents that direct chemical reactions.

Credit: Alicia Magann.

FORETELLING MATERIAL PROPERTIES

Harvard University's **Jennifer Coulter** models materials' electronic structures to understand how well they conduct heat or electricity, speeding the design of compounds for new applications. Coulter has studied single-atom-thick materials such as graphene and examined how bending or straining a material changes its electrical conductivity. To streamline simulations, she and her colleagues released Phoebe, high-performance computing (HPC) software to predict transport in materials by accounting for microscopic scattering properties of electrons and phonons (crystal lattice vibrations). The package can boost efficiency on several computer architectures, including those with graphics processing units (GPUs).

DEMANDING PROBLEM

At the University of Texas at Austin, **Morgan Kelley** studies how chemical companies can optimize production to cut energy use and operating costs. "If we can predict what our electricity prices will be, we can design a plant schedule so that when electricity is cheap, they overproduce" chemicals, Kelley says. Then they can store those fuels and distribute them when power demand and prices peak. With Michael Baldea and Ross Baldick, she models air-separation units, which segregate oxygen, nitrogen and argon from the atmosphere. She reduced the simulation, omitting low-impact factors, and reframed the problem, cutting runtime from up to 97 hours to under a minute. Results showed her demand response methods could cut electricity use by up to 15 percent.

"Alicia had a steep hill to climb to learn advanced aspects of quantum mechanics, get herself on the frontier edge of it and then come up with a challenging problem. But she's an extremely driven person," says Rabitz, whose 12-person lab thrives on a mix of experimental and theoretical researchers.

Although lab experiments have demonstrated many aspects of the quantum control of chemical reactions, modeling these systems via computers – "one of the original dreams in this field," Rabitz says – remains elusive. Thus, unlike the virtual prototyping of airplanes, for example, researchers can't yet use computers to design ideal quantum controls, including for quantum computers.

Magann's thesis research is aimed at helping change this. "I find ways to make quantum control simulations easier and cheaper to do," she says.

A central challenge is that "with quantum control calculations you need to simulate the behavior of a quantum system," Magann says of this self-referential problem. Whereas conventional computational resources, such as speed and memory, scale arithmetically (two processors can do twice the work of one), quantum systems experience the curse of dimensionality – the computational resources needed to represent them scale exponentially. As a result, fully capturing the quantum interactions of just a few particles is too computationally demanding for even DOE supercomputers, among the world's most powerful.

Computational scientists overcome this by making approximations. Magann's early Ph.D. research demonstrated that a technique called the time-dependent Hartree approximation could simulate the optimal quantum control of weakly interacting molecular rotors. These molecules can only rotate, in contrast to also moving in other natural ways, such as stretching and twisting.

"The approximation makes a huge difference," she says. "I can do calculations that are absolutely not possible without it."

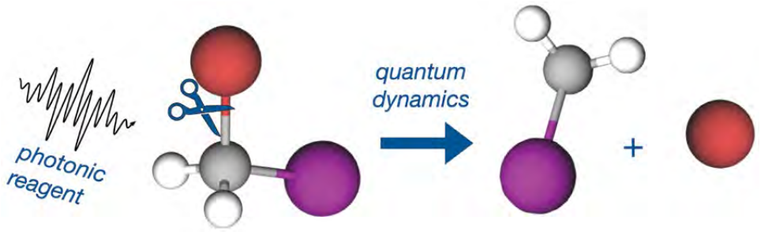
Magann extended this exploration to accelerating the task of designing the controls – the lasers – resuscitating a technique that originated in control engineering: quantum tracking control.

"Tracking control has a long history," Rabitz says. "Its appeal is that as a designer you write down a track that you want a quantum observable to follow and then you invert the track mathematically to find the control. It looks superficially extremely easy, but this has bedeviled the control community."

That's because until now equations used in this quantum control technique experienced singularities: At times they resulted in infinities, "the killer of tracking control," Magann says. But in a 2018 *Physical Review A* paper, she demonstrated equations to effectively apply quantum tracking control to molecular rotors. "This opens up a new application area where quantum tracking control can be used to accelerate the design of quantum controls."

In another co-authored paper with Rabitz and Tulane University researchers, Magann showed that this tracking control technique could design a laser pulse that enhances the distinguishability of chemical mixture components.

As she became more familiar with the field, Magann realized that to ideally optimize quantum control simulations, she'd have to explore a frontier technology that itself relies on quantum control. "I started hearing more and more about quantum computers."



Quantum control theory originally was inspired by the goal of selectively manipulating chemical reactions at the smallest scales. In this example, a super-short laser pulse (black squiggle) serves as a photonic reagent that breaks a selected chemical bond and steers a reaction toward a set of desired products. Today, researchers apply quantum control in chemistry, biology, materials science and quantum computing. *Credit: Alicia Magann.*

Rabitz knew the ideal place for her to pursue that subject. His former Ph.D. student Matthew Grace is a quantum control and quantum information researcher in Sandia National Laboratories' Extreme-Scale Data Science and Analytics group. He became Magann's first practicum mentor.

Grace connected her to a colleague, Mohan Sarovar, an engineer and physicist who leads Sandia's Optimization, Verification and Engineered Reliability project as part of the lab's ambitious effort to create a quantum computing test bed. Launched in 2018, the program aims to develop techniques and tools that will make near-term quantum computers, so-called noisy intermediate-scale quantum (NISQ) computers, for practical tasks.

With Grace and Sarovar, Magann mapped out her idea to develop simulation methods for quantum control that leverage quantum computers' power. "That turned out to be an insightful observation," Sarovar says. The practicum research led to a joint paper with Rabitz and her Sandia mentors on using a hybrid quantum-conventional computer to simulate quantum molecular dynamics and control.

The research was so promising that Sarovar hired Magann as a year-round, part-time remote intern, encouraging her to attend conferences and meetings and to learn and scour the field for key, tractable problems. As a result, during her second Sandia practicum (a virtual one due to COVID-19) Magann devised a quantum algorithm for optimization, such as complex delivery routing and timing problems.

Discrete optimizations are "very difficult problems, and she developed a new approach for doing these optimizations that looks like it might be suitable for near-term NISQ quantum computers," says Sarovar, who's interested in identifying tasks best suited to a NISQ machine.

From that initial drive to combine control engineering and quantum mechanics, Magann knows she's serendipitously captured a powerful research wave. She's working hard to contribute, having presented several talks and posters since 2019, including an invited talk in the Quantum Control of Light and Matter Gordon Research Conference.

Determined to avoid theoretical dead ends, she knows that, paradoxically, she has to help build a quantum computer to find out just how good her quantum control algorithms really are.

Says Magann, "We need to keep the momentum going, to realize the full potential of quantum computing."

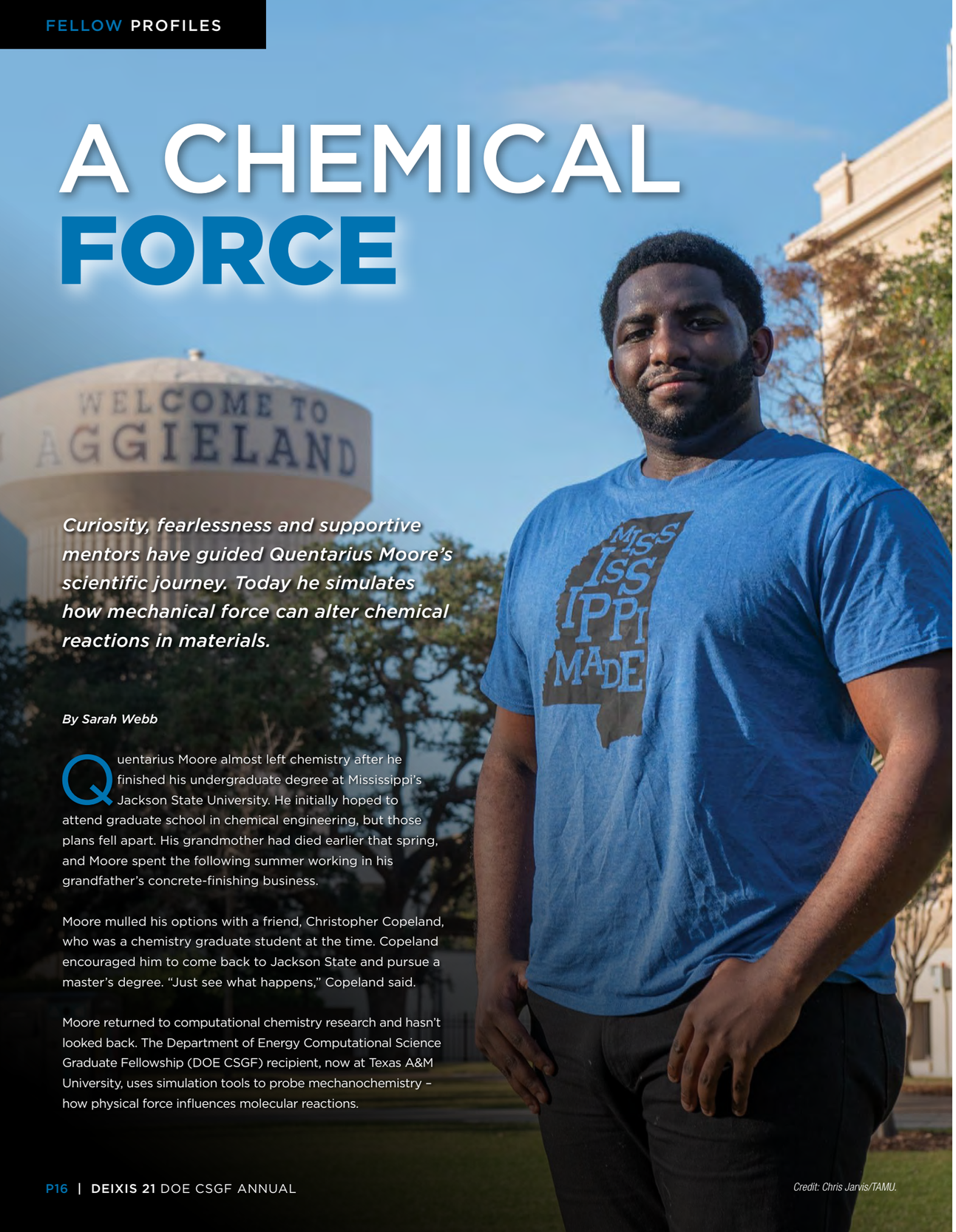
CREATURE RESEARCHER

Kari Norman loved the outdoors side of ecology research, but a semester at the University of Helsinki turned her to computational methods. With Carl Boettiger at the University of California, Berkeley, she improves ecological measurements over time. They focus on functional diversity, which analyzes how species vary and interact by summarizing each community in a single number describing physical traits, such as a bird's beak length, that are vital to their ecological role. Norman researches how much functional diversity she would expect to see by chance. She repeatedly samples the species pool, calculates functional diversity for each and uses statistics to correct the observations. Her models can help direct conservation efforts.

MOLECULAR MATH

Anya Katsevich aims to develop theoretical mathematical methods, but her projects often have practical uses. One of them, with Afonso Bandeira, her New York University advisor, relates to cryogenic electron microscopy, a means of imaging molecules at the atomic level. Meaningless information clouds the pictures, and the molecules may lie in unknown orientations. The data emerge as a distribution, a mixture of signals of interest that obscure each other, and researchers need to find the most likely version. Katsevich and Bandeira use data about the distributions to calculate a function that gauges how close guesses are to the real value. Katsevich uses expectation maximization to augment this function.

A CHEMICAL FORCE



Curiosity, fearlessness and supportive mentors have guided Quentarius Moore's scientific journey. Today he simulates how mechanical force can alter chemical reactions in materials.

By Sarah Webb

Quentarius Moore almost left chemistry after he finished his undergraduate degree at Mississippi's Jackson State University. He initially hoped to attend graduate school in chemical engineering, but those plans fell apart. His grandmother had died earlier that spring, and Moore spent the following summer working in his grandfather's concrete-finishing business.

Moore mulled his options with a friend, Christopher Copeland, who was a chemistry graduate student at the time. Copeland encouraged him to come back to Jackson State and pursue a master's degree. "Just see what happens," Copeland said.

Moore returned to computational chemistry research and hasn't looked back. The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient, now at Texas A&M University, uses simulation tools to probe mechanochemistry – how physical force influences molecular reactions.

Credit: Chris Jarvis/TAMU.

His science interests date back to watching *Mythbusters* on the Discovery Channel as a teenager. Moore liked the puzzle of mathematics and chemistry and seeing how everyday processes work. "I wanted something that was quintessentially hard," he says. "I liked the challenge of it."

As a freshman, Moore joined a peer-mentoring program that matched him with a junior and a graduate student who worked in computational chemistry and gave Moore his first taste of the subject. Moore also tried experimental research on nanoparticles. In 2014, he grew two-dimensional chemical films while in a National Science Foundation summer research program at the University of Alabama. His advisor, Hung-Ta Wang, also urged him to go to graduate school.

Two years later, that summer research project helped Moore connect with his future Ph.D. advisor, James Batteas. They met at a conference where Moore described listening to Bruno Mars while coaxing molybdenum disulfide (MoS_2) films to grow in Wang's lab. After the talk, Batteas and Moore discussed music, mutual science interests and Moore's future. Batteas and his colleagues were launching a project on MoS_2, and he thought Moore's computational expertise would be a key asset. "We have all these big ideas," Batteas told Moore, "and I think you could be the right person for this." Moore visited Texas A&M for several weeks that summer and explored research in Batteas' group before applying to the Ph.D. program in 2017.

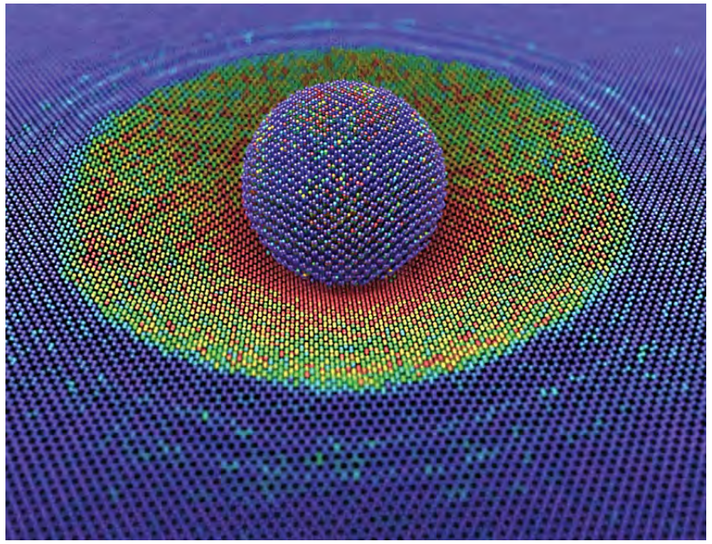
Chemists have carefully studied how light, heat and electricity affect chemical reactions, Moore says. But "we don't understand how force alters reaction energy and pathways," factors that are important as researchers consider solid lubricants. The atomic and nanoscale jagged edges on these surfaces can cause wear and tear or make them vulnerable to chemical reactions such as oxidation. The research also has implications for devices that must function in extreme environments. "If you shoot a satellite into space and you want something to actuate and it doesn't actuate, that's a big problem."

Moore studies two-dimensional systems such as graphene – carbon in sheet form. Its surface is known for being relatively inert, but graphene lubricants demonstrate reactivity under wear and tear. Defects and pokes that bend the surface out of plane can cause the carbon atoms to react with free-radical molecules.

The MoS_2 work includes computational materials scientists at Sandia National Laboratories in New Mexico, where Moore has completed two practicums with Michael Chandross. MoS_2 can work well as a solid lubricant, Chandross says, but exposing it to water and air can drastically increase friction. Composite coatings can help overcome this problem, but so far it's unclear how and why they work, which limits their use. So the team's focus is helping researchers understand these chemical details to help build better lubricants.

When Moore arrived at Texas A&M, he had used only density functional theory (DFT), a computationally intensive tool that can become too demanding when simulating a large number of atoms. Through his Sandia research, he learned a molecular dynamics method, LAMMPS, that lets researchers probe larger periodic systems such as graphene and MoS_2 while including approximations. More recently he's incorporated plane-wave DFT, a technique that offers advantages of both approaches, into his research.

Moore is the lone computational chemist in Batteas' group, where other researchers use atomic-scale microscopes to probe chemical surfaces. Moore plans to do experiments, too, which would provide new insights for his computational work. For example, he thinks that artificial intelligence methods offer an opportunity to glean new details from the Batteas group's extensive experimental datasets that follow chemical reactions occurring on surfaces. The group recently received a



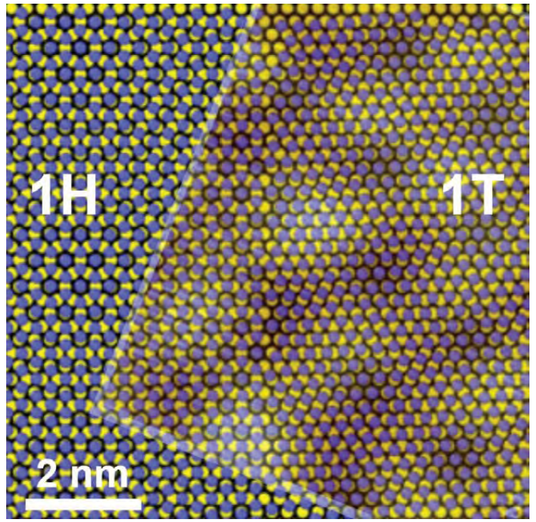
A molecular dynamics simulation snapshot in which a 6-nanometer diamond particle (central sphere) indents a graphene sheet. Red areas on the surface show greater downward mechanical stress than green areas. Force can change graphene and other materials, increasing their chemical reactivity. *Credit: Quentarius Moore.*

CLEVER CLIMATE

Benjamin Toms' Lawrence Berkeley National Laboratory practicum with Karthik Kashinath and Prabhat inspired him to refocus his Ph.D. research, with Colorado State University's Elizabeth Barnes, to machine learning for climate predictions. They combined physical theories about how ocean patterns affect precipitation and temperature and incorporated them into neural networks. "Then we try to understand what the neural network has learned so we can learn something new about the system itself," Toms says. He and his colleagues believe they can predict near-term climate, up to several years ahead. He's launched a company to build models for that purpose.

(QU)BIT PLAYER

Annie Wei's Massachusetts Institute of Technology (MIT) quantum algorithm research unites her interests in computer science and physics. Her methods are designed to run on quantum computers that use qubits, computer bit equivalents that also can represent both one and zero simultaneously, boosting computational power and efficiency. But today's quantum computers are small and error-prone, so Wei often uses HPC systems to simulate quantum algorithms. She's built techniques to solve several problems, including analyzing mountains of data from giant particle accelerators. Wei also creates methods with both classical and quantum-mechanical parts to employ the best features of each kind of computer.



Molybdenum disulfide can form sheets with two distinct crystal patterns: 1H, which acts like a metal; and 1T, which acts like a semiconductor. Combining these two in a single device could help with the design of new electronic devices. This image overlays Quentarius Moore's calculations of these structures on microscope images from the Batteas group. *Credit: Quentarius Moore and Michael Chandross.*

$1.8 million National Science Foundation grant to found a center, with the University of California, Merced, the University of Pennsylvania and others, for research, outreach and entrepreneurship focused on mechanochemistry. Moore is a key link within the center's computational work, Batteas notes, collaborating with researchers at other institutions to set up simulations.

"Quentarius is one of the hardest-working Ph.D. students that I've ever had," Batteas says, but he remains relaxed, even when working through stressful situations. "He's a really calming force in the lab." Moore also injects fun into what could be routine tasks, such as organizing the group's regular research meetings. Recently he assigned lab members to two teams and modeled the meeting structure after the popular video game *Among Us*. "Nothing with him is boring," Batteas says. Chandross appreciates Moore's independence, attention to detail and grasp of the big picture. "He's eager to learn and is also unafraid."

Moore has helped with Texas A&M's annual chemistry open house, and he plans to continue that outreach while building resources for chemistry instruction back in Mississippi. He had few childhood science role models, he says, and wants future generations to see the full range of such career opportunities.

Moore's longtime interest in photography and videography could support those projects. While at Jackson State, he freelanced for ESPN, providing technical support for Division I college football games in Alabama, Mississippi and Louisiana and at Memphis bowl games. Much of the work involved running along the sidelines and supporting camera operators as they got action shots. He reprised that role for a 2019 Texas A&M game.

Chandross has arranged for Moore to become a Sandia intern, allowing him to split his time between New Mexico and Texas until he finishes his degree in 2022. Moore is exploring a range of research career options. The DOE CSGF program of study was difficult yet rewarding and increased his interest in computer graphics, visualization and statistical techniques, he says. "The CSGF hasn't narrowed my career choices but instead blossomed my interests to be more than I ever expected."

COMBATING CLIMATE CHANGE

A fellow combines public policy credentials with artificial intelligence expertise to optimize power systems and reduce greenhouse gas emissions.

By Sarah Webb

Since high school, Priya Donti has wanted to work on climate change solutions. First she thought of developing new solar panels and pursued chemical engineering at Harvey Mudd College in Claremont, California. But she soon discovered she enjoyed computer science more and struggled to combine that interest with a project that would clearly affect climate change.

Then a computer science professor sent her an article about how artificial intelligence could help incorporate renewable energy sources into the power grid and reduce greenhouse gas emissions. The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient has worked on these problems ever since.

Donti has pursued a rare dual Ph.D. in computer science and public policy at Carnegie Mellon University in Pittsburgh. That choice "requires a lot of initiative," says computer science professor Zico Kolter, one of Donti's advisors, who says she stands out for her persistence, strong technical skills and desire to effect change. And others are noticing: She was named to *MIT Technology Review's* 2021 list of Innovators Under 35.

Donti grew up in Massachusetts and was interested in everything from poetry to math and science. But the desire to improve human wellbeing shaped her path from an early age. Regular visits to India, her parents' birthplace, helped her recognize her own opportunities and the needs of disadvantaged communities around the world. In India, "you often see a stark contrast of real poverty juxtaposed against real wealth."

Donti's high school biology teacher set aside two weeks for a sustainability unit. As the class discussed climate change, she learned how this crisis would disproportionately harm the world's most marginalized populations.

Donti graduated from Harvey Mudd in 2015 and embarked on a yearlong Thomas J. Watson Fellowship. She traveled to five

Credit: Carnegie Mellon University.

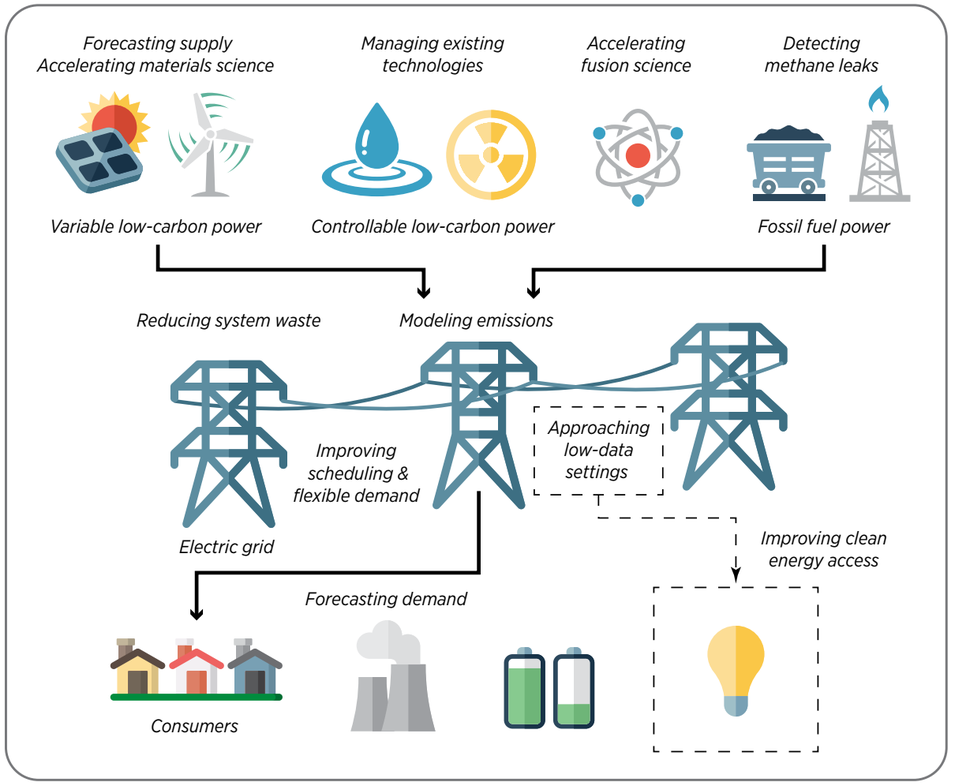
countries – Germany, India, South Korea, Japan and Chile – to learn how each was modernizing its electrical system. Donti conducted more than a hundred interviews. When she asked subjects to define smart grid, "I got a hundred pretty different answers." She saw how social and political factors shaped the way countries pursue modernization. For example, Germany pushed to move grids from private to public ownership; India did the opposite. The experience strengthened her interest in the technical and public policy challenges of using renewable energy to combat climate change.

In some of her research, Donti has tried to forecast renewable energy supplies and electricity demands so that grid operators can continually balance production and consumption. There's a built-in uncertainty to decisions that dictate power demand, she notes, and the ebb and flow of renewable energy further complicates matters. "The amount of solar and wind power you get depends on what the weather is. And that's not something you can control ahead of time."

Donti also must consider the context in which her machine-learning algorithms are used. For instance, AI researchers want their forecasts to be as accurate as possible. But accuracy isn't always the most important factor in many real-world settings, Donti says, particularly in complex situations where a forecast sometimes includes mistakes. "You ultimately care about whether the power-system operator was able to make a good decision on the basis of your forecast."

A key challenge: navigating the various research communities' different cultures. Machine-learning practitioners like to move fast and seeing where systems fall apart can be a natural part of the research process. But power grid managers' first priority is keeping the lights on; their aim is to build systems that can't break. Donti also grapples with the tension that can arise between academic productivity and societal impact. "Papers are great, but in the end, I really want the things I'm developing to help us actually reduce greenhouse gas emissions."

During her 2018 National Renewable Energy Laboratory (NREL) practicum, Donti wrote code to assess and improve the power grid so it better integrates solar energy. The consumer-facing part of the system, the distribution grid, traditionally has been a one-way street, delivering electricity from power plants to homes and businesses. But rooftop solar panels complicate the system, and power engineers must grasp how to best monitor and manage the resulting bidirectional flow.



Machine learning can help to reduce greenhouse gas emissions from electrical systems through a variety of strategies, such as forecasting energy supply and demand, managing energy sources, reducing system waste and accelerating the discovery of new clean energy technologies. *Credit: Rolnick, David, et al. "Tackling climate change with machine learning." arXiv preprint arXiv:1906.05433 (2019).*

The NREL team had struggled with this project, but Donti was eager to take it on, says Andrey Bernstein, NREL's group manager of Energy Systems Control and Optimization. He says she solved the team's issues, improved the algorithms and was a key contributor to a resulting paper in *IEEE Transactions on Smart Grid*.

Bernstein praised Donti's leadership, enthusiasm and depth of knowledge. "She was passionate about technical aspects as well as the overall topic, renewable energy and climate change questions." Her theoretical and mathematical skills were impressive, he adds, particularly when considering her work's broad, interdisciplinary scope.

Donti also co-chairs Climate Change AI, an international volunteer community of a few thousand machine-learning researchers addressing climate change. The group launched in 2018 after a luncheon at NeurIPS, a machine-learning conference. Key members, including DOE CSGF alumna Kelly Kochanski (featured on page 28), kept in touch through a Slack discussion group. Donti wrote the electrical grid section and co-presented the report at the United Nations Climate Change Conference in Madrid that December. The group followed up with workshops at top machine-learning conferences, assembled online resources and a discussion forum for broader community engagement. They also are creating further educational and funding programs. "It's a really awesome and dynamic group of people who really care about tackling climate change," Donti says.

In most respects, collaborating with Donti is more like working with a CMU junior faculty member than with a graduate student, Kolter says. She's worked hard to build her own research agenda, developing and engaging with new ideas and even raising money for large-scale projects.

"It's really a full-time job, just her work with Climate Change AI" to spread awareness about the impact researchers can have on these issues, Kolter says. "And that's in addition to her work on the computer science side of things."

Donti also donates her time and computing skills to improve Pittsburgh. She and a few other CMU graduate students have launched Tech4Society, which encourages technically skilled students to volunteer with community organizations. Members have helped with affordable housing and public transportation and offered cybersecurity clinics for activists.

Not least, Donti has worked on predictive-policing accountability – exposing inherent structural biases in the computational tools used to forecast where crimes occur and who commits them. Her group helped stop a secret predictive-policing test that Pittsburgh officials were conducting. As a result, city and county councils are weighing regulating such techniques and other controversial law-enforcement tools like facial recognition.

Donti plans to finish her Ph.D. in 2022 and is open to working on climate change through research, entrepreneurship, public policy or a mix of those options. "I am really looking for things that combine intellectual challenge with real world, on-the-ground impact."

UNPACKING THE BIG BANG

At the University of Illinois at Urbana-Champaign **Zachary Weiner** models the fleeting events preceding the Big Bang, when the universe exploded and swelled over the course of 13.8 billion years. To account for the model's flaws, physicists postulated that inflation, accelerated expansion spanning just 10^{-34} seconds, enlarged the universe first and resulted in nearly identical temperatures throughout the cosmos. But inflation has no way to produce the particles that comprise everything. With advisor Peter Adshead, Weiner models how the homogeneous energy driving inflation fueled particle production that reheated the universe, leading to synthesis of light elements. He studies preheating, an initial phase of violent particle creation that would produce a background of gravitational waves. Weiner's codes predict how spectra of those waves would appear, providing information that constrains early-universe models.

IONIC SITUATION

For **Malia Wenny**, part of chemistry's fun comes from the interplay between laboratory experiments and computational tools. With Harvard chemist Jarad Mason, she's studied ionic liquids, fluids that are made of charged particles and do not evaporate. She concentrates on their molecular structure and capacity to absorb molecules such as oxygen, which could make them useful as artificial blood and for other applications. Wenny works with Boris Kozinsky to simulate these materials' structures. Meanwhile, her 2019 Argonne National Laboratory practicum led to a collaboration to measure the compressibility of ionic liquids with small-angle X-ray scattering at the lab's Advanced Photon Source.

Longer versions and additional profiles are available:

krellinst.org/csgf/fellows/fellow-reflections

OPTIMIZED FOR DISCOVERY

A computational mathematician finds a national lab an ideal place for a highly collaborative career to grow.

Credit: Mark Lopez/ Argonne National Laboratory.

By Jacob Berkowitz

Stefan Wild came to Argonne National Laboratory in the summer of 2006 for what was to be a four-month summer practicum. He's never really left.

Wild discovered a highly collaborative, open-science research environment that's optimal for him. It's fostered Wild's dynamic career, including a 2020 DOE Early Career Research Program award.

"I would never have predicted then that I'd be at Argonne for more than a decade, and the only reason I'm here is because of my practicum," says Wild, a 2005-2008 Department of Energy Computational Science Graduate Fellowship (DOE CSGF) alumnus who completed his Ph.D. in operations research at Cornell University.

Wild's scientific specialty is developing mathematical optimization techniques to improve how models and simulations perform on high-performance computers. On his practicum he developed an important algorithmic addition to TAO, the lab's toolkit for advanced optimization, and on graduation was hired as an Argonne Director's Postdoctoral Fellow. For the past dozen years Wild has steadily risen through the scientific and management ranks to his current position directing the Laboratory for Applied Mathematics, Numerical Software and Statistics (LANS).

Wild says Argonne computing's flat organizational structure has been perfect for his professional growth. He oversees about 60 scientists and engineers but still spends about three-quarters of his time on his research. The interdisciplinary team-based culture helps Wild find intriguing ideas, whether while playing on Argonne's Ultimate Frisbee club (which has led to novel lab collaborations) or leading brainstorming meetings of LANS' dozen-member senior research council.

This environment also nurtures Wild's math-with-a-mission research approach. "What really attracts me is doing math to advance the basic sciences," says Wild, who in late 2020 was elected chair of the Society for Industrial and Applied Mathematics Activity Group on Computational Science and Engineering.

His approach has led to a remarkably wide range of collaborations, from using computational techniques to improve cancer research to automating production processes for novel nanomaterials.

An early collaboration with practicum advisor Jorge Moré led to Wild's focus on optimization for scientific machine learning, a core artificial intelligence sub-technology. In 2011 they developed POUNDERS, an optimization code that dramatically reduces the time required to calibrate atomic nuclei simulations on supercomputers, as part of DOE's cross-lab Universal Nuclear Energy Density Functional SciDAC (Scientific Discovery through Advanced Computing) collaboration. "What used to take physicists a year could now be done in a couple hours," Wild says.

machine-learning efforts, including in preparation for one of the first exascale supercomputers, Aurora, developed with AI in mind and coming to Argonne in 2022. Near-term noisy intermediate-scale quantum computers DOE labs are pioneering also are ripe for black box optimization, Wild says.

Asked if managing the $2.5 million early-career award feels onerous, Wild laughed over Skype from his pandemic-period home office.

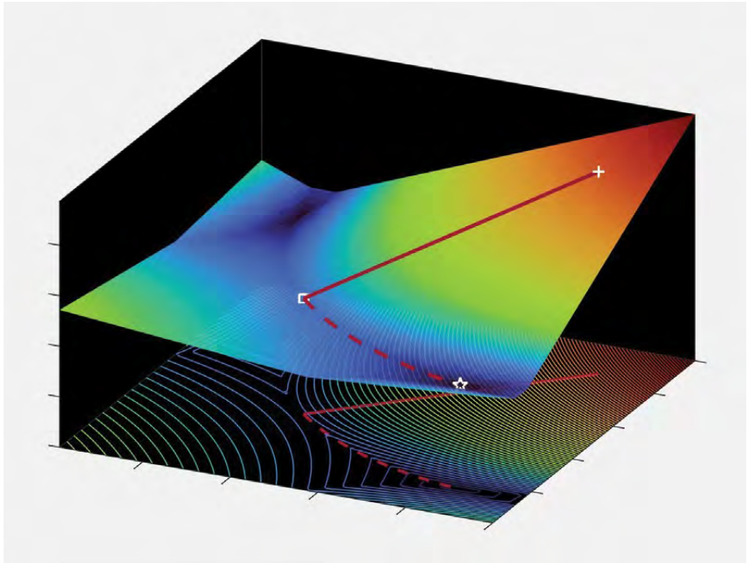
'It's like a Magic 8 Ball: You ask it a question, and you shake it up, and then it gives you an answer.'

Now with his DOE early-career award he's focused on a five-year effort to tackle one of the gnarliest optimization challenges: derivative-free optimization. In classical mathematical methods, a system is optimized by precisely modeling the effect an input variable has on the system and tuning the variable to get a desired outcome. For example, the optimization could explore the ideal number of running processors to minimize the energy a supercomputer uses for a simulation. However, researchers use derivative-free, or black-box, optimizations for systems that are so complex that they don't have all the underlying mathematical equations to describe them.

"The only thing that you know about a black-box system is what you get back from evaluating it," explains Wild, who with Argonne colleagues co-wrote a 2019 *Acta Numerica* cover-story review of state-of-the-art derivative-free optimization methods. "It's like a Magic 8 Ball: You ask it a question, and you shake it up, and then it gives you an answer. You learn something about that Magic 8 Ball from that sort of oracle or input-output relationship and use this to optimize the system."

Black-box optimizations are a foundational component of scientific

"That's the fun part," he says. "I get to choose what I work on and expand my group to have postdoctoral researchers and students working with me on these foundational problems. And so, this is really exciting because I get the chance to allow some of my enthusiasm and the fact that I love my job inspire the next generation of researchers."



A back box optimization algorithm can increase a multigrid simulation's efficiency. Seen here: a three-dimensional application of an unoptimized simulation (plus sign) and an improved, faster approach (box). The star indicates a valley, or a computational-energy low point with a shorter simulation run time than possible without the algorithm. *Credit: Stefan Wild.*

Credit: Laura Morton.

GERM WRANGLER

Sarah Richardson's company aims to harness bacteria to benefit humans and the planet.

By Thomas R. O'Donnell

As founder and chief executive of a biotechnology company, Sarah Richardson solicits venture capital, buys lab equipment, coordinates staff – and sometimes gathers chicken droppings.

"There was a month period where I was going around getting chicken poop from various people," says Richardson, a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient from 2007 to 2011. Her firm, MicroByre, aims to identify bacteria that have unique and useful abilities, then "get them to do stuff they were already inclined to do or already doing. We have to help them or encourage them or edit them to do it" profitably.

If all goes well, the company's domesticated microorganisms could produce fertilizers, fuels and drugs or help remediate biological contamination and reduce greenhouse gas levels.

But first MicroByre must find the germs. "It's not the best use of my people's time to drive around" visiting poultry farmers instead of isolating bacteria or writing genetic analysis software – "a lot of stuff I can't do," Richardson says. "I can go charm a lady who has a bunch of chicken poop."

Richardson's staff searched the guano for bacteria that control the growth of other germs in the chicken's gut. The probiotic chemical they secrete also can be used to make adhesives and polymers that would otherwise come from petroleum.

MicroByre paid for the samples to secure its claim to the bacteria as intellectual property. But for the chicken producers, cash was just a side benefit, Richardson says. "Honestly, they're all very nice and excited to be part of something."

MicroByre's biologists and programmers developed procedures to identify and isolate useful bacteria from the multitude found in the manure. The team discovered organisms "we were looking for, and they're doing exactly what we wanted better than we've ever seen."

The company's robotic and computational pipeline gathers information about individual strains: what they do well, how they interact with other organisms, what they consume and what they produce.

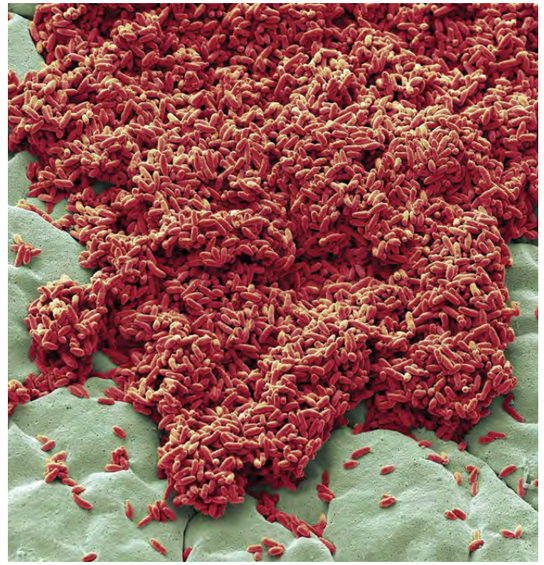
With that knowledge, researchers align bacterial functions with human needs. With an understanding of a bacterium's quirks, MicroByre technicians use various methods, including genome editing, to make a strain easier to grow in a lab or factory and maximize desirable functions or compounds' production.

MicroByre doesn't want to be a biomanufacturer, Richardson says. It will license its customized strains to other firms. MicroByre also may provide its bacteria-wrangling tools to companies so they can create or improve their biomanufacturing processes.

For now, "we are just flat-out grinding on data," with robots sequencing DNA and technicians sifting the results. DNA sequences aren't useful until they're labeled, Richardson says, but MicroByre is producing information needed to model organism function and expects to tap high-performance computing (HPC) systems at some point.

Richardson didn't yearn to be an entrepreneur when she finished her Ph.D. at the Johns Hopkins University School of Medicine in 2011. Her research focused on synthetic biology – essentially redesigning a yeast genome. She first was a postdoctoral researcher at Lawrence Berkeley National Laboratory's Joint Genome Institute, which probes genetics for renewable energy, bioremediation and other tasks. She later moved to the Joint BioEnergy Institute, another Bay Area DOE facility focused on developing plant-based renewable fuels.

Richardson loved working at the facilities but believed they needed new genomic tools and infrastructure to advance. She realized that her labors to build them were unlikely to advance her career. "Not that the work wasn't valuable or being used immediately by everyone around me," she says. "The incentive structure wasn't lined up for me to do what I thought needed to be done. And maybe I'm just hard-headed."



A scanning electron micrograph of *Acidiphilium cryptum*, a bacterial species that prefers acidic conditions and is found in areas contaminated with radioactive materials and heavy metals. MicroByre is studying this organism for cleaning hazardous waste sites and other uses. *Credit: Steve Gschmeissner, Science Photo Library.*

preparing her to seek capital. It gave her fellow entrepreneurs with whom she could commiserate, celebrate and share advice.

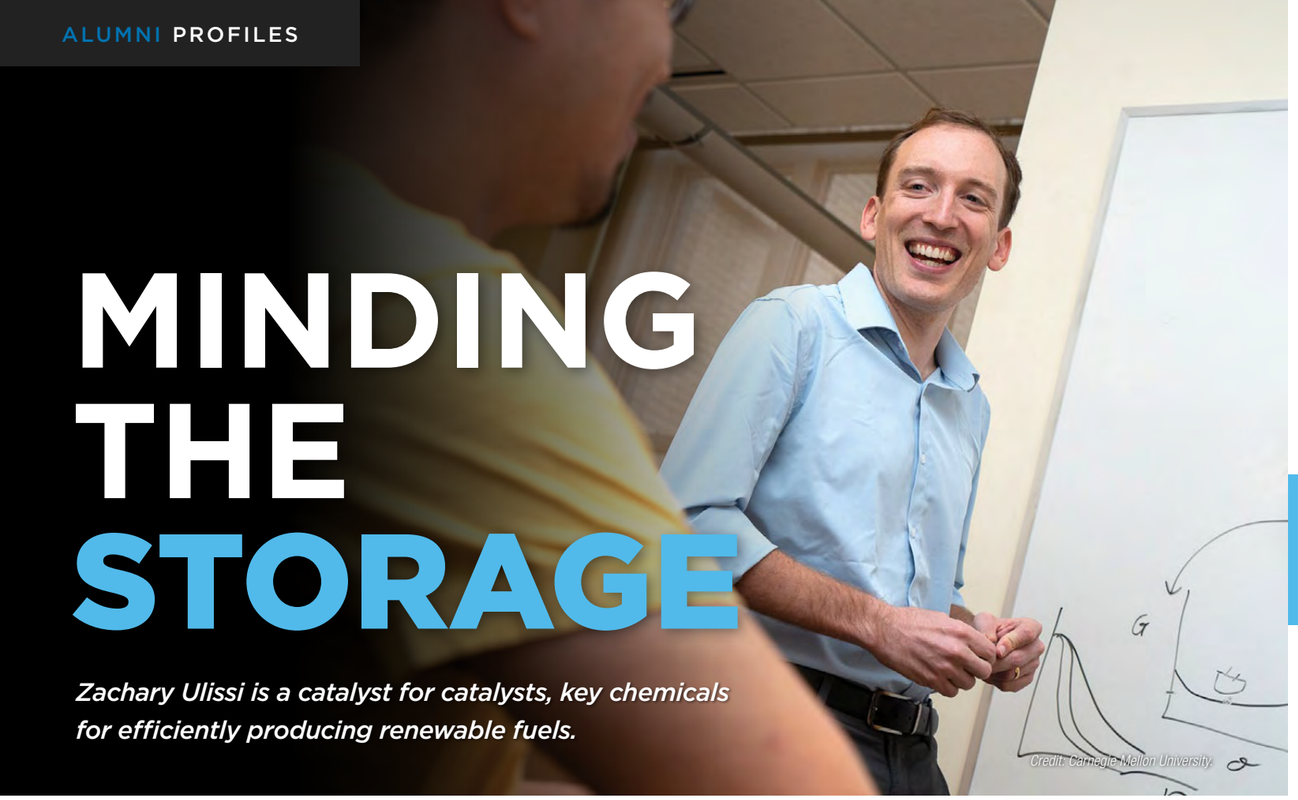
The DOE CSGF, meanwhile, taught Richardson the languages of computer science, HPC and applied math as well as molecular biology. That experience lets her coordinate a team with skills in all those fields. "My favorite part is getting out of the way and letting people who are better than me get it done."

'I can go charm a lady who has a bunch of chicken poop.'

She reluctantly left and launched MicroByre. The company was one of 10 chosen in 2017 to locate at Cyclotron Road, a Berkeley Lab innovation center. For two years it gave the company access to space, equipment and expertise to launch a capital-intensive business before facing investor demands for progress.

Perhaps more importantly, it provided mentors that helped Richardson avoid mistakes and learn the language of business,

MicroByre already has raised seed money from investment firms that focus on climate change solutions and industrial biotechnology. In the next year it hopes to finish validating its technology, begin product development collaborations with industrial partners, and double its workforce. But the goals go beyond profit. "We think this is a tech that can really impact the planet in a positive way," Richardson says. "I want to give it its best possible shot."



Credit: Carnegie Mellon University

MINDING THE STORAGE

Zachary Ulissi is a catalyst for catalysts, key chemicals for efficiently producing renewable fuels.

By Andy Boyles

Chemical engineer Zachary Ulissi wants renewable energy to fill more of the world's electricity needs. But solar, wind and other such sources are limited because the power industry has no cost-effective way to store energy. When the wind doesn't blow and the sun doesn't shine, and when hydro or nuclear power aren't available, fossil fuels must meet energy demands.

Ulissi and his colleagues have taken on this energy-storage problem. They're seeking ways to efficiently break the stubborn molecular bonds in carbon dioxide, nitrogen and water, then rearrange the atoms into molecules that store energy as fuel.

The group's plans hinge on materials called electrocatalysts. Like other catalysts, they facilitate chemical reactions while remaining unaltered. The difference: An electrocatalyst lies on the surface of an electrode and relies on an electric current to do its job.

Ulissi notes that two recent changes have set the stage for this work. First, electricity-driven chemical reactions and separations have made many industrial processes more efficient. Second, renewable energy costs are declining. The goal of green energy that both fills immediate needs and produces fuel for later consumption seems nearly within reach.

"We're still at the beginning of figuring out which chemical transformations can be replaced with these new methods, and catalyst design is at the center of these challenges," says Ulissi, assistant professor of chemical engineering at Carnegie Mellon University and a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) alumnus (2010-2014).

The team already has gained attention for using machine learning to screen for promising electrocatalysts. For example, in a May 2020 *Nature* paper, the researchers reported the most highly electrically efficient catalyst yet discovered – a copper-aluminum alloy – for transforming carbon dioxide and water into oxygen and ethylene. Ethylene can be a hydrocarbon fuel and is common building block for consumer polymers. Part of the project used resources at DOE's National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory.

Ulissi foresaw this research direction even as an undergraduate at the University of Delaware. He had chosen a major in physics and chemical engineering with minors in chemistry, math, materials science and computer science. Besides those ambitious goals, he took a job in the chemical engineering lab of Dionisios Vlachos, where he soon saw how his many interests could converge.

Vlachos and his colleagues use high-performance computing (HPC) to create models and simulations of a wide range of chemical structures. Ulissi worked on catalysts. "That was super fun," he says. "It convinced me that I wanted to be doing more in the computation and the math side."

He saw that of the many traits that might single out efficient catalysts, the right amount of stickiness, or adsorption, showed promise. Some potential catalysts seize reactants in a viselike grip that changes chemicals but can't release them. Others let reactants slide past like ice skaters, too fast for a chemical reaction to occur. But a catalyst that makes reactants cling transiently, like wool socks to polyester pants, holds the chemicals just long enough for the desired reactions to take place, then lets them go.

'We're still at the beginning of figuring out which chemical transformations can be replaced with these new methods.'

Ulissi pursued this research path, almost always involving HPC, from graduation in 2009 through a master's degree in advanced mathematics at Cambridge University in 2010 and his doctoral degree from the Massachusetts Institute of Technology in 2015. During his Ph.D., he and several other DOE CSGF recipients, including Anubhav Jain and Brenda Rubenstein, met through the fellowship program and later began collaborations that continue today.

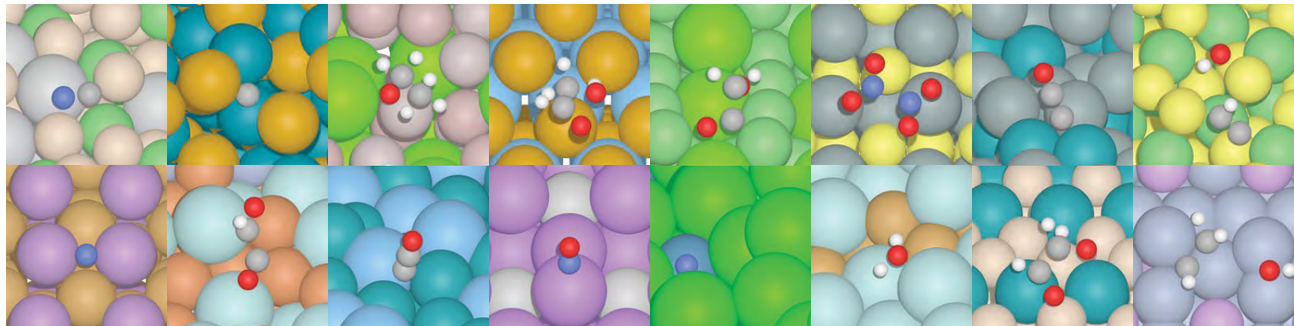
To address larger catalysis problems beyond the *Nature* paper, the Ulissi team developed the Open Catalyst 2020 (OC20) database, a list of possible catalysts and adsorbates. Over about a year, the group collaborated with Facebook Artificial Intelligence Research to create the dataset.

They started with thousands of crystal structures from the Materials Project, a Berkeley Lab initiative to calculate the properties of known and predicted compounds. The group cut the crystals to expose hundreds of thousands of potential catalyst surfaces and considered how various adsorbates might bind and interact. The team used density functional theory (DFT), a technique to model the electronic structure of the material, for about a million of these configurations. Now the researchers have a catalog of electrocatalyst stickiness, ready to be used for catalyst screening or machine-learning models.

They are now using the OC20 dataset to train larger and more accurate machine-learning algorithms to predict these properties thousands of times faster than the DFT simulations. They plan to use these methods to tackle catalyst design beyond the copper-aluminum system. For example, Jain and Ulissi are collaborating to identify catalysts that might be helpful for water-quality applications. Much of their work is done on NERSC's Cori, a Cray XC40 machine. The team also has earned a spot as one of the first users of Perlmutter, a Cray system at NERSC that will have three to four times Cori's performance.

Ulissi has high hopes for electrocatalysts because researchers who use machine learning to sift hundreds of thousands of candidate materials now share openly with one another. "The accelerated materials design community is really fun," he says. "Everyone collaborates to release new code and datasets. The things that we're working on are really trying to make better resources for the community to make rapid progress."

A random sampling of molecules and adsorbing surfaces included in the Open Catalyst 2020 (OC20) database. Zachary Ulissi and his colleagues use this dataset to train machine learning algorithms that can assist with designing new catalysts. Their paper about this work was published in April in *ACS Catalysis. Credit: Zachary Ulissi/CMU.*



SCATTERING WAVES AND TRACKING SNOW

Anderson and Kochanski chosen for math and modeling, outreach and mentoring.

By Thomas R. O'Donnell

Thomas G. Anderson

Kelly Kochanski

A mathematician who has advanced wave-scattering calculations and an earth scientist who has modeled the interactions that produce snow formations shared the 2021 Frederick A. Howes Scholar in Computational Science award.

A committee of alumni and friends of the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) chose Thomas G. Anderson and Kelly Kochanski for the annual award, whose namesake was the DOE's leading applied mathematics official until his death in 1999. The award recognizes recent fellowship alumni for excellent research and outstanding leadership, integrity and character.

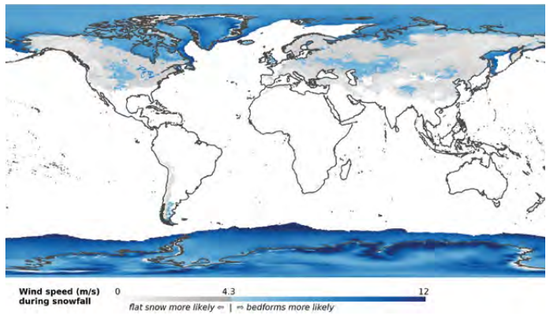
Anderson, a fellow from 2014 to 2018, completed his applied and computational mathematics Ph.D. at the California Institute of Technology in 2020. He's now a postdoctoral assistant professor of mathematics at the University of Michigan. Kochanski, a fellow from 2016 to 2020, earned a geological sciences Ph.D. from the University of Colorado Boulder last year. She's now a senior data scientist for McKinsey & Company, part of a team that advises clients on the effects of climate change.

Kochanski's computing background often proves useful as companies seek information on how changing climate may affect specific sites. "To do this, we need to do significant parallel processing of climate model data," she says.

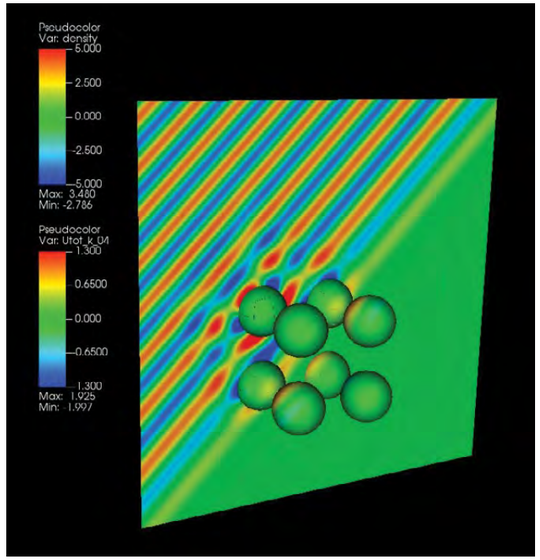
The job doesn't require the field work Kochanski did for her Ph.D., something she misses despite the often brutal weather in the Rocky Mountains. Over three winters she and a team of undergraduates gathered video of windblown snow forming shapes across the ground. These dunes and ridges can influence energy exchanges between Earth's surface and atmosphere, details climate models largely omit. With the data, Kochanski modified a sand-dune simulation code into Rescal-snow, the first multiphysics model of windblown snowform evolution.

Anderson has spent much of his professional life on the surface where objects meet their environments. Boundary integral equations, which elucidate this interplay, are the key elements connecting his projects. "We understand how waves move through free space pretty well," Anderson says. "It's the obstacle itself that poses a challenge – or poses a barrier, literally." Surface features from one area can inform researchers about the nature of solutions for an entire domain.

At Caltech, Anderson focused on how waves – generally sound or electromagnetic waves – and complex objects interact. At Michigan, he uses boundary integral equation techniques to study fluid flow, especially quantifying and optimizing fluid mixing. "This isn't an easy problem to tackle in anything but the simplest cases," he says. "I'm excited because these questions are not well-studied."



Average 10-meter wind speed during snowfall onto sea ice or snow-covered land, 2010-2020. Wind speeds above 4.3 meters per second are more likely than not to generate snow bedforms. *Credit: Kelly Kochanski.*



Scattering of a wave from a trapping geometry, one of the most complex known obstacles where, despite trapping, waves still decay exponentially. Solutions in the presence of other common trapping obstacles exhibit slower decay, an area of active research. The time snapshot depicts the total acoustical pressure (the desired solution) on a slice of the domain volume as well as the normal derivative of this same quantity on the spheres' surfaces. Computations are done on the boundary and the resulting surface quantities provide the means to produce a solution in the volumetric region. *Credit: Thomas G. Anderson.*

Anderson was active in the Caltech computing and mathematical sciences department, serving on advisory councils to improve the academic environment for graduate students. He codeveloped an undergraduate course on ethics in computer science and participated in the Caltech Y's Rise tutoring program in underserved areas of Los Angeles.

Anderson also helped lead the Caltech Argentine Tango Club, an opportunity, he says, for graduate students "to expand their sense of self beyond just the lab. That was a big factor for me: to have personal growth opportunities apart from grinding out research."

Kochanski also fostered student growth, mentoring nearly a dozen undergraduates, including those who helped on her thesis research and while on practicums. "I put a lot of thought into designing projects that gave them opportunities to learn and develop the skills they were interested in while doing real science," Kochanski says. Mentoring was "probably the most meaningful thing I did as a grad student."

Her work extended across borders. In 2015 she and other recent Massachusetts Institute of Technology graduates adapted the International Young Physicists' Tournament program and traveled to Santiago, Chile, to teach secondary students. Kochanski helped sustain the program and hand it off to later MIT students.

Kochanski also has helped introduce machine learning to climate science. She and other researchers (including fellow Priya Donti, featured in this issue on page 19) produced a major paper on using artificial intelligence for climate change research. They formed Climate Change AI, which seeks to blend climate science and machine learning.

Similarly, Kochanski worked with the Community Surface Dynamics Modeling System, an initiative to encourage sharing among researchers who use computation to investigate processes occurring at Earth's surface. She was a member of the organization's AI and machine-learning committee and encouraged researchers to explore the technology.

Meanwhile, Kochanski shared her expertise outside academic circles through the question-and-answer website Quora, where her more than 200 essays have received more than 3 million views. The instant feedback from readers helped her develop "a much more concise and snappy way of writing, which has really been powerful," Kochanski says.

Kochanski will continue pursuing technology at the frontier of computer and earth sciences. "I feel lucky to be working in a growing field with social importance."

Anderson's "goal is to always be contributing good work and good ideas." His advice to young investigators: Understand your field's literature and how your ideas differ from previous ones. "It's OK to not initially know exactly where your research will fit in, and it's OK to take risks with ideas."

ABOUT FRED HOWES

The Frederick A. Howes Scholar in Computational Science award, first presented in 2001, has come to stand for research excellence and outstanding leadership. It's a fitting tribute to Howes, who was known for his scholarship, intelligence and humor.

Howes joined DOE in 1991 and advocated for the fellowship and for computational science as manager of the Applied Mathematical Sciences Program. He died unexpectedly in 1999 at age 51. Colleagues formed an informal committee to honor him and chose the DOE CSGF as the vehicle. The award is sustained through donations from the Howes family and others.

ASCENDING TO EXASCALE AND OTHER HEIGHTS

For the fellowship's graduates, the program's 30th was a very good year.

The Department of Energy's (DOE's) Exascale Computing Project (ECP) named **Daniel Martin** (1993-1996) the team lead for application development in earth and space science. Martin will help oversee and develop exascale-capable projects to explore the universe's structure and astrophysical phenomena and to better model earthquakes and clouds. Martin is a computational scientist and leader of the Applied Numerical Algorithms Group at Lawrence Berkeley National Laboratory.

DOE's Princeton Plasma Physics Laboratory touted **Noah Mandell's** work to improve a model of the plasma edge in tokamak fusion reactors. Mandell (2015-2019) extended the Gkeyll code to handle magnetic fluctuations. The simulations may help physicists understand and avoid machine-damaging heat bursts.

Qiskit interviewed **Sukin (Hannah) Sim** (2016-2020) on its YouTube channel for a four-part series on her career and quantum circuits research. Sim, then a Harvard University doctoral candidate, also spoke about optimizing parameter-heavy circuits at QHack's 2021 Quantum Machine Learning Hackathon. She is now a research scientist with Zapata Computing.

Columbia University biomedical engineering professor **Tal Danino** (2006-2010) was among seven researchers who received the 2020 Pershing Square Sohn Prize for Young Investigators in Cancer Research. The award provides $200,000 a year for up to three years. Danino's lab programs probiotic bacteria to target tumors and deliver lung cancer therapeutics. Danino also was chosen by the Cancer Research Institute for its Lloyd J. Old STAR (Scientists Taking Risks) award, providing $1.25 million in project support over five years.

Amanda Randles (2010-2013), a Duke University biomedical sciences professor, delivered the virtual keynote talk at the 2021 Rocky Mountain Advanced Computing Consortium's High-Performance Computing (HPC) Symposium. Her group received a DOE INCITE grant of 290,000 hours on Summit, the HPC system at the Oak Ridge Leadership Computing Facility (OLCF), to model how cancer cells circulate. And the team's HARVEY code, which models the circulatory system, will be among the first to run on Aurora, the exascale computer planned for the Argonne Leadership Computing Facility (ALCF).

The Duke Arts website featured **Clay Sanders** (2016-2020) and his artwork, focusing on a commissioned painting that the campus arts center exhibited. He's now a mechanical engineer at Sandia National Laboratories, California.

Hannah De Jong (2014-2018) and her Stanford University colleagues developed a high-throughput, scalable method for sequencing the coronavirus genome while collecting DNA data about the human host.

MIT's new Center for Exascale Simulation of Materials in Extreme Environments, including alumnus Asegun Henry, will focus on exascale simulation of materials in hypersonic flow conditions. Applications include hypersonic vehicles like the one in this visualization. *Credit: U.S. Defense Advanced Research Projects Agency.*

Massachusetts Institute of Technology mechanical engineering professor **Asegun Henry** (2005-2009) was lead author of a *Nature Energy* paper outlining five key ways that thermal energy could help stem global climate change. Henry also was named a co-primary investigator for MIT's new Center for Exascale Simulation of Materials in Extreme Environments. The center aims to predict how materials degrade when used in space flight, industry, nuclear safety and other punishing conditions.

The online magazine *POWER* interviewed venture capitalist and entrepreneur **Leslie Dewan** (2010-2013) about using nuclear energy technology to cut carbon emissions while minimizing or consuming radioactive waste.

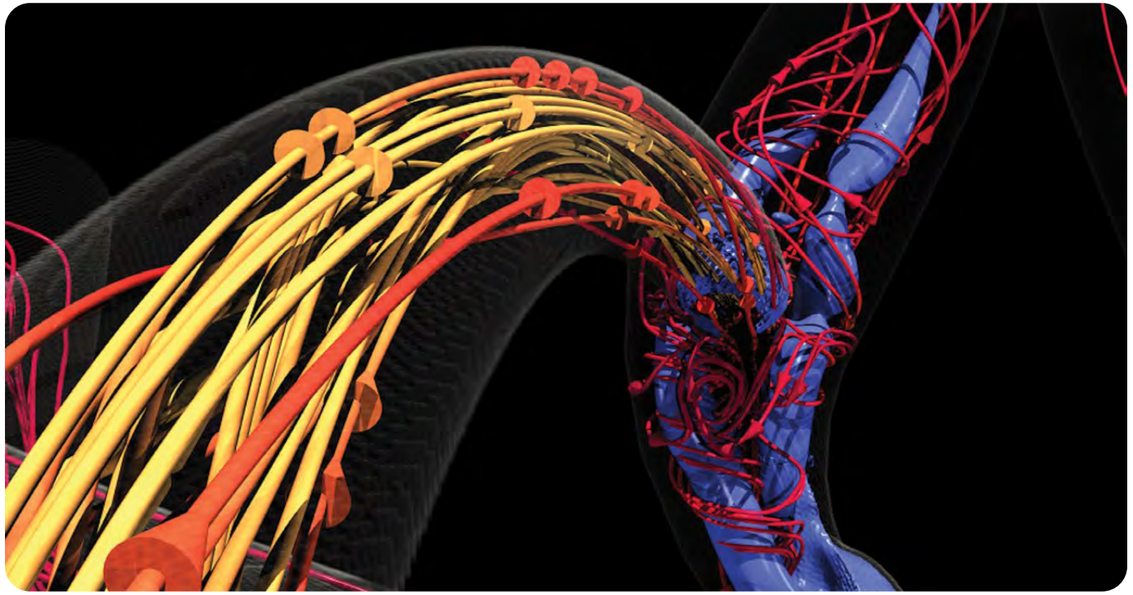
Julia Ebert (2016-2020), who is finishing a computer science Ph.D. at Harvard, was named a 2021 Siebel Scholar. The program recognizes exceptional students from the world's leading graduate schools of business, computer science, energy science and bioengineering. Honorees receive $35,000 to support their final year of studies.

Derek Macklin (2012-2016), a senior data scientist at the healthcare company Grand Rounds, was lead author on a *Science* paper in which he and colleagues compared results reported for the *E. coli* bacterium across millions of datasets from thousands of academic papers. After correcting for some initial inconsistencies, they showed that the model could be predictive.

Ars Technica highlighted **Danielle Rager's** (2014-2018) side gig, in which she uses her programming skills to perform as {arsonist}, an electronic musician who concocts description-defying compositions. By day, she is a researcher at Intel Labs.

Hal Finkel (2007-2011) left the ALCF to join the DOE Office of Advanced Scientific Computing Research as a computer science program manager. Finkel was a co-primary investigator on numerous ECP projects and helped develop the HACC cosmology code, a two-time Association for Computing Machinery (ACM) Gordon Bell Prize finalist. Finkel and **Nicholas Frontiere** (2013-2017) were on a team that ran HACC a final time on the ALCF's now-retired Mira supercomputer. Their simulation tracked dark matter structure formation in the universe.

A team that included alumnus **James Phillips** (1995-1999) and fellow Anda Trifan won a Gordon Bell Special Prize for HPC research addressing the COVID-19 pandemic. The award was presented at the Supercomputing 2020 (SC20) conference. Phillips is a senior research programmer at the National Center for Supercomputing Applications, based at the University of Illinois at Urbana-Champaign, where Trifan is a theoretical and computational biophysics doctoral candidate. She's also an intern at Argonne. The multi-institutional team developed an artificial intelligence-driven workflow to investigate the SARS-CoV-2 spike protein, the main means by which the virus infects cells. As part of the research, they modeled all of the virus' 305 million atoms.



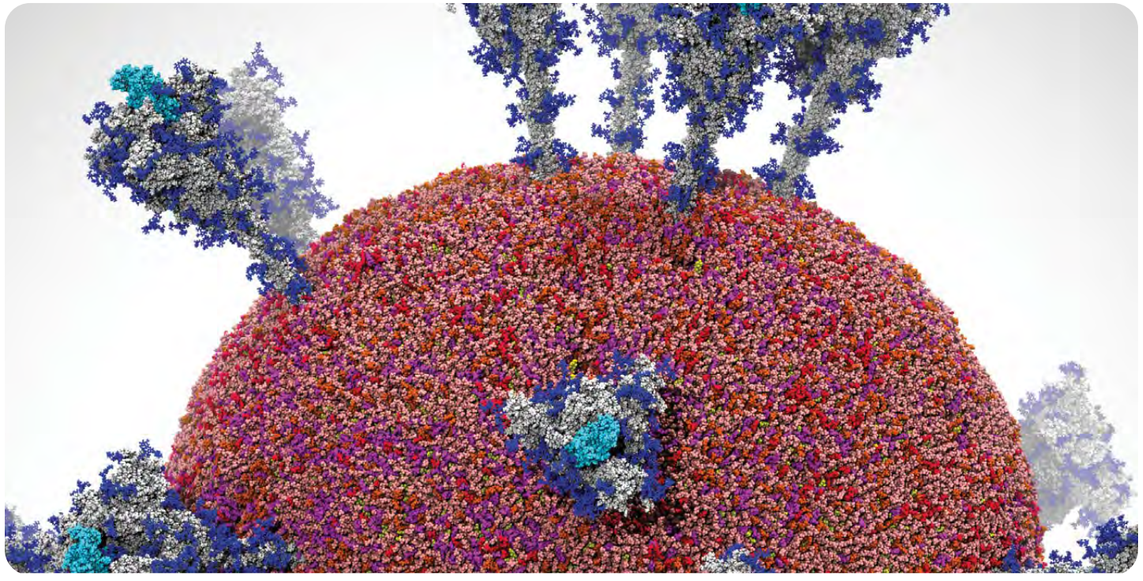
Duke University researchers, led by Amanda Randles, will use the new Aurora exascale HPC system to investigate the role that biological parameters play in determining tumor cells' paths through the circulatory system. *Credit: Joseph Insley, Argonne National Laboratory.*

"Rehearsal" by Clay Sanders was chosen to hang in Duke University's Rubenstein Arts Center. *Credit: Clay Sanders.*

Joshua Vermaas (2011-2016) and **David Rogers** (2006-2009), both at Oak Ridge National Laboratory, were finalists for the special Gordon Bell prize. They were on a multi-institutional team that created a virtual laboratory on Oak Ridge's Summit supercomputer and simulated how more than a billion compounds interact with SARS-CoV-2.

Richard Barnes (2015-2019) of the University of California, Berkeley, won second prize at SC20 in the ACM Student Research competition for his presentation, "Communication-Avoiding Large Graph Algorithms for Flow Modeling." In the project, Barnes developed a way to accelerate HPC hydrology models that help depict how landscapes evolved.

Alumni now hold three of four offices leading the Society for Industrial and Applied Mathematics (SIAM) Special Interest Group on Computational Science and Engineering. Members elected **Stefan Wild** (2005-2008, featured this issue, page 22) as chair, **Jeff Hammond** (2005-2009) as vice chair and **Judith Hill** (1999-2003) as program director. Wild is a computational mathematician in Argonne's Laboratory for Applied Mathematics, Numerical Software and Statistics. Hammond is a principal architect at NVIDIA. Hill is a computational science project leader at Lawrence Livermore National Laboratory.

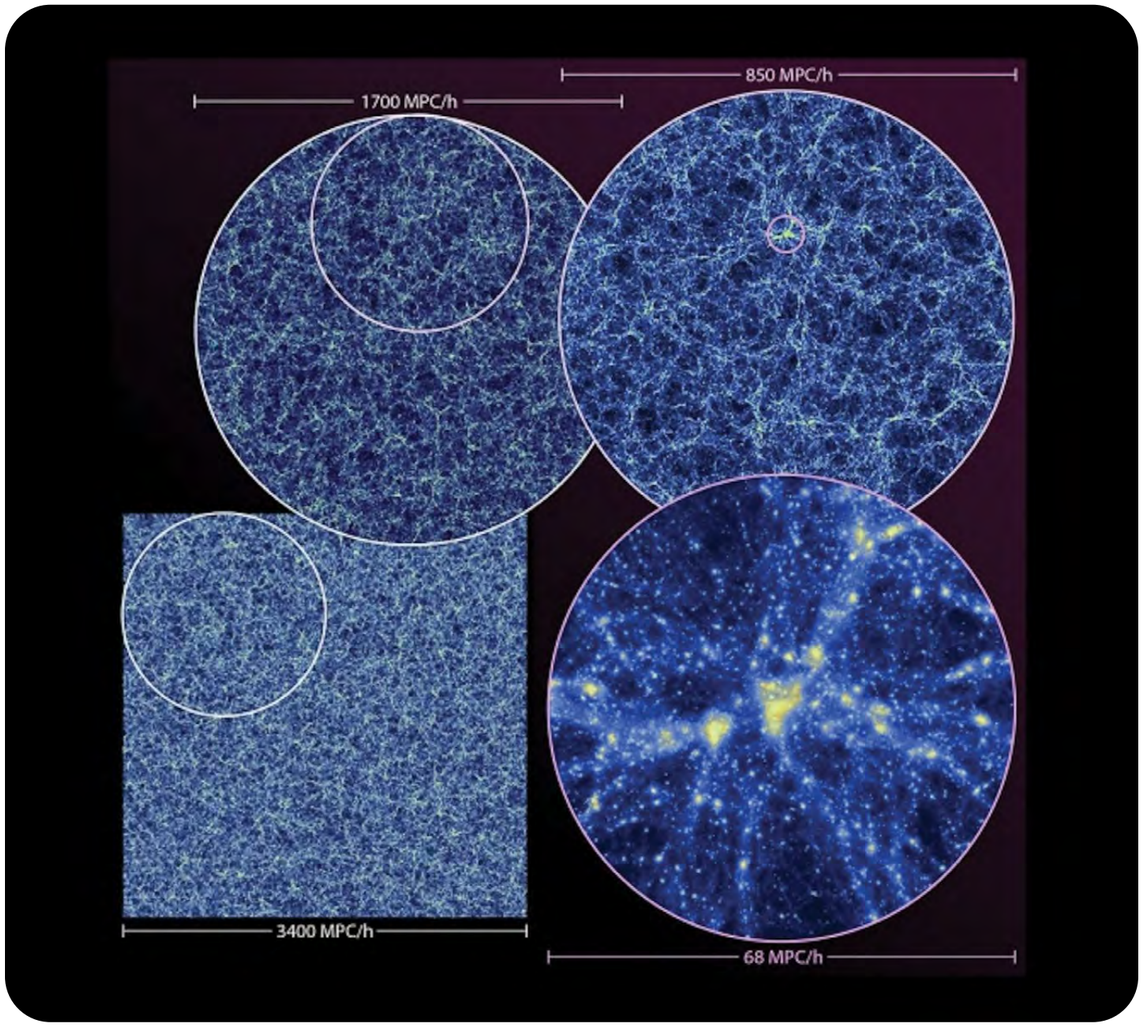


A snapshot of a visualization of the SARS-CoV-2 viral envelope comprising 305 million atoms. Alumnus James Phillips and fellow Anda Trifan were part of the team behind the award-winning project. *Credit: Rommie Amaro, University of California San Diego; Arvind Ramanathan, Argonne National Laboratory.*

Eileen Martin (2012-2016), a Virginia Tech professor, delivered a tutorial on arrays at Stanford's virtual Women in Data Science 2021 Worldwide Workshop. She will join the faculty at the Colorado School of Mines in January 2022.

Google's **Jarrod McClean** (2011-2015) and fellow Alicia Magann (featured this issue, page 13) of Princeton University are among the authors of a perspective in the online journal *PRX Quantum*. The team proposed using quantum optimal control to improve variational quantum algorithms, a technology for probing noisy intermediate-scale quantum computers.

Jeffrey Hittinger (1996-2000) was honored with the 2021 James Corones Award in Leadership, Community Building and Communication by the Krell Institute, which manages the DOE CSGF. A panel of judges chose Hittinger, director and division leader of Livermore's Center for Applied Scientific Computing, for his work moving applied mathematics toward exascale computing, his support for the fellowship and his ability to communicate to technical and nontechnical audiences.



Visualization of the Last Journey simulation, a project that included alumni Nicholas Frontiere and Hal Finkel. The large-scale structure of the universe is shown as a thin slice through the full simulation (lower left). Other images zoom in on the structure at different levels. The lower right panel shows one of the largest structures in the simulation. *Credit: Argonne National Laboratory.*

CLASS OF 2021

Peter Ahrens
Massachusetts Institute of Technology
Computer Science
Advisor: Saman Amarasinghe
Practicum: Sandia National Laboratories, New Mexico

Morgan Kelley
University of Texas at Austin
Process Systems
Advisor: Michael Baldea
Practicum: Argonne National Laboratory

Benjamin Toms
Colorado State University
Atmospheric Science
Advisor: Elizabeth Barnes
Practicum: Lawrence Berkeley National Laboratory

Robert Baraldi
University of Washington
Applied Mathematics
Advisor: Aleksandr Aravkin
Practicum: Lawrence Berkeley National Laboratory Argonne National Laboratory

Claire Kopenhafer
Michigan State University
Astrophysics
Advisor: Brian O'Shea
Practicum: Sandia National Laboratories, New Mexico

Steven Torrisi
Harvard University
Materials Physics
Advisor: Efthimios Kaxiras
Practicum: Lawrence Berkeley National Laboratory

Matthew Carbone
Columbia University
Chemical Physics
Advisor: David Reichman
Practicum: Brookhaven National Laboratory

Miriam Kreher
Massachusetts Institute of Technology
Nuclear Engineering
Advisor: Benoit Forget
Practicum: Los Alamos National Laboratory

Annie Wei
Massachusetts Institute of Technology
Quantum Information
Advisor: Aram Harrow
Practicum: Fermi National Accelerator Laboratory

Jennifer Coulter
Harvard University
Computational Materials Physics
Advisor: Boris Kozinsky
Practicum: Oak Ridge National Laboratory

Alicia Magann
Princeton University
Quantum Control
Advisor: Herschel Rabitz
Practicum: Sandia National Laboratories, California (2019, 2020)

Zachary Weiner
University of Illinois at Urbana-Champaign
Cosmology, High Energy
Advisor: Peter Adshead
Practicum: Argonne National Laboratory

Priya Donti
Carnegie Mellon University
Computer Science and Public Policy
Advisor: Zico Kolter
Practicum: National Renewable Energy Laboratory

Quentarius Moore
Texas A&M University
Chemistry
Advisor: James Batteas
Practicum: Sandia National Laboratories, New Mexico (2018, 2019)

Malia Wenny
Harvard University
Chemistry
Advisor: Jarad Mason
Practicum: Argonne National Laboratory

Anya Katsevich
New York University
Applied Mathematics
Advisor: Jonathan Weare
Practicum: Los Alamos National Laboratory

Kari Norman
University of California, Berkeley
Ecology
Advisor: Carl Boettiger
Practicum: Oak Ridge National Laboratory

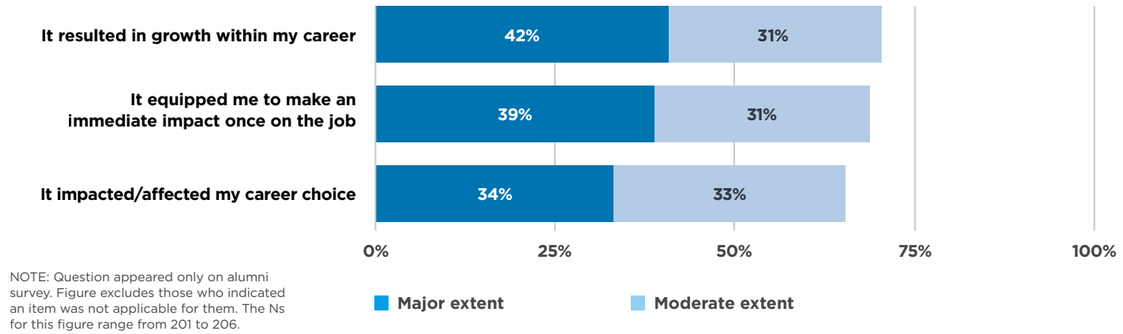
Jonas Kaufman
University of California, Santa Barbara
Computational Materials Science
Advisor: Anton Van der Ven
Practicum: Lawrence Livermore National Laboratory

Kevin Silmore
Massachusetts Institute of Technology
Chemical Engineering
Advisor: James Swan
Practicum: Oak Ridge National Laboratory

DOE CSGF: TAKING HPC INTO CLASSROOMS, BOARDROOMS AND LABS

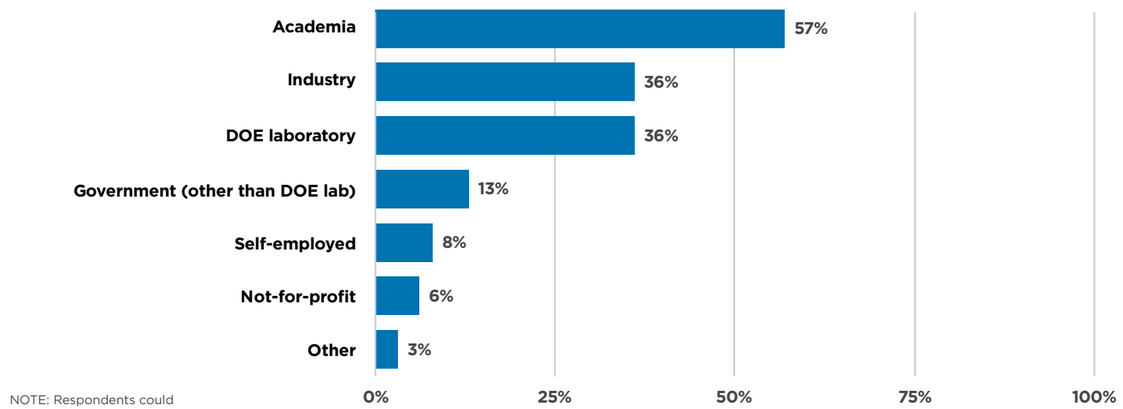
Alumni of the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) overwhelmingly say the program's combination of studies in an application field, such as physics or chemistry with high-performance computing and mathematics, influenced the employment they chose and boosted their on-the-job impact and career growth. Most have worked in academia, industry or government laboratories, helping to establish supercomputing as a tool for solving problems of national importance. *Source: https://www.krellinst.org/csgf/about-doe-csgf/2017-longitudinal-study.*

Percent of alumni reporting the extent to which exposure to HPC has had an impact on their career

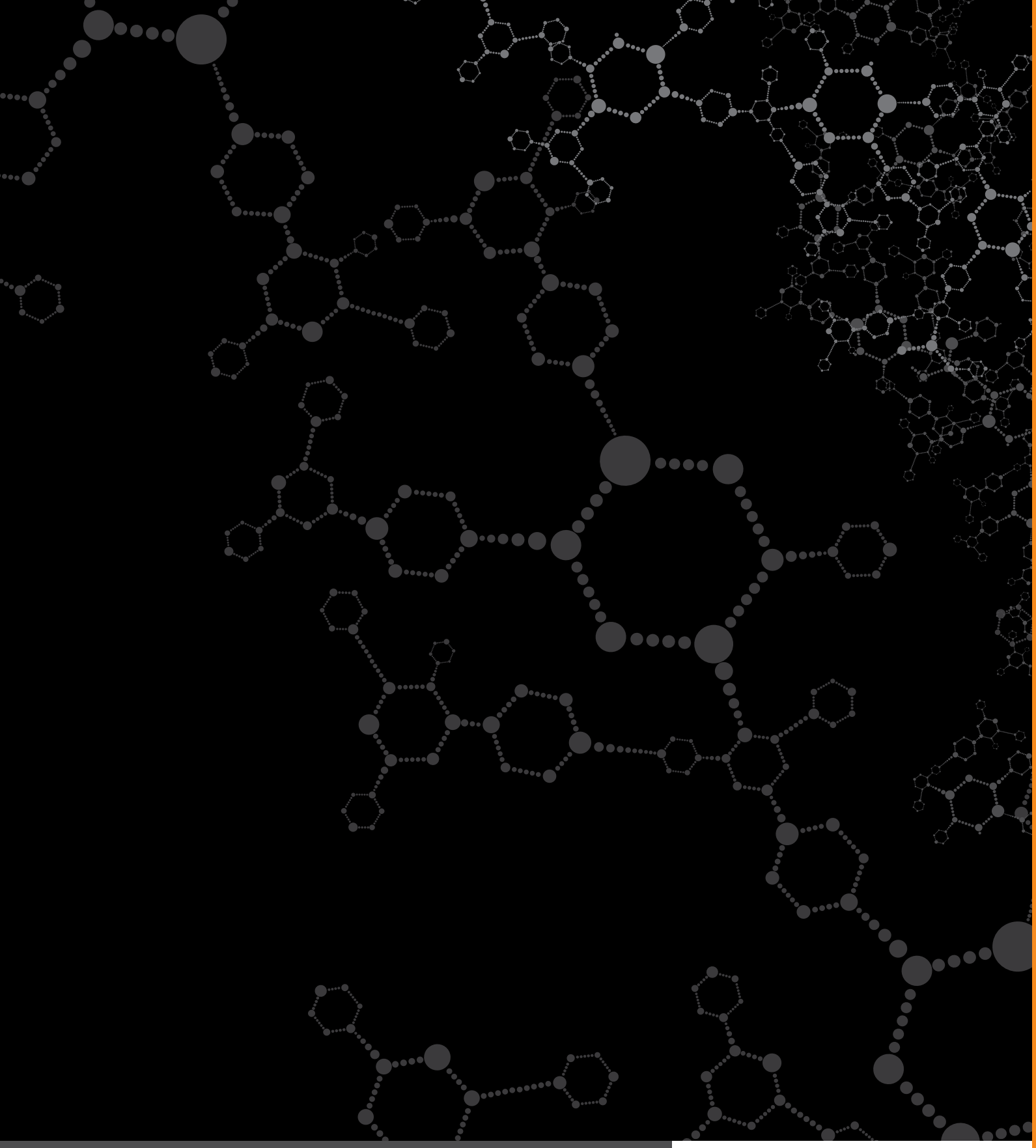


NOTE: Question appeared only on alumni survey. Figure excludes those who indicated an item was not applicable for them. The Ns for this figure range from 201 to 206.

Percent of alumni reporting the professional settings in which they had worked since completing the DOE CSGF (N=198)



NOTE: Respondents could select multiple sectors.



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