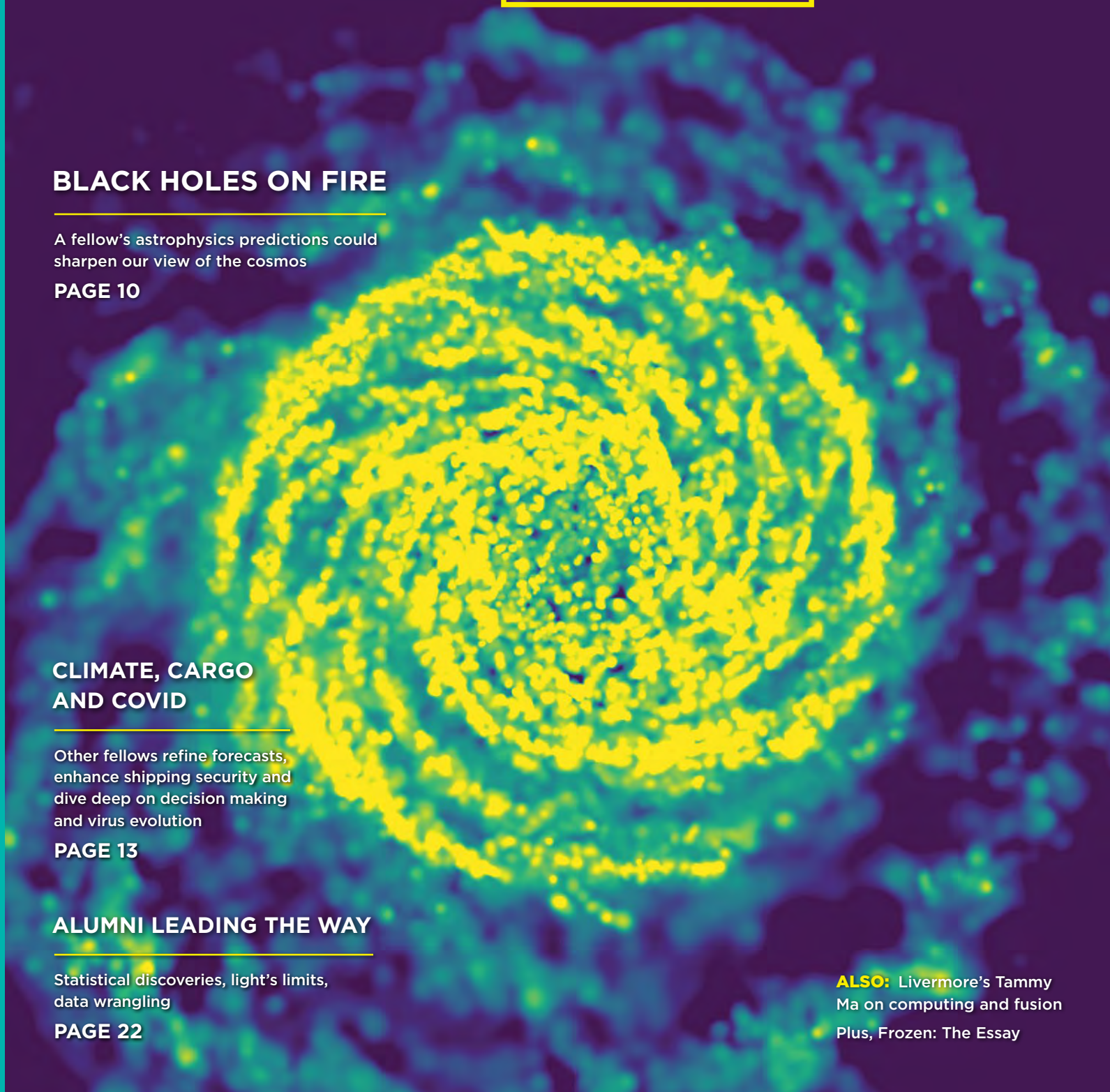
THE DOE CSGF ANNUAL

2023

DEIXIS

DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP



BLACK HOLES ON FIRE

A fellow's astrophysics predictions could sharpen our view of the cosmos

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ALUMNI LEADING THE WAY

Statistical discoveries, light's limits, data wrangling

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ALSO: Livermore's Tammy Ma on computing and fusion

Plus, Frozen: The Essay

EXPANDING REACH: THE INCOMING DOE CSGF CLASS

The Department of Energy Computational Science Graduate Fellowship has increased its incoming class, welcoming 39 fellows in 2023-24. They represent 25 institutions and will pursue research in computational geophysics, environmental fluid mechanics, applied mathematics and much more.

Zachary Andalman
Princeton University
Astrophysical Sciences

Alexandra Bardon
Massachusetts Institute of Technology
Computational Neuroscience

Luke Bhan
University of California, San Diego
Intelligent Systems, Robotics and Control

Amanda Bowden
University of Colorado Boulder
Atmospheric Science

Amelia Chambliss
Columbia University
Plasma Physics

Lauren Chua
Massachusetts Institute of Technology
Polymers and Soft Matter

Cameron Coles
Cornell University
Ecology and Evolutionary Biology

Luis Delgado Granados
University of Chicago
Theoretical and Computational Chemistry

Amil Dravid
University of California, Berkeley
Computer Science

Mohit Dubey
University of California, Berkeley
Environmental Engineering

Isabella Dula Razzolini
Stanford University
Atmospheric Science

Michelle Garcia
Dartmouth College
Theoretical/Computational Chemistry

Jacob Halpern
Columbia University
Plasma Physics

Emma Hart
Emory University
Computational Mathematics

Juampablo Heras Rivera
University of Washington
Mechanical Engineering

Iran Hernandez Imbert
Duke University
Mechanical Engineering

Elyssa Hofgard
Massachusetts Institute of Technology
Electrical Engineering and Computer Science

Benjamin Holmgren
Duke University
Computer Science

Abigail Keller
University of California, Berkeley
Ecology

Patrick Kim
Princeton University
Plasma Physics

David Krasowska
Northwestern University
Computer Science

James Larsen
University of Michigan
Applied and Interdisciplinary Mathematics

Adam Lechowicz
University of Massachusetts Amherst
Computer Science

Brandon Lee
Princeton University
Plasma Physics

Fiona Majeau
University of Colorado Boulder
Electrical Engineering

Ethan Meitz
Carnegie Mellon University
Molecular Simulation and Heat Transfer

Joshua Melendez-Rivera
Texas A&M University
Computational and Surface Chemistry

Marlo Morales
Washington State University
Physics

Benjamin Moyer
University of Maryland, College Park
Computational Geophysics

Kirill Nagaitsev
Northwestern University
Computer Science

Jennifer Paige
University of California, Davis
Applied Mathematics

Melissa Rasmussen
Stony Brook University
Astronomy

Pavan Ravindra
Columbia University
Chemical Physics

Gabriel Rios
Princeton University
Atmospheric Science

Kathlynn Simotas
University of California, Santa Barbara
Astrophysics

Joseph Torsiello
Temple University
Nuclear and Particle Physics - Theory

Cristian Villatoro
University of Notre Dame
Applied and Computational Mathematics and Statistics

Michael Walker
Princeton University
Fluid Mechanics

Sienna White
University of California, Berkeley
Environmental Fluid Mechanics

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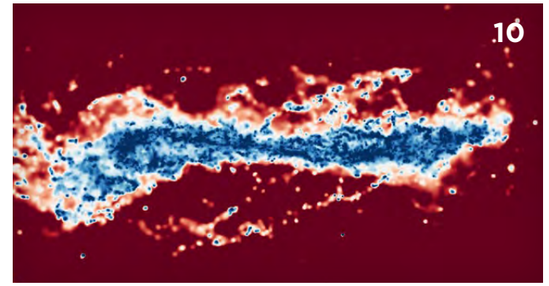

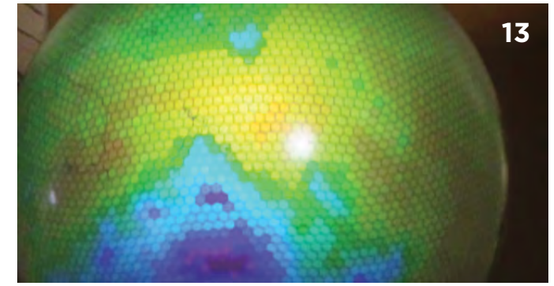

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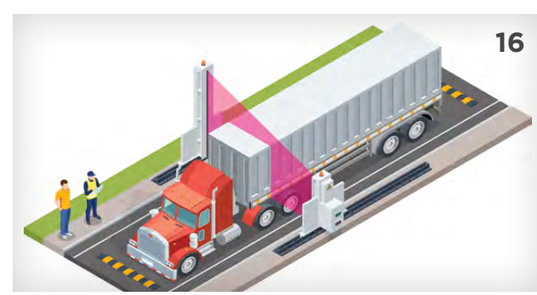

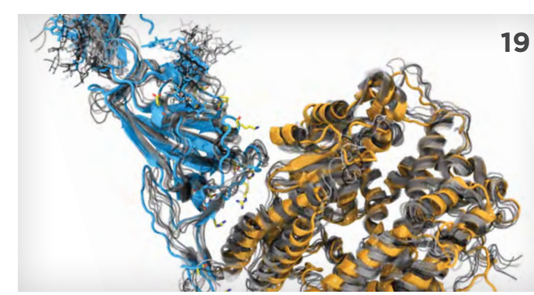

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For additional information about the DOE CSGF program, the Krell Institute or topics covered in this publication, please go to: www.krellinst.org/csgf

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

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

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Science Media Editor — Thomas R. O'Donnell
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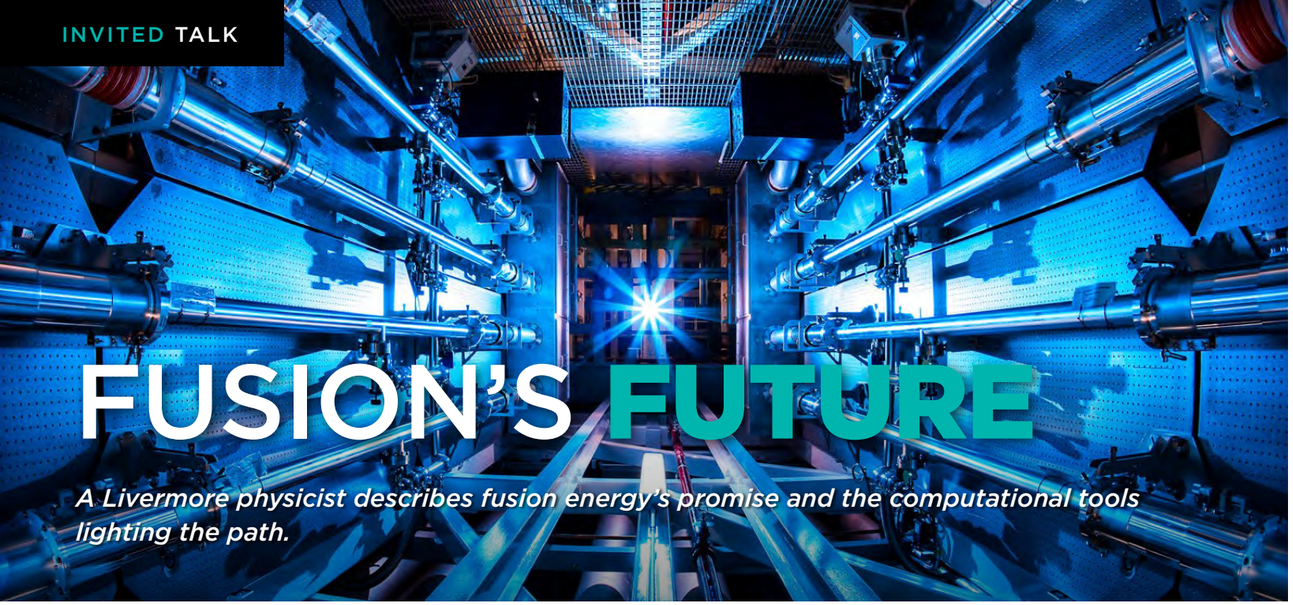
ON THE COVER: An enormous galaxy encircling a supermassive black hole simulated by Lindsey Byrne of Northwestern University using the FIRE (feedback in realistic environments) model. The assembled hot gases are blue and cold gases are yellow. *Credit: Lindsey Byrne.*



FUSION'S FUTURE

A Livermore physicist describes fusion energy's promise and the computational tools lighting the path.

The National Ignition Facility's preamplifier support structure, which helps boost laser power for inertial confinement fusion experiments. *Credit: Damien Jemison.*

Tammy Ma

As a plasma physicist at the National Ignition Facility (NIF), Tammy Ma leads the Lawrence Livermore National Laboratory Inertial Fusion Energy Initiative and was a member of the team that achieved inertial fusion ignition in late 2022. She's received numerous honors, including the 2023 James Corones Award in Leadership, Community Building and Communication.

DEIXIS: HOW DID YOU GET INTERESTED IN FUSION RESEARCH?

Tammy Ma: Fusion is one of the grand challenges of science and technology. If we can harness fusion, it could be a clean, limitless energy source. It could help us with climate security, with energy security and with bringing up standards of living everywhere.

I also love working on big science projects – big teams, big facilities – things that in some cases only national labs can make happen.

WHAT NIF INNOVATIONS GOT US FROM NEAR-IGNITION TO IGNITION?

The idea of driving a fusion reactor with lasers started in the 1940s and '50s. We had to build successively bigger lasers to make it happen. In 2021, we achieved burning plasma: enough fusion reactions to feed back on itself and make more fusions happen. But we had yet to get more energy out, what we call ignition, than we put in with the lasers. In the intervening year, we turned up the laser energy about 8% and made it more precise.

We also improved the target. The little fuel capsule that holds the deuterium-tritium fuel has to be nearly perfect, with few nicks, bumps or divots on its surface. And we made a few design changes. By turning up the laser energy, we could make the wall of that capsule a bit thicker, which makes it more stable.

WHAT ROLE DID COMPUTING HAVE IN THOSE ADVANCES?

In any one of our experiments, more than 10,000 different physics parameters can be changed: the laser energy put in, the laser pulse shape – its power output as a function of time – where the lasers point, the material thickness of the target's capsule wall.

How do you know what to change? Computing plays an enormous role. We have to use our high-fidelity, 3D simulation tools to model the entire reaction, from every bump on that capsule to exactly how the lasers delivered. We put that into the simulation codes and see if the result matches what came out of the experiment.

The computers never get it exactly right. A simulation is only as good as the data we feed it. So data from the last experiment are put in, and then we try to improve the codes and then run it again on the next experiment. Our modeling and simulation team is as big as the experimental side. That's how important it is.

WHAT ARE THE CHALLENGES IN MAKING CLEAN ENERGY WITH INERTIAL FUSION?

With inertial fusion we're using lasers to compress and hold fuel together long enough to get it to fuse. You're relying on the inertia of the target itself. To turn this into a power plant, it's envisioned you would have to repeat the reaction 10 times per second. Today we do a shot every four to eight hours or so on NIF.

HOW MIGHT MAGNETIC AND INERTIAL FUSION COMBINE TO REALIZE FUSION ENERGY?

Both concepts have challenges to overcome, but they both have a lot of potential. Both are fusion plasmas, so there's a lot of overlap as well. In magnetic fusion you use these huge, strong magnets to hold your plasma together long enough that it can fuse. One of the big challenges is keeping the plasma from touching the fusion reactor walls – it quenches and you have what we call a disruption, which stops the reaction. On the inertial side, we manage target-pellet imperfections and adjust the laser to optimize the reaction.

In both cases we're talking about using machine learning and AI for real-time feedback loops so that you can do the best experiment that you can.

WHAT COMPUTATIONAL SCIENCE TOOLS WILL BE IMPORTANT IN FUSION ENERGY'S FUTURE?

One thing that's important for fusion's future is continuing to improve that predictive capability – when simulation tools have been tuned to real data so that they can forecast what will happen in an experiment. If you're trying to run a physics simulation of a reaction, you might start at the atomic scale.

In plasmas, ions move separately from the electrons. To understand how the plasma moves, you need a hydrodynamics code to model wavelike motion or other collective effects. You also have to model the lasers coming in. Then how do we combine all those codes at different scales to get a complete picture?

We have to do the same sort of experimental integration from atomic physics up to the biggest lasers in the world, like NIF's.

And then there's integrating research from across the different DOE labs, plus universities and private industry. How do we combine all the knowledge that we have and leverage it all to build a full picture?

The combination of that interconnectedness and supercomputers that can handle all this information – that's one of the big frontiers for us going forward.

WHAT ARE THE CRITICAL QUESTIONS THAT GET YOU UP IN THE MORNING?

I'm excited about doing something that has never been done and charting that path. I'm not just asking scientific questions. I also think about how to bring together players across the U.S. to help realize how important fusion energy is.

Science has a huge policy aspect. We scientists have a responsibility to help move society and our country where we think is best based on scientific knowledge.

For me, fusion energy is such an important potential solution, but that level of science requires a huge amount of support, buy-in from your legislators, from DOE and the national lab system. I get the chance to bring it all together, learn new things and grow as a scientist and as an individual.

WHAT ADVICE DO YOU HAVE FOR EARLY-CAREER RESEARCHERS?

Science is hard. You're doing technology development; you are trying to do things that have not been done. That's risky. There are a lot of unknowns and failure. Everybody goes through that, but hopefully you have a good team to do it with. Stick with it, and just know that you're not alone.

WHAT ELSE WOULD YOU LIKE TO MENTION ABOUT FUSION AND COMPUTING?

The advances in fusion research and computing technology set us on a path to increased understanding and faster development. This work also helps with the U.S. national security mission because the same simulation codes underlie the safety, security and reliability of our nuclear stockpile.

When I give NIF tours, I always pause at the window before you enter the laser bay overlook and point out the building that houses Sierra, the world's sixth fastest supercomputer. NIF would not exist without that supercomputer and the ability to model our experiments. It's essential.

The National Ignition Facility's target chamber (blue) at Lawrence Livermore National Laboratory, where Tammy Ma and colleagues achieved fusion ignition in late 2022. *Credit: Damien Jemison.*

THE ARCTIC OCEAN, WITH A GRAIN OF SALT

Carlyn Schmidgall on Arctic sea ice, with the R/V Woldstad research vessel in the background. A boat hook is to the right. *Credit: Jim Thomson.*

The DOE CSGF Communicate Your Science & Engineering Contest gives fellows and alumni the opportunity to write about computation and computational science for a broad, nontechnical audience. The author of this year's winning essay studies physical oceanography at the University of Washington.

By Carlyn Schmidgall

The boat hook is frozen again. It's one of the simplest and most useful tools aboard the ship, an extendable pole with a U-shaped plastic hook on one end, used to deploy and recover all manner of oceanographic equipment. It took less than an hour for wind chill and the Arctic Ocean's freezing spray to encase its joints in a thin ice layer.

From years of debugging code and fixing faltering hardware as a researcher, I've learned that the simplest solution often is the best. In this case, banging the boat hook on the rail a few times sends the ice clattering to the deck, freeing the joints to extend the pole to its full length. This is the seagoing version of turning our instrument off and on.

Granted, the middle of the ocean isn't a typical workplace for a computational scientist. With a crew of 11 other researchers and engineers, I traveled aboard the R/V Woldstad to the Beaufort Sea as a member of the NASA Salinity and Stratification at the Sea Ice Edge (SASSIE) field campaign.

The Arctic Ocean is one of the planet's most rapidly changing environments under human-caused climate change, with temperatures rising nearly four times faster than the global average. Better understanding the Arctic's rapidly evolving ice-ocean-atmosphere system will improve climate predictions. The SASSIE mission aimed to collect data on upper-ocean properties – such as salinity, temperature and current velocity – that can affect sea-ice formation in the polar autumn.

The ocean is like an onion: It has layers. In oceanography, we call this stratification – levels of lighter water sit atop heavier, deeper ones, leading to stability in the water column. Two variables set ocean stratification: the temperature and the salinity, which have compounding and occasionally competing effects.

For much of the global ocean, temperature sets stratification, since the sun heats water, lightening it at the surface and enhancing its stability. The polar oceans are an anomaly to this trend because there salinity sets stratification as fresh, cool layers sit atop warm, saltier, deeper layers. This salinity stratification protects sea ice from stored subsurface heat, which, if bought to the surface, could delay ice formation or precipitate melt.

The Arctic Ocean poses a particular challenge in this regard because the present generation of climate models qualitatively misrepresents its stratification. Broadly, they predict surface waters that are too salty compared with real ocean observations. They also miss much of the interesting subsurface variability in salinity and temperature, such as the warm, salty layer of Pacific water that flows into the western Arctic in the summertime. Thus, to leverage models as a powerful tool to understand the Arctic Ocean's state now and into the future, we must understand why they fail to replicate its stratification and complex dynamics as observed in nature.

One aspect that interests me is the role of eddies in modulating Arctic Ocean stratification. These are swirling water masses, the oceanic equivalent of atmospheric storms and weather patterns. As they move, they can trap and transport seawater, nutrients and marine life and play a significant role in global ocean dynamics.

'From years of debugging code and fixing faltering hardware as a researcher, I've learned that the simplest solution often is the best.'

Before the SASSIE expedition, I was most familiar with using numerical models to study the atmosphere and seas. These take the governing fluid dynamics equations and cast them onto a grid of points spanning the region we're modeling, allowing us make predictions about how fluid flow will evolve.

Large-scale climate models can't track individual raindrops, wind gusts or waves. So, to account for the cumulative impact of an uncountable number of tiny components, we parameterize processes that are too small for our models to resolve – we define their effects based on observed, real-world values. To develop these parameterizations, we must understand the ocean's physical state, which requires observations like those the SASSIE campaign collected.

For my Ph.D., I intend to help bridge the gap between modeling and observational oceanography, working with a variety of models plus ground-truth measurements to understand the oceanic system from multiple perspectives. Our models are better, and thus our science is better, when we have the measurements to back them up.

Eddies are computationally challenging. Their small size means models must have high enough resolution to capture their dynamics, or instead must accurately parameterize their effects. Furthermore, eddy structure depends on stratification, so any model errors in this property will lead to inaccuracies. The data I helped collect on the SASSIE cruise will let me contribute to a theoretical understanding of eddies and their impact on the near-surface Arctic Ocean, with the goal of linking them to impacts on ice formation.

The specter of climate change looms over all earth science disciplines, motivating the urgency of our work. As a computational scientist, I plan to contribute to the next generation of climate models, giving us tools to monitor the climate in the present and make predictions.

Conducting research can sometimes feel like acting as a tiny raindrop, individual wind gust, or lone wave – but the cumulative impact of this work will bring us closer to understanding our climate system. And, in this way, I hope to do my part to protect it – one frozen boat hook, or frozen computer, at a time.

FEEDING SUPERMASSIVE BLACK HOLES

With a leading model, a fellow teases apart the most awesome objects in the cosmos.

By Jacob Berkowitz

When Lindsey Byrne arrived at Iowa's Grinnell College in 2014 to begin a physics undergraduate degree, she had an inkling the stars might play a role in her future. She'd loved astronomy sleepover camp as a middle schooler and was attracted to Grinnell partly because of its small observatory. But she wasn't expecting to discover a powerful new way of exploring the cosmos: via computing.

"When I heard about computational astrophysics, I thought it seemed really cool," says Byrne. "The limited exposure I had to astronomy before that was to observational astronomy. I had not thought about computational, theoretical astrophysical simulations, so it was definitely a new perspective. But I've always had an interest in computers and computation, and I was interested in developing more of those skills."

With Grinnell astrophysicist Charlotte Christensen, Byrne simulated the influence of dust shielding on star formation. That led to a 2019 first-author paper in *The Astrophysical Journal*.

Now on a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) at Northwestern University, Byrne uses a leading cosmological model and supercomputers to elucidate the galactic role of some of the most awesome objects in the cosmos: supermassive black holes.

"Typically, when we think of black holes, we think of ones that form at the end of the lifetime of a massive star," Byrne says. "The supermassive black holes I'm studying are much bigger than that; they're millions or billions of times the mass of the sun and they exist at the centers of most, if not all, galaxies." The most famous of the supermassive black holes – or SMBHs for short – is Sagittarius A* at the core of our Milky Way galaxy.

In modeling the place of SMBHs in galaxy evolution, Byrne is addressing a cosmological grand challenge: bridging the vast scales involved. Cosmologists focus on dark matter and dark energy and the emergence of large-scale structure, with galaxies often the smallest resolved elements in their models. For astrophysicists, galaxies are the big structures, the birthing grounds of stars.

Credit: Bonnie Robinson.

A model called FIRE – for feedback in realistic environments – attempts to integrate across these vast cosmic scales, says Byrne's advisor, Claude-André Faucher-Giguère, who co-created the code a decade ago as a postdoctoral researcher. The model creates cosmological simulations of galaxies from the Big Bang's initial conditions to today's observable universe. "What's novel about the FIRE simulations is that we also have resolution inside individual galaxies and can carry out physics calculations of how star formation occurs," he says.

Byrne's undergraduate work had involved hydrodynamical modeling. FIRE also does hydrodynamical simulations – fundamental physics models that integrate gravity (how matter is drawn together) and the hydrodynamics (temperature, pressure, density and movement) of the cosmic gas that clumps to form stars.

When it came to deciding on a graduate program, Byrne says Faucher-Giguère's lab offered the best of all worlds: a welcoming lab group of a half-dozen graduate students and post-docs that's also part of the larger, international and multi-university FIRE collaboration.

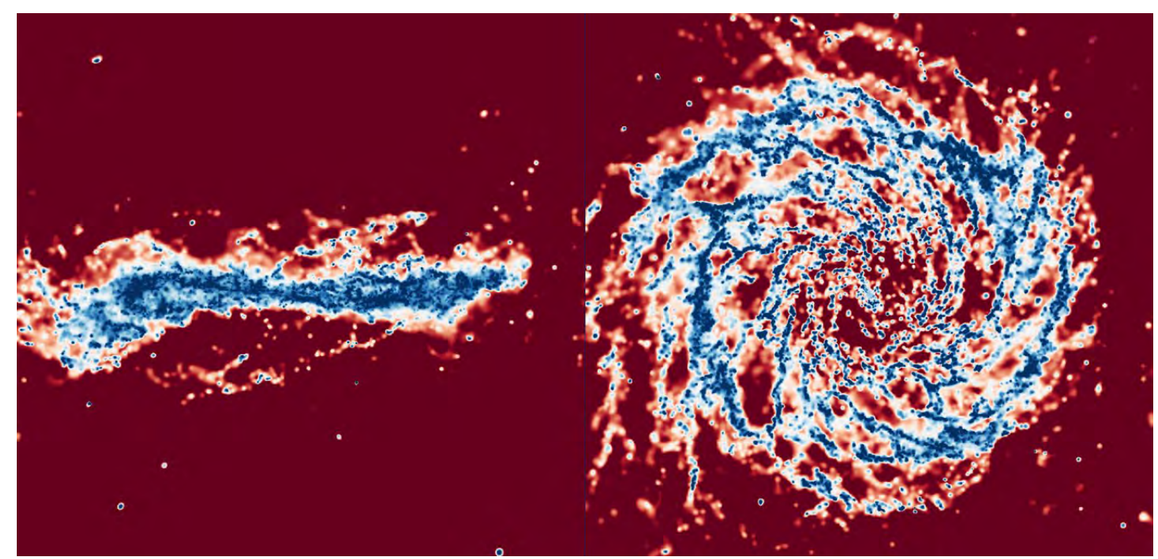
His group also provided an ideal foothold on the leading edge of computationally exploring black-hole dynamics. "Modeling the growth and feedback of supermassive black holes is a very important component of capturing the formation of galaxies," says Faucher-Giguère, an associate professor of physics and astronomy.

Earlier FIRE simulations had revealed two stages of SMBH growth: an intermittent stop-and-start stage followed by a tipping point leading to steady, much more rapid growth, Byrne says. Her initial thesis research has focused on explaining the physical basis for this growth transition, notably the key role of gas availability.

In a recent paper with FIRE collaborators at five other universities, first-author Byrne presented her analysis of 16 detailed galaxy simulations with sizes ranging from dwarf-mass to Milky Way-mass and beyond, exploring the factors involved in giant black holes' growth transition.

A black hole's gravity creates a surrounding, spiralling accretion disk of infalling gas. As the gas passes the event horizon – the point at which not even light can exit – it becomes part of the black hole. "A supermassive black hole grows by eating up the gas around it," Byrne explains. In this way, an SMBH can grow a thousand times more massive over the course of a billion years. "On an astronomical time scale, that's quickly."

But Byrne's analyses of the FIRE simulations, which ran on Northwestern's Quest and the Texas Advanced Computing Center's Stampede2 supercomputers, showed that during the early, low-mass period of SMBH growth, supernova explosions ejected gas from the galactic nucleus. This repeatedly starved the black hole and made gas accretion highly intermittent. "The SMBHs begin to grow more steadily on average once galaxies develop a stable gas reservoir," Byrne says.



A simulation of massive galaxies and their hot (red) and cold (blue) gases encircling supermassive black holes viewed edge-on (left) and face-on (right). These simulations use the FIRE (feedback in realistic environments) model. Following page: Another edge-on galaxy view with hot (blue) and cold (yellow) gases. *Credit: Lindsey Byrne.*

GREEN EVOLUTION

Princeton University's **Claire Zarakas** studies how plants can mediate and mitigate human-caused warming. But the opposite aspect – how climate affects plants – also fascinates the atmospheric sciences student. "Looking at both sides is really important and not something we give enough attention to as a scientific community," she says. Zarakas's simulations dissect plant-climate interactions, which models currently capture with only broad estimates of water and carbon uptake. There also are few observations of how elevated carbon dioxide affects tropical ecosystems, necessary information for improved models. Zarakas also studies how such uncertainties can affect physical climate projections.

LITTLE AND LUMINOUS

When **Lauren Zundel** joined Alejandro Manjavacas's nanophotonics lab as a University of New Mexico undergraduate, she knew she wanted to do physics research. Her focus immediately landed on how light interacts with materials at the tiniest scales, and she's worked in the same group ever since. For her Ph.D., Zundel has used high-performance computing to simulate how repeating particle patterns – arrays tens to hundreds of micrometers in size – behave and how to manipulate their responses to light. The results could help researchers develop novel thermoplasmonic devices that produce heat from light or new tools for solar energy applications.

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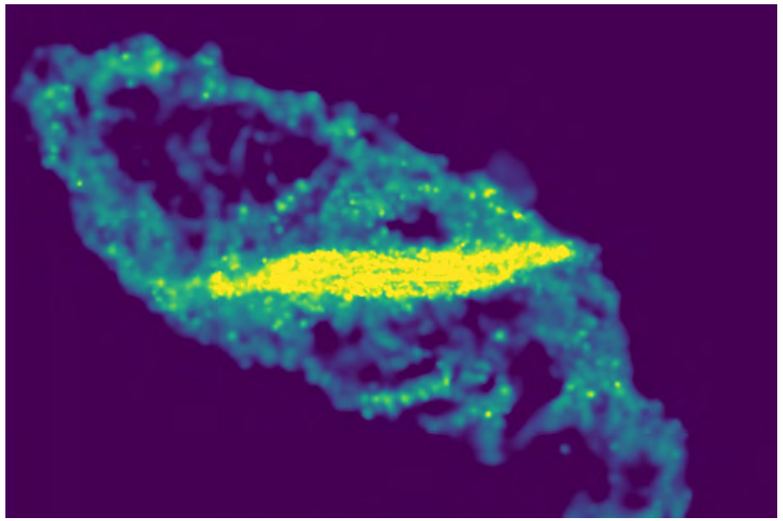


Determining the cause of gas reservoir stabilization proved harder than expected, she says. "Trying to understand what was actually going on and the theoretical basis led me to go down lengthy rabbit holes as I was trying to understand the things that I was finding, and as a result the project ballooned."

Her simulations revealed that, at the transition point, a galaxy's overall structure changed in major ways, including the total stellar mass, the black hole's mass and the inward pressure from gas in the medium surrounding the galaxy.

Says Faucher-Giguère: "It was a real challenge to try and disentangle the various elements. It's a complex interaction."

Notably, Byrne's computational conclusions make testable predictions about these black holes that the James Webb Space Telescope might detect for the first time in early, low-mass galaxies. The FIRE simulations predict that these starved black holes will be smaller than the currently observed SMBH-to-galaxy scaling ratio predicts.

In a second phase of her thesis research, Byrne models how well-fueled SMBHs, also called active galactic nuclei (AGN), come to play a critical role in energetically shaping galactic evolution. "SMBHs give off incredible amounts of energy as they grow, and this energy could have a substantial impact on how the galaxy around them grows and evolves," she says.

Her AGN thesis research is informed by her autumn 2021 practicum with Zarija Lukić, a research scientist at Lawrence Berkeley National Laboratory's Computational Cosmology Center. Lukić is a principal author of Nyx, a highly parallel hydrodynamics solver for cosmological simulations. Byrne updated and further developed the code's AGN model, including porting parts from outdated Fortran code to C++ and, updating some computationally intensive parts to run on graphics processing unit accelerators, boosting the model's efficiency.

In September 2022 Byrne traveled to Reykjavik, Iceland, to present at a conference called What Drives the Growth of Black Holes: A Decade of Reflection. The event was a transition for the computational astrophysicist, now making discoveries in her own right, she says. "People were interested in my research and asked lots of questions."

LEARNING CLIMATE

A Colorado State fellow employs machine learning for climate modeling, putting provenance behind predictions.

By Thomas R. O'Donnell

Weather so fascinated Jamin Rader in his high school years that he would compile forecasts for analysis. He went to websites – weather.com, Accuweather, the National Weather Service and others – to collect data, then calculated the most probable outcomes.

Rader, a Colorado State University climate dynamics doctoral student, didn't know then that he was creating an ensemble forecast. "It's funny how much of what I did as a kid is actually, in a lot of ways, what I do now."

It wasn't until his parents told him, however, that Rader understood his obsession could be his career. Now the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient applies machine learning to atmospheric science and climate, probing predictability in forecasts extending months, years and beyond.

Machine-learning techniques are relatively new to his field, Rader says, so he can "explore their capabilities that we don't fully understand yet and, maybe even more so, explore their limitations."

One aspect of Rader's research is capsulized in the difference between two phrases, *this looks like that* and *this looks like that there*. They relate to interpretable neural networks, which seek to resolve a major machine-learning issue: how it works is mostly a mystery.

In simple terms, researchers feed neural networks and other machine-learning models known information – in this case, weather maps and data. This trains them to identify similar features in unlabeled, previously unseen data, then extrapolate predictions from them. The approach is powerful, but "the how-and-why the model makes its predictions is inscrutable," says a July 2022 *Journal of Advances in Modeling Earth Systems* paper Rader coauthored with his advisor, Elizabeth Barnes, and two others.

Few models are always perfect, Barnes says, so scientists need reasons to trust their results. Interpretable models provide them, with information on how the algorithms reached their predictions. "Purely understanding the approach can be incredibly helpful for gauging trust" in a model's output.

Credit: Jayme DeLoss.

Machine-learning models also can be overfit – learning to rely on meaningless noise that doesn't reflect the real physical world. To make a network interpretable, researchers usually constrain the model, forcing it to learn in specific ways, Barnes says. "You've tied its hands, if you will, a bit." Those constraints, however, often provide a better result because the model is more likely to learn the real physical relationships rather than spurious ones.

Rader says the interpretable machine-learning approach "comes from the idea that we can make neural networks that think a little bit like us," helping scientists understand more complex aspects of climate and climate predictability.

For the paper, the team extended the prototypical part network (ProtoPNet) that Duke University's Chaofan Chen and colleagues described in a 2019 publication. ProtoPNet's approach, focusing on bird classification, is *this looks like that*. Much as a human ornithologist would, the technique identifies the species of previously unseen birds by comparing images of them with prototypes – examples of known species from training data.

The advantage: ProtoPNet's decisions can be linked to features found in both the input bird image and in a relatively small set of species-specific training prototypes, the *Advances in Modeling Earth Systems* paper says. That shows how the algorithm made its prediction.

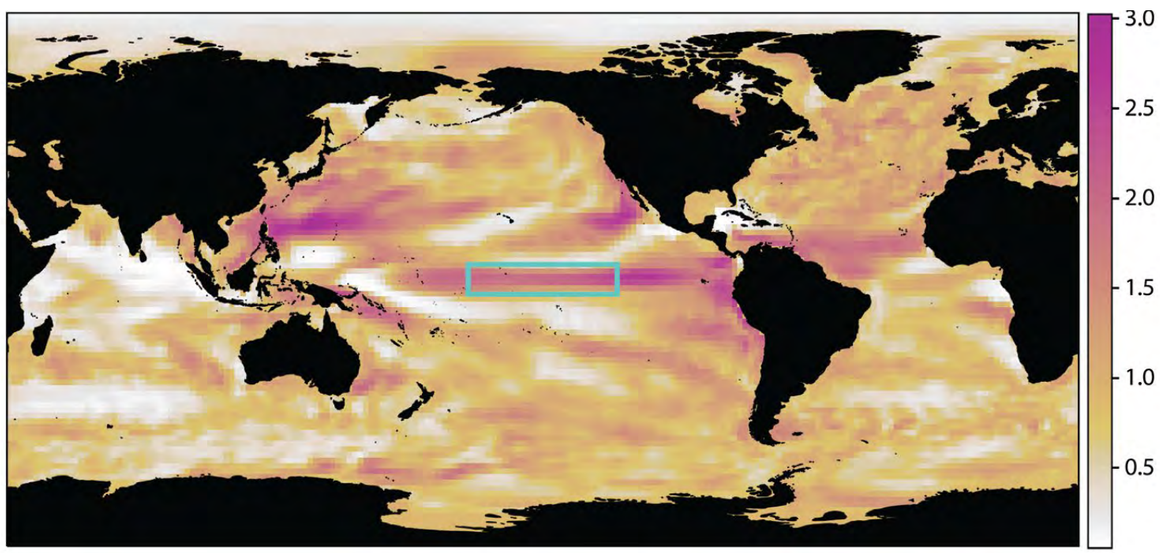
Barnes, Rader and their colleagues added location to ProtoPNet, extending it to *this looks like that there* and naming it ProtoLNet, for prototypical location network. For weather and climate forecasting, a neural network must do more than identify similar features in data, Rader says. The features also must be in similar locations. Greater convection and rainfall over the western Indian Ocean, for example, may herald a cyclical rainfall pattern. In another place, such as over land or another ocean, they may indicate something different.

With ProtoLNet, researchers can see the set of past patterns the code used to produce a forecast. The team believes the approach is useful for science, but "we also hope it will inspire other scientists to improve upon these methods."

Now Rader is devising an interpretable neural network from scratch, Barnes says, exploring how to "develop other tools that are applicable to different types of climate problems that *the this looks like that there* algorithm is not right for."

Life has forced Rader to innovate. He was 18, a high school cross-country runner, when he felt ill on a Sunday night and went to bed. He rose when he realized something was wrong.

What happened next, he says, was "almost cinematic, like 'steps out of bed, the next step isn't quite as strong, the third step is, oh man, I need to lay down on the ground.'"



Regions of importance, as learned by an AI model, for predicting wintertime Niño3.4 sea surface temperature (SST) anomalies – indicators of central tropical Pacific El Niño conditions – given wintertime SST anomalies a year before. Purples highlight regions that are most important for predicting the anomalies, while whites highlight regions that are not important for predicting them a year in advance. The teal box indicates the Niño3.4 region the machine learning task targets. *Credit: Jamin Rader.*

Rader had transverse myelitis. Doctors believe his immune system attacked his spine, damaging its nerve fibers and paralyzing his lower body.

Going from able-bodied to paraplegic in minutes was difficult, but Rader says he benefitted from the chance to radically improve. It was "a huge challenge where I get to get really, really good at something." Each day he could "experience being better, even if that started off as just being, 'now I can sit up.'"

Rader spent the summer after his University of Washington freshman year studying weather and climate at the University of Oklahoma. For another three summers he was at the University of Colorado Boulder under SOARS (Significant Opportunities in Atmospheric Research and Science), a program for underrepresented groups. "That was when I made the transition from wanting to do weather and weather forecasting to being more interested in large-scale climate problems."

During his 2021 virtual Pacific Northwest National Laboratory practicum, Rader worked with earth scientist Po-Lun Ma to improve how autoconversion – cloud droplets colliding to form rain – is represented in DOE's Energy Exascale Earth System Model (E3SM).

Autoconversion and how aerosols – tiny airborne particles – affect it lead to uncertainty within earth systems models, says Ma, who oversees a multi-institutional effort studying aerosols and their interactions with clouds. Present models use a 20-year-old approach based on data from a single cloud type. Studies found they don't effectively describe autoconversion under other conditions.

Rader used cloud measurements from DOE and other agencies to calculate autoconversion rates under various circumstances. He identified important factors affecting autoconversion and built a prototype machine learning-based emulator that accurately simulates it, but with a low computational cost.

Lab researchers will evaluate the approach's performance, including within E3SM, DOE's flagship Earth systems model, to determine whether it improves on the standard method. "Then this can be part of the next-generation E3SM," Ma says.

Rader expects to graduate in 2024. He'd like to continue working with machine learning, but he avoids making plans because they rarely develop as expected. Instead, "if you just ride the wave, you'll get to the right spot."

Alongside research, Rader visits elementary schools a few times each year to talk about weather with students. His presence shows "you don't have to be a typical white-lab-coat scientist we see in old books. You can be a young disabled scientist."

Barnes marvels at Rader's energy, enthusiasm and quick grasp of difficult concepts. "He's undaunted by technical skills that he may not have yet," eagerly learning new approaches. "That's something that's so fun with him."

Rader spends much of his off-research time playing and traveling with a sled hockey team. "It's the sport that most emulates the feeling of running," he says. When racing across the ice, "it's the closest thing to freedom that you can get."

Continued from page 12

TAKING CHARGE

Thermodynamics uses few variables to describe chemical systems, but the ones **Christopher Balzer** studies are complex. "That's what keeps me interested," says Balzer, a Caltech chemical engineering Ph.D. candidate. "When you do get an answer, it's quite satisfying." He focuses on polymers, chains of similar atomic units, and polyelectrolytes, in which some units carry a charge. Both are found in everything from shampoos to adhesives. Balzer's models help experimentalists understand how to fine-tune the compounds. For example, he and two colleagues, including advisor Zhen-Gang Wang, studied polyelectrolyte complex coacervates – oppositely charged polyelectrolytes. When combined they can generate droplets that wet solid surfaces. Balzer found that manipulating the surfaces' electrostatic condition can control wettability, an important finding for adhesives and other applications.

HARNESSING QUBITS

The nascent nature of her quantum algorithm research engrosses Harvard University's **Madelyn Cain**. The computers she taps use qubits, which can be 1 and 0 simultaneously, promising to vastly accelerate calculations. Cain studies combinatorial optimization, problems that seek the best solution from myriad options by finding a system's lowest energy state. "It's expected that no computer can really solve these problems efficiently because it's so difficult." For a *Science* paper, Cain and an international team tested algorithms for one such puzzle on a quantum computer composed of 289 coupled qubits. The team found significant speedup over classical algorithms in some instances, depending on difficulty. Sometimes the fragile qubit configuration deteriorated before completing its calculations. Cain is developing new algorithms to improve performance.

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SHORING UP SHIPPING

Building on his nuclear security interests, a fellow simulates strategies for scanning cargo containers.

By Andy Boyles

Whether stacked on ships, aligned on rails or cruising highways, cargo containers are the lifeblood of international commerce.

They're also a potential security vulnerability. For his Ph.D. at the Massachusetts Institute of Technology, Peter Lalor simulates ways to non-intrusively scan cargo containers for nuclear materials, shoring up shipping safety.

More than 30 million cargo containers enter the United States annually, and they could carry smuggled goods, including nuclear materials. The infiltration and detonation of a nuclear device this way is exceptionally unlikely, says the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient, but the human and economic consequences of such an incident at a major port or border crossing would be devastating.

Lalor understood nuclear security's significance long before he chose to work in the field. He grew up near Lawrence Livermore National Laboratory and interned there for three summers as a University of California, Berkeley, physics undergraduate. "You show up, and there are guards with rifles and everyone's talking about nuclear bombs all the time," he says. "So that was the intro to nuclear security."

Initially, he focused his undergraduate studies on dark matter. But in his first Livermore research project, Lalor worked on computer simulations aimed at wringing optimal statistical power from imperfect (and classified) imaging scenarios. Next, he tried nuclear engineering with Bethany Goldblum's Berkeley group, helping simulate methods to detect contraband nuclear materials via their neutron emissions.

Credit: Martha Stewart.

With Goldblum's encouragement, Lalor applied to graduate programs in nuclear engineering, landing in Areg Danagoulian's MIT group. Danagoulian uses computational and experimental physics to design methods that reduce nuclear threats. For example, the team wants to improve the detection of special nuclear materials, such as plutonium and uranium, that adversaries might smuggle into the United States.

A nuclear security purpose also drove Lalor's 2021 DOE CSGF practicum at Los Alamos National Laboratory with Emily Casleton, deputy leader of the statistical science group. Lalor helped model radioactive materials transport in a nuclear facility, laying the groundwork for simulating comparable activities at places that house different nuclear material types behind various shield arrangements.

U.S. Customs and Border Protection screens every cargo container that enters the country and scans high-risk ones with penetrating radiation. Lalor's Ph.D. centers on improving such devices.

A cargo scanner projects dual radiation beams of different energies to image what's inside. The beams are in the range of several millions of electron volts (MeV), up to 100 times higher than a medical X-ray. Those scans flag materials based on their density – large quantities of uranium or plutonium, for example, or the lead or tungsten used for shielding.

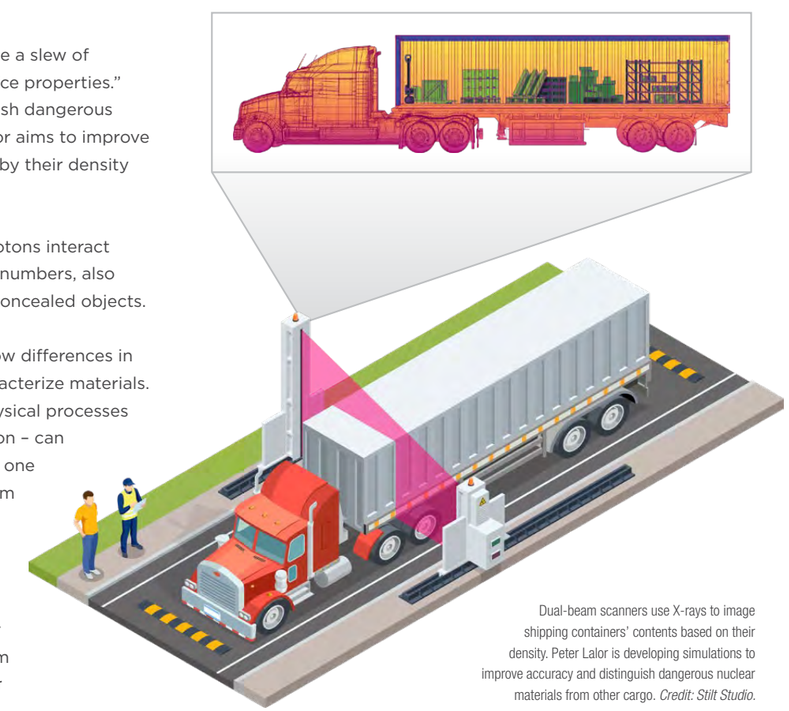
"When you go to higher energy, you introduce a slew of problems," Lalor says. "You lose all sorts of nice properties." Today's cargo scanners can't always distinguish dangerous materials from benign dense substances. Lalor aims to improve scanners' ability to detect materials not only by their density but also by chemical makeup.

Applying the physics of how high-energy photons interact differently with atoms based on their atomic numbers, also known as Z, Lalor looks for ways to identify concealed objects.

He started with simulations that examined how differences in transparency to X-rays could be used to characterize materials. He discovered that competition from two physical processes – photoelectric absorption and pair production – can make high-Z materials indistinguishable from one another. The two processes block photons from passing through materials and reaching a device's detector. In the former, an atom absorbs a photon and ejects an electron. A different electron replaces it, emitting another, lower-energy photon. In pair production, a photon interacting with an atom generates both an electron and its antimatter counterpart, a positron.

To test whether materials might be sorted based on Z, Lalor simulated how well the lower- and higher-energy scanner beams penetrated individual objects inside a container. At lower energies, photoelectric absorption blocked more incoming photons than other processes, capturing them as they collided with atoms. Pair production becomes increasingly important at higher energies. Boosting photon energy increased the pair production rate – and lowered the photoelectric absorption rate. As atomic number increased, the probability of both interaction processes also increased. Therefore, most materials were more transparent to one beam than the other. The ratio between the high-beam and low-beam transparencies handily sorted steel from aluminum, for example, and both of those from carbon. Greater differences between the two beams' energies produced both larger transparency differences and more accurate atomic number estimates.

But these dual-beam cargo scanning systems have limits. They can't distinguish much heavier materials – plutonium, uranium, lead and tungsten – from each other and are less accurate on thinner chunks of material. In such substances, the photoelectric effect becomes so significant that it begins to outcompete pair production, giving the same measurements for different materials.



Dual-beam scanners use X-rays to image shipping containers' contents based on their density. Peter Lalor is developing simulations to improve accuracy and distinguish dangerous nuclear materials from other cargo. *Credit: Stilt Studio.*

Continued from page 15

MUTUAL ATTRACTION

Gabriel Casabona has probed the astrophysics underpinning space's densest objects. Much of his Northwestern University research has revolved around unique features of merging neutron stars, whose superfluid interiors and solid exteriors cram the sun's mass into a Manhattan-sized area. He's modeled the dynamic physics at their centers and examined the extreme forces when these objects interact. For his Los Alamos National Laboratory practicum, Casabona modeled how the intense gravity between neutron stars could crack their crusts, releasing energy surges. Casabona already belongs to a large international mission – the Laser Interferometer Space Antenna (LISA) – that will detect gravitational waves from space and is scheduled to launch in the next decade. After Northwestern, he hopes to join NASA's core LISA team.

DOWNSIZING TASKS

Scientists with big data puzzles come to researchers like **Koby Hayashi**: computer scientists able to shrink tasks. "We want to reduce the size of problems in a way that is theoretically sound," says Hayashi, a Georgia Institute of Technology student. In one project, Hayashi and colleagues implemented low-rank approximation with parallel processing and GPUs. They used nonnegativity constraints, ensuring the calculations produce numbers 0 and greater for improved interpretability. To do this, they created the PLANC code, for parallel low-rank approximation with nonnegativity constraints. On Oak Ridge National Laboratory's Titan, the code ran up to seven times faster than on standard processors only. PLANC also scaled well when analyzing mouse brain images. Now Hayashi focuses on randomized methods that quickly encapsulate key data aspects.

MESHING MODELS

Climate researchers use both complex and simplified models because each has its strengths. But what if the two types could mesh? University of Wisconsin-Madison's **Jason Torchinsky** and Ph.D. advisor Samuel Stechmann, a DOE CSGF alumnus, have sought to link models so they communicate as they compute. They've shown that a simulation could rely on one model that accurately predicts the climate's mean state but use another better suited to understand moisture variability. "The idea is to get them to communicate relevant information," as if they were collaborating on a project, Torchinsky says. Researchers could apply the idea to other scientific areas that have models with complementary strengths. During the COVID-19 pandemic, Torchinsky founded a virtual monthly meetup for DOE CSGF recipients and alumni.

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Armed with models for various photon fates, Lalor compared his transparency techniques with traditional cargo-scanning approaches. Those methods based their probes of container contents on empirical databases built from scans of many material samples. The techniques take an X-ray image and match its characteristics with reference materials in an empirical database.

Because he lacks the security clearances to access such data, Lalor compared his earlier simulations with an off-the-shelf model that assumes that all detected photons simply pass straight through a container and its contents without interaction. As he expected, that approximate model was only somewhat accurate for identifying material transparencies.

Lalor wanted to improve that old model with a semi-empirical approach that accounted for photons that reach the detector after interacting with the material. He incorporated a physical effect called Compton scattering. In this case, a photon interacts with an atom's outer electron. Instead of being absorbed, the photon loses some of its kinetic energy and caroms off in a new direction. As is well known, Compton scattering deflects many photons away from the detector, but some are diverted only slightly and still strike it. Other photons can be scattered twice, zig-zagging their way to the detector.

This semi-empirical model represents materials not just through the photons they block but also through those that reach the detector via these circuitous pathways. Using simulated scans that mimicked empirical data, he showed that just three scans could generate enough data to distinguish a range of materials of various thicknesses. As a result, the new, semi-empirical model, based on Lalor's transparency simulations, was an improvement. Compared to the off-the-shelf model, it wrangled materials' outcomes into alignment with their true values, flagging them by their atomic numbers. "Here's a more accurate model that we can use in the context of these systems, which would enable more accurate material identification," he says.

Eventually, Lalor would like to see his semi-empirical approach tested in the field, fine-tuning it with data from actual container scans. His next logical step would be to verify and develop his findings, perhaps by collaborating with investigators whose security clearance would give them access to experimental data. However, establishing such partnerships is a challenge in this field.

Until he does, Lalor is moving forward the best he can, simulating loaded containers. "I would love to have access to infinite data," he says. "But that's a problem that every Ph.D. student in my situation runs into, which is that this is stuff that the national labs are doing, and it's harder as an academic. You have to kind of approach it at a different angle."

DECISIVE ACHIEVEMENT

A third-year fellow models COVID-19 virus variants and examines how people weigh complex decisions.

By Sarah Webb

When COVID-19 loomed as a public health threat in early 2020, Danilo Pérez-Rivera was a neurobiology research technician at the University of Puerto Rico Medical School and applying to graduate school. The pandemic was poised to exacerbate entrenched challenges on the island, including a lack of health leadership and a medical personnel shortage. Though only 24 years old at the time, Pérez-Rivera was recruited as part of an interdisciplinary team of scientists, mathematicians, engineers and artists to fill an urgent need: building a data-based system to track testing, hospitalizations and more as the foundation of the island's pandemic response.

The effort, now known as SMICRCPR (the Spanish acronym for the Puerto Rico Municipal Case Investigation and Contract Tracing System), eventually grew to more than a thousand people, with Pérez-Rivera the project's scientific advisor and keeper of the data dashboard and its website's daily updates. Even after he chose New York University for graduate school, he delayed his move until January 2021 to support the team's work.

The project demonstrates how Pérez-Rivera has applied his broad interests in math, health, neuroscience, chemistry and computing to societal problems, particularly in Puerto Rico, his mother's birthplace and his home since he was 8. "When I saw science could save lives, I really wanted to dedicate myself to do something meaningful so that I was contributing to my community."

Credit: Hollenshead/NYU Photo Bureau.

Pérez-Rivera has continued that work as a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient. During his 2022 Argonne National Laboratory practicum, he contributed to an artificial intelligence-based model, GenSLM, that predicted how new SARS-CoV-2 virus variants evolve. That project was awarded the 2022 Gordon Bell Special Prize for High-Performance Computing-Based COVID-19 Research.

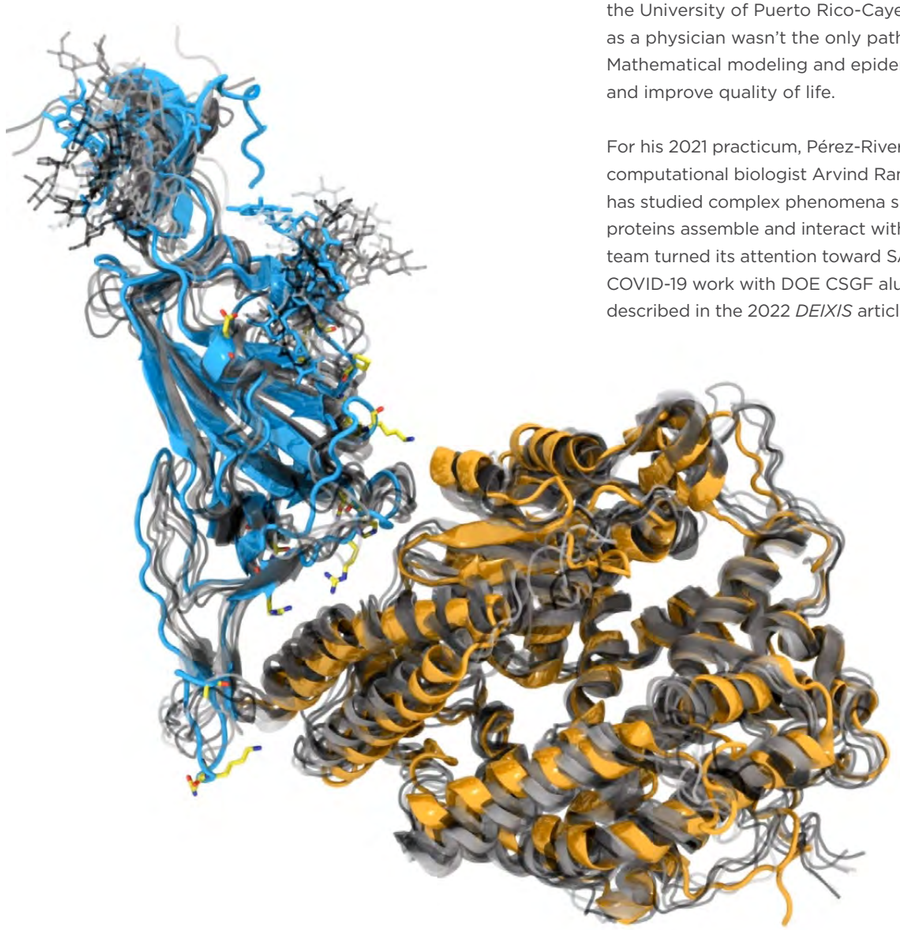
He grew up in Puerto Rico public housing. In school, Pérez-Rivera stood out in English because, born in the Bronx, it was his first language. His teachers encouraged him to pursue technical subjects. The rules and precision, particularly in math, appealed to him because other parts of his life felt unstable, he says. "It's having a clear set of structures that you could operate within and generate creative, self-sustaining solutions."

Pérez-Rivera's mentors helped him gain admission to the Puerto Rico Department of Education's flagship residential school, 90 minutes from home. Advanced electives there introduced him to scientific research, and he made friends who shared his love of rocks and the stars.

Through Math Olympiad competitions, he learned about modeling and became interested in generating problems and experimenting with ideas that could be tested with simulations and derivations. Pérez-Rivera pursued an undergraduate major in chemistry because it was interdisciplinary – and required both quantitative and experimental work. "I felt like it would give me the basic tools I would need," either to pursue medicine or to study astrochemistry and more. He did a research project modeling Type 1 diabetes, an interest that became personal because his then-girlfriend had the disease.

Pérez-Rivera's mentor on that project, Mayteé Cruz-Aponte of the University of Puerto Rico-Cayey, showed him that working as a physician wasn't the only path to improving health. Mathematical modeling and epidemiology could guide policy and improve quality of life.

For his 2021 practicum, Pérez-Rivera worked with Argonne computational biologist Arvind Ramanathan. Ramanathan has studied complex phenomena such as how disordered proteins assemble and interact with small molecules, and his team turned its attention toward SARS-CoV-2 in 2020. (Earlier COVID-19 work with DOE CSGF alumna Anda Trifan was described in the 2022 *DEIXIS* article, "Decoding Disease.")



The GenSLM algorithm used an AI-based model to predict COVID-19 variants of concern, an achievement that was recognized with the 2022 Gordon Bell Special Prize for HPC-based COVID-19 research. Here the blue and yellow ribbons show the model's predicted variant of the SARS-CoV-2 spike protein laid over the protein structure observed in the BQ.1 variant (gray), which was widespread in late 2022. *Credit: Defne G. Ozgulbas/University of Illinois Urbana-Champaign.*

Pérez-Rivera joined a 30-person team working on the AI-based language model designed to analyze viral genes and rapidly identify how they could mutate into potentially harmful variants. These models are expensive to train, so the team wanted to study individual proteins for gene variations of interest.

Working closely with Argonne's Max Zvyagin, Pérez-Rivera curated data for the SARS-CoV-2 spike protein and ran an initial analysis that helped the team identify sequence clusters tied to later variants. Ramanathan notes that the result "let us prepare for the GenSLM models, which is a much larger-scale effort."

Although the team trained the model on data from the pandemic's first year only, he says, "we were able to robustly identify what would eventually emerge to be the variants of concern, such as omicron, and even BQ.1. And how we did that is really a testament to how far artificial intelligence has brought us."

For his NYU doctoral research, Pérez-Rivera studies value-based decision-making, or how humans or animals make choices centered on the options' perceived worth. This fundamental neuroscience question has applications in policy, economics and medicine. Understanding why people make certain choices can unearth bias and help nudge people toward better decisions.

In a classic scenario, a person might be offered $5 immediately but could hold out for the result of a coin flip and receive either $10 or nothing, Pérez-Rivera says. If the decision involves higher stakes – thousands or even millions of dollars – the person might choose differently. A host of other factors, such as mental health and neural differences, can alter how an individual weighs the options. Members of Christine Constantinople's NYU lab have been studying the relevant reward circuits in rats' brains to see how they respond to these sorts of situations, and the team will do related studies in humans.

Pérez-Rivera also works with NYU's Cristina Savin to build computational models that help researchers tease out dynamic factors and neural differences that drive individual choices. Motivation, attention and how recently a subject has received a reward each work on different but interacting timescales, Constantinople says. Most methods for characterizing neural activity have focused on a single timescale.

Pérez-Rivera expects to finish his Ph.D. in 2025 and plans to bring his technical skills and research connections back to Puerto Rico. Whether a career in academia, government or the private sector, he's certain of one thing: "I very much see myself pursuing what I call citizen-facing science."

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WASTE NOT

With a father in the field, **Michael Toriyama** was raised in materials science. Now a Northwestern University Ph.D. candidate, he seeks high-efficiency thermoelectric materials that convert heat to electricity. "Imagine being able to harness all or most of the energy expelled as waste heat from, say, nuclear power or industrial plants, and converting that into usable electrical energy," Toriyama says. His computational chemistry simulations focus on topological insulators that conduct electricity at the surface but are insulating underneath. The compounds are usually used for things like low-temperature superconductors. He was part of a team that simulated a compound of the abundant elements sodium, calcium and bismuth that could have high thermoelectric efficiency, even at room temperature. It's a possible replacement for chemical coolants in air conditioners and refrigerators.

DIVIDE AND CONQUER

Stanford University Ph.D. student **Amalee Wilson** applies HPC techniques to a problem that has been difficult to parallelize: solving satisfiability modulo theories (SMT). This automated reasoning strategy can decipher myriad problems, from room scheduling to verifying that computer hardware designs work as intended, but it's devilishly difficult to break into digestible pieces that can be computed across multiple processors. Until recently, researchers who'd tried parallelization found that dividing an SMT problem could result in worse performance. Wilson has developed an algorithm that splits these tasks and improves performance. After finishing her Ph.D., she plans to seek a research position at a national laboratory or in industry.

TOPOLOGY TO BIOLOGY

As an undergraduate, **Boyan Xu** was a pure mathematician, but he then started his University of California, Berkeley, Ph.D. using topology to decode neuron firing in rats, keying on signal patterns to map a roaming rodent's location. With Ksenia Krasileva, he also has modeled how plants' immune proteins acquire mutations to fight pathogens. Xu recently returned to topology to incorporate shape features within AI-based protein structure prediction, work that can help biologists understand forces that constrain evolution. Increasingly, Xu thinks of himself as a biologist. "I love working with organisms, and I love thinking about evolution." During an ORNL practicum with Dan Jacobson, he used mathematical approaches to discover associations between and infer functions of plant genes in a known network.

STATISTICALLY SIGNIFICANT

A LANL statistician helps cosmologists and epidemiologists grasp their data and answer vital questions.

By Thomas R. O'Donnell

Applied statistician Kelly Moran spans disciplines at Los Alamos National Laboratory (LANL) like a journeyman carpenter, dipping into her mathematical toolbox to help researchers make discoveries.

"We want to make sure their data are what they need to answer that question and build models and systems to help them do the answering," she says.

Moran joined LANL's Statistical Sciences Group in the Computer, Computational and Statistical Sciences (CCS) division in 2020 after working at the lab occasionally over five years. While a Clemson University undergraduate, she contacted a LANL epidemiology group about a paper it produced – and got a job there. Moran left after a year to pursue a Duke University statistics doctorate with a Department of Energy Computational Science Graduate Fellowship (DOE CSGF), leading to 2017 and 2018 practicums and a 2019 summer job at Los Alamos.

Her early projects mostly focused on epidemiology, analyzing data, such as internet search traffic, to forecast global disease and medical trends, but Moran has expanded to other fields since joining LANL permanently.

"At Los Alamos, the opportunity to work on lots of different application areas is easy to come by," she says. It's often "saying yes or being in the room when someone happens to say they need a statistician." More options "means more chances to cherry-pick what I want to work on."

Moran's latest research takes her to space. She analyzed data from the Interstellar Boundary Explorer (IBEX), a NASA satellite that collects data used to map the heliosphere, where the sun's particles meet outer space. IBEX has three particle-detecting sensors – including one LANL technicians built – whose data can track interactions between the heliosphere and space. Those passing through all sensors are qABC (qualified ABC) events, "our gold standard observations," Moran says. But qBC events, in which just two specific instruments detect particles, also interest astrophysicists and are more plentiful than qABC events.

Moran explored whether the same underlying heliosphere signal could produce both kinds of events. She generated the statistically most likely heliosphere signal based on the data and found that the two event types could plausibly share it.

Moran also helps probe cosmic structure, writing an emulator – a simpler surrogate for computationally demanding code – to predict the matter power spectrum for the Mira-Titan Universe simulation. This model was devised by an international team, led by Argonne National Laboratory researchers, and named for the two DOE supercomputers it ran on.

The matter power spectrum contrasts matter's density – the degree to which it clumps – between relatively small, local scales and a universe-wide scope. Large-scale structures grow linearly; theory is sufficient to describe them. Smaller-scale structures develop more randomly, requiring demanding simulations.

Moran based the emulator on data from 111 high-resolution simulation runs. The model spans multiple scales and lets researchers tweak parameters, such as dark-matter behavior, to grasp their influence on cosmic structure. She used statistical modeling to learn the relationship between these parameters and the resulting matter power spectrum so that supercomputers can make predictions at new parameter settings in seconds instead of weeks.

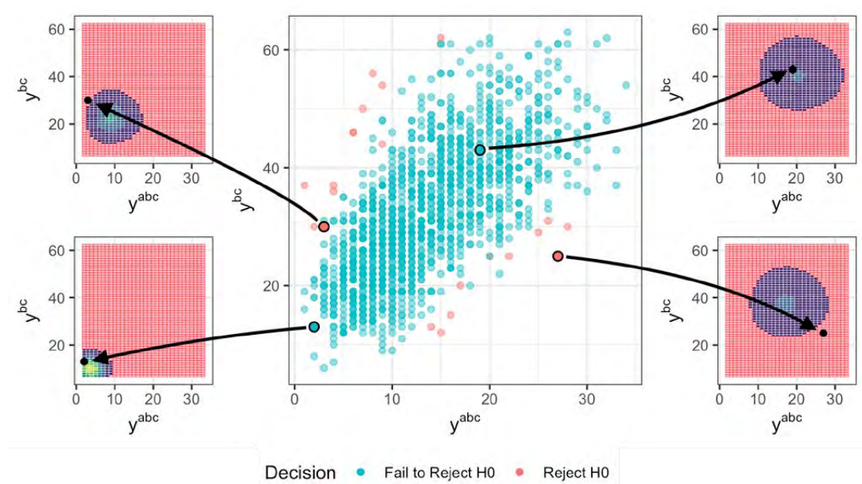
In 2021, Moran studied the spread of viral variants during the COVID-19 pandemic. With statistician Lauren Beesley and other colleagues, she analyzed data to understand what influences the speed with which mutant strains, such as delta and omicron, become dominant. "We were looking at how those takeovers happened across different locations, both national-level and some subnational-levels" to track the role of demographics, such as age and vaccination rates.

The researchers found a country's strong natural immunity, following recent COVID-19 infection peaks, was associated with a later transition to a new variant compared to other countries. Higher vaccination rates often led to slower transitions to variants, but not always: omicron resisted vaccine-produced antibodies.

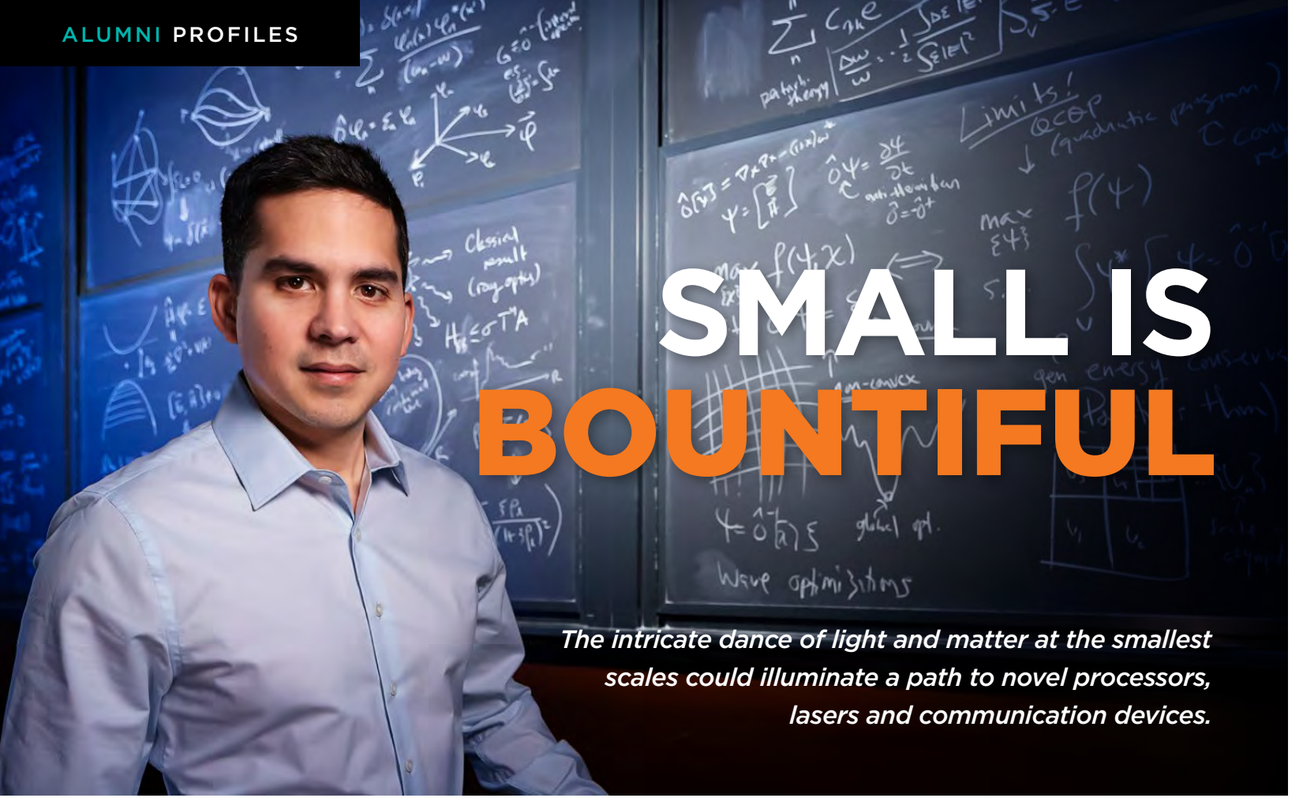
Moran has used her coding skills to help automate the LANL Occupational Safety and Health Division's system to test and monitor employee health and hazard exposure. She's also on a CCS panel that fosters social, professional and funding opportunities for early-career and new LANL workers. She uses the role to promote the Statistical Sciences Group's warm and open culture throughout the division.

Moran was the only woman in her Ph.D. cohort. "I identify as under the LGBT umbrella," too, and science "doesn't always feel like a friendly place" for either group or for people of color, she says. "Trying to make small steps so that that isn't true feels like an important task."

'We want to make sure their data are what they need to answer that question and build models and systems to help them do the answering.'



For each pair of qABC and qBC event counts, denoted y^{abc} and y^{bc}, seen during an orbit of the IBEX-Hi satellite, Kelly Moran and colleagues tested a hypothesis: that some shared underlying signal rate could plausibly have generated both counts. The center plot shows hypothesis test results for each observation. The four highlighted observations point to sub-plots showing the regions in which the hypothesis would be rejected (pink) and where the count pair actually fell (black points) in the subplots, indicating whether they were consistent with the hypothesis. This let the researchers assess whether and how heliospheric scientists can use both qABC and qBC data in their analyses. *Credit: Kelly Moran. Previous page: Los Alamos National Laboratory.*



SMALL IS BOUNTIFUL

The intricate dance of light and matter at the smallest scales could illuminate a path to novel processors, lasers and communication devices.

By Jacob Berkowitz

Alejandro Rodriguez talks about physics with the passion of a baseball or jazz aficionado. In this, his Princeton University students can hear echoes of one of his heroes: Richard Feynman, the conga-playing physics popularizer who in his 1959 lecture "Plenty of Room at the Bottom" famously predicted the nanotechnology revolution.

Rodriguez, an associate professor and director of Princeton's program in materials science and engineering, is exploring exactly how much room there is for creating optimized nanophotonic, or light-based, devices.

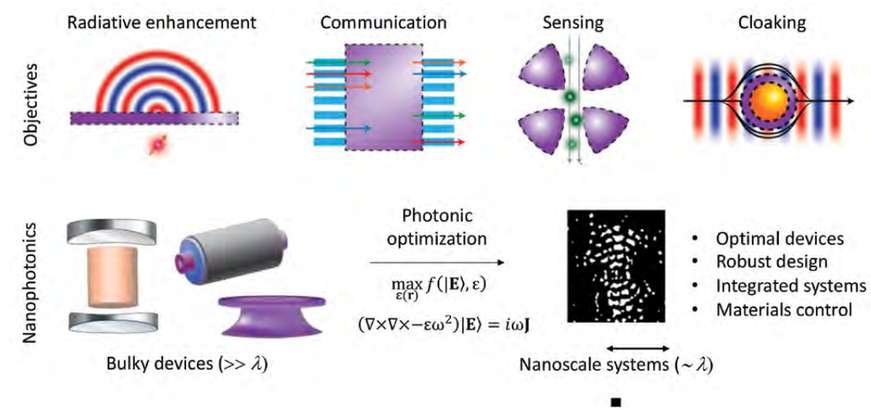
In what he describes as a marriage of physics and engineering, Rodriguez is identifying fundamental limits on light manipulation, energy transfer and other nanoscale interactions. The 2006 to 2010 Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient at the Massachusetts Institute of Technology also is developing the mathematics and algorithms that will lead to ideal electromagnetic devices. Nanophotonics, he says, is ultimately about how to build devices and systems that manipulate light at various wavelengths. This includes optical chips that could one day power all-optical supercomputers and ultraviolet nanolasers.

As Rodriguez explains it, in the past couple of decades, increases in high-performance computing have fueled the rise of inverse design, also known as large-scale optimization – simulating thousands of different possible nanophotonic structures in search of the one that outperforms all others.

"But it turns out," he says, "even when large-scale optimization problems are solved using brute-force computational methods that search through hundreds of thousands of design parameters, you are never guaranteed to find the best possible solution because the problem is highly multidimensional. It's a non-convex optimization problem."

Imagine, Rodriguez says, dropping a marble into a bowl. It rolls to the very bottom. That's a convex problem with an easy-to-calculate absolute bottom, or minimum. In contrast, a non-convex problem resembles an upside-down cragged mountain peak; there are numerous local depressions in which a marble might get stuck before reaching, if ever, the absolute, or global, minimum.

Rodriguez co-wrote a 2022 *Nature Reviews Physics* paper that was first to describe a generalized mathematical framework that accounts for the absolute physical limits on light-matter interactions, determining the global optimum for a range of factors in any nanoscale structure.



Alejandro Rodriguez's mathematical and computational techniques provide a strategy to shrink bulky systems such as millimeter-scale lasers and fiber-optic communication systems (bottom left) to nanometer-scale devices (bottom right) able to integrate with existing microelectronic architectures. Such devices could help with a range of problems (top left to right), including enhancing radiation from quantum and nanoscale emitters for quantum processors, high-efficiency light-emitting diodes, lasers and more; new communication systems that can move high-bandwidth data over short (micron-scale) distances; ultra-small devices with increased light sensitivity for medical imaging, diagnostics and sensing; and cloaking devices that work across visible and infrared spectra. *Credit: Alejandro Rodriguez. Previous page: David Kelly Crow.*

Rodriguez, recipient of a 2019 National Science Foundation Presidential Early Career Award for Scientists and Engineers, calls the result "the most exciting discovery of my career. It guarantees that you can assess nearly best-possible solutions to many electromagnetic problems." He's presented the finding to colleagues at major conferences since the paper came out.

The research has its roots in his doctoral research on the Casimir force, electromagnetic attraction or repulsion between objects nanometers apart. The force results from quantum electromagnetic fluctuations of the atoms comprising the objects. Rodriguez developed algorithms that let researchers compute the Casimir force between objects with complex geometries, such as those on silicon chips.

'You are never guaranteed to find the best possible solution because the problem is highly multidimensional.'

This work established a career-long approach: Extend the understanding of a fundamental force to the nanoscale and apply this to develop shape-agnostic computational solutions to the inverse design of nanophotonic devices.

For example, in papers published in *Physical Review Letters*, Rodriguez and colleagues, including graduate student Prashanth Venkataram, used computational modeling and algebraic techniques to show that microscopically close objects can radiate millions of times more heat than previously theorized. The formula was the first major amendment to the math that describes radiative heating – the Stefan-Boltzmann law – since its establishment in the late 19th century. It also provided a critical insight on a fundamental limit in nanodevice design.

Rodriguez and his mother came to the United States from Cuba via Mexico and gained political asylum when he was a teenager. "I grew up in poverty and had to endure the hardships of emigrating and adapting to a whole new life in the U.S.," he says. "Learning to live with that kind of uncertainty has been very instrumental in helping me navigate academia."

Rodriguez says there's still plenty of room to investigate the realm of the very small. In 2021 he received a Princeton X research grant, designed for creative, risk-taking projects, to extend his large-scale optimization techniques to terahertz devices, the next level of wireless communication.

"More often than not, I find myself feeling my way through science. You have to ride the wave of knowledge and not worry too much about the final destination. I've learned that this helps me be more scientifically productive and lead a happier life."

WORKING THE SYSTEM

A recent fellowship graduate embarks on a career in metadata management, cloud storage and ethics in high-performance computing.

By Sarah Webb

As a Dartmouth College undergraduate, Margaret Lawson pursued computing by accident. She was considering a psychology major when she took a computer science course to fill a requirement and help snag a research position.

"I really loved it, but I wasn't sure if I had a place in the field," she says. A professor, Tom Cormen, encouraged Lawson to major in computer science and consider graduate school. That was a first step on a research career that led Lawson to a Department of Energy Computational Science Graduate Fellowship (DOE CSGF) from 2019 to 2022 and to high-performance computing (HPC) challenges at the national laboratories and Google.

As a software engineer at the company's Kirkland, Washington, campus since summer 2022, Lawson has worked to expand its cloud storage offerings.

With growing HPC-driven data sets, storing information can be costly and moving it can be a bottleneck. Engineers could overcome some of these challenges by storing data in the cloud for easy retrieval when parallel processors need them. DAOS – an object storage platform developed by Intel – already is part of Aurora, the Argonne Leadership Computing Facility's exascale supercomputer, and has performed well on input-output benchmarks.

At the SC22 supercomputing conference, Lawson demonstrated how DAOS performs on Google's cloud platform, particularly with HPC workloads that involve many small files, such as deep-learning applications. It's a step toward moving more HPC workloads into the cloud.

Her work is rooted in Dartmouth's unique undergraduate requirements and in a research internship. Students must take courses during the summer after their sophomore year but remain off campus during another quarter. That meant Lawson had five months available in early 2017.

She talked with an acquaintance, who had worked at Sandia National Laboratories, about computer science internships. That person connected her with Jay Lofstead, a Sandia software engineer who was pursuing strategies to help scientists track salient information in the sea of data they collect and store. Lofstead's pitch: This work will be incredibly difficult and confusing. How's that sound?

Lawson embraced the challenge and loved her time at Sandia. She realized that "grad school was the way I could keep doing it," and continued her collaborations with Lofstead even while working on a computer science Ph.D. at the University of Illinois Urbana-Champaign.

Supercomputers' expanding power has produced a data explosion in recent years. As a result, metadata – date created, author, file size and more details that help identify and classify information – have ballooned to giga- and terabyte scales and continue to grow.

"How can we manage this large amount of information efficiently?" Lawson says. "A lot of scientists in HPC are not computer science experts. They really want something that's usable, intuitive." The initial design she and Lofstead developed used dedicated computing nodes for metadata management. The system would write to or query them as needed. That made the information available but degraded system performance.

That's because metadata are many small messages that tie up communication in high-bandwidth networks.

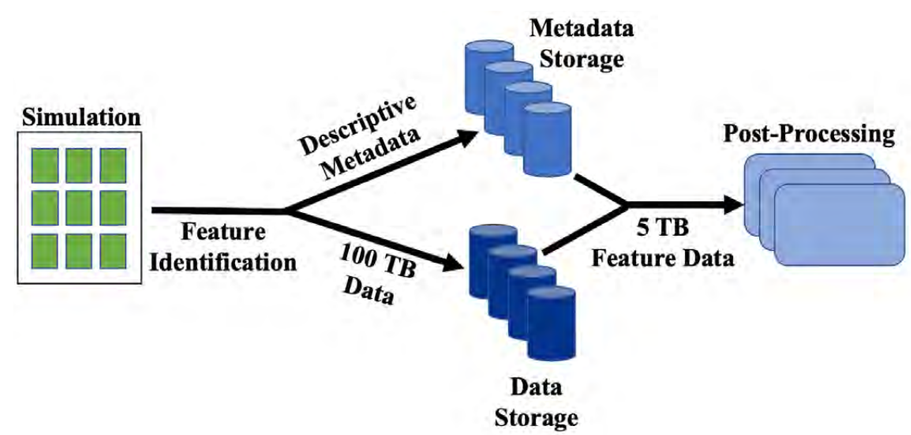
Lawson developed a local version of the management system that embedded metadata servers within compute nodes as an option. The team adopted her solution as the system design. It started by tackling the easiest case: applications that use regular computational meshes, making it straightforward to track metadata based on gridlike coordinates. Lawson's Ph.D. research expanded the approach to more complex meshes, including completely unstructured ones. "It gets a lot more complicated when you're using an unstructured mesh," she says, "because you can't make any assumptions about the mapping between a location in the application space and the stored data."

Sandia gave Lawson access to many cores for system testing and to computational scientists and their day-to-day research challenges. A longstanding joke in systems research is that people end up developing systems that no one wants or needs. It's important designers ensure they're solving real problems, she says. "I think one of the most important ways of doing that is talking to the people."

'A lot of scientists in HPC are not computer science experts. They really want something that's usable, intuitive.'

For her Lawrence Livermore National Laboratory practicum, Lawson studied *in situ* analysis and visualization – that's done as a program runs. "It was a chance to look at another piece of the general workflow," she says, and to collaborate with and learn from a new team. "My job as a researcher was to better understand the entire lifecycle of an HPC application, the entire workflow of HPC scientists, and this was just insight into another piece of that."

Since 2019, Lawson also has co-led recurring SC-conference discussions about HPC and ethics, shining a light on technology creators' responsibilities to use HPC fairly and to manage global equity and access to computing resources at all levels. "There are just so many topics for ethical considerations because of the scale at which we do things and the industries in which the technology is being used."



In this workflow for descriptive metadata management, the algorithm first identifies potential features of interest and stores information about them as descriptive metadata. Scientists can use these descriptors in post processing to identify which data include an identified feature of interest and should be loaded for analysis. *Credit: Margaret Lawson. Previous page: Malcolm Smith.*

OSCILLATIONS AND INTERPLAY

Dipti Jasrasaria promotes community and computationally characterizes nanocrystals.

By Thomas R. O'Donnell

Dipti Jasrasaria

Interactions illuminate Dipti Jasrasaria's life. She prizes exchanges with colleagues and anticipates their needs. As a University of California, Berkeley, Ph.D. student, she helped develop a program to boost incoming chemistry graduate students over an academic hurdle, catalyzing contacts with their more experienced peers.

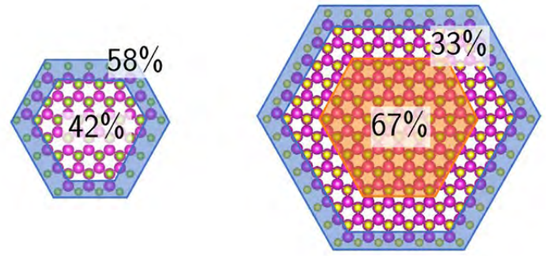
And Jasrasaria's research has tracked previously discounted interactions influencing the properties of such rising technologies as quantum dots or semiconducting nanocrystals, structures so tiny that quantum physics governs their behavior.

In recognition of her outstanding research, character and leadership, Jasrasaria, a Columbia University postdoctoral researcher and a 2018 to 2022 Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient, is the 2023 Frederick A. Howes Scholar in Computational Science.

Jasrasaria fell for chemistry's broad applicability in high school. As a Harvard University undergraduate, she vowed to take courses in the subject until she didn't like them anymore. That didn't happen, but her first research experience was mixed. Jasrasaria loved working with genetics professor and 2009 Nobel laureate Jack Szostak and enjoyed the team's camaraderie as it probed life's chemical origins. Wet lab tasks were less appealing.

Meanwhile, Jasrasaria's quantum mechanics and computer science classes introduced her to computational chemistry. "I realized there was this exciting field that combined both of those things and allowed me to do research without being in the lab." She worked with computational chemist Alán Aspuru-Guzik on the Clean Energy Project, which seeks high-efficiency solar cell materials.

Jasrasaria broadened her computational science experience on a Harvard fellowship to England's University of Cambridge, earning a master's degree with chemical physics professor David Wales. She joined Eran Rabani's lab to pursue her doctorate.



The large contribution of surface modes to the reorganization energy – a measure of exciton-phonon coupling – in small cadmium-selenide nanocrystals (left) can be mitigated by adding a passivating cadmium-sulfide shell (right), lowering the overall reorganization energy from 33 milli-electron volts to 7 milli-electron volts. *Credit: Dipti Jasrasaria.*

At Berkeley, first-semester graduate chemistry courses are challenging, Jasrasaria says. Especially for physical science students, "the quantum mechanics and statistical mechanics courses moved super-fast and required a lot of math background that students often didn't have." Constantly feeling one or more steps behind can harm students' mental health, contributing to impostor syndrome and feelings they don't belong. The classes seemed to be "having an impact on people's self-efficacy and self-concept as a scientist in a pretty long-lasting way."

With three colleagues, Jasrasaria developed a five-day boot camp so incoming graduate students could revisit math concepts they'd previously studied or learn about ones they hadn't. They offered the first program via teleconference in summer 2020.

"We got a lot of excitement from the chemistry department," Jasrasaria says. Administrators provided a grant to continue the camp and analyze results to improve outcomes. Now they've essentially adopted the program. "To have a student-run space to start graduate school has been really helpful," she says, and has made "students feel like they deserve to be in the department."

Meanwhile, Jasrasaria's research seeded a new obsession: phonons, quantum carriers of vibrational energy (heat and sound) from atoms' constant oscillations. Besides acoustic phonons, there are higher-energy optical ones that light excites directly. Phonons are important because they're ubiquitous, she says.

Modeling phonons' interactions with electrons, however, is computationally demanding. Each atom contributes three phonon modes, and nanocrystals can have hundreds of atoms. Small structures are easier to model but less relevant to real-world experiments and applications. Nanocrystals' hallmark optoelectronic properties depend on their size.

To make the problem manageable, models often omit phonons and focus on electrons. "But if you're trying to model a real material, for example, you really need to include those phonons or those vibrations because they impact electronic properties in a tangible way," Jasrasaria says. Electron-phonon interactions also might provide tools to tailor nanoscale materials for specific uses.

These obstacles have produced disagreements over how phonons interact with excitons – electrons and the holes they leave behind after energy, usually from light, boosts them to higher-energy states. Excitons are the physical entities behind solar power. Scientists differ over whether excitons in nanocrystals interact with acoustic phonons, optical phonons or both, and on the impact of such interplay.

During her Ph.D., Jasrasaria studied exciton-phonon interactions computationally in nanocrystals like those used in experiments and devices.

To make the calculations feasible while retaining important details, she and Rabani discarded a common approximation that ignores vibrations and adopted others they found valid. They modeled eight cadmium-selenide nanocrystals of four different sizes, one set bare and the other encased in cadmium-sulfide shells. They found that excitons couldn't couple to acoustic phonons as well in core-shell nanocrystals, matching experiments. That meant phonons didn't affect properties, such as the light wavelength the nanocrystals emitted and how fast it's emitted, as much in core-shells as they did in the simple core structures.

The calculations ran on Cori, a Cray XC40 machine at DOE's National Energy Research Scientific Computing Center, and led to a *Nano Letters* paper. The work, Jasrasaria says, provides a way to account for phonons and shows that omitting them misses important phenomena.

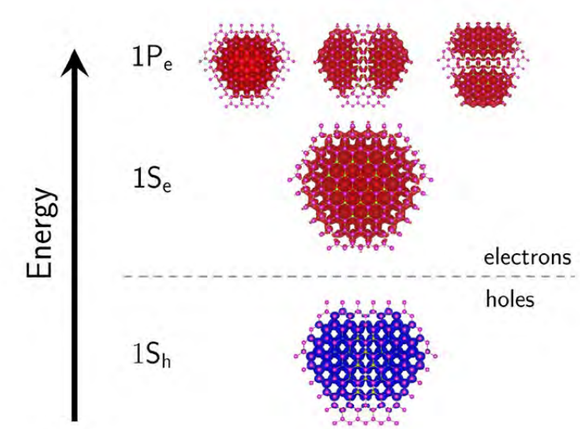
Jasrasaria and Rabani also probed phonons' role as high-energy excitons release energy to reach equilibrium. The models found an exciton could emit multiple phonons as it dropped to a lower energy level. This contradicted theories suggesting that multi-phonon processes would be ponderous and that an exciton primarily changed energy levels by emitting a single phonon at a time.

The research, posted on the arXiv preprint server, describes a process that happens in just femtoseconds (quadrillionths of a second) in the cadmium-selenide nanocrystals but is up to 10 times slower in core-shell nanocrystals. Slow-relaxing excitons could improve solar cell efficiencies, but the opposite may be true for lasers, Jasrasaria says. So "being able to understand and then tune that timescale, depending on what application you want, would be the ideal."

In Timothy Berkelbach's Columbia group, Jasrasaria now mainly focuses on materials with anharmonic vibrational structure, in which phonons are strongly coupled to each other.

Jasrasaria enjoys academia. At Berkeley, she learned to navigate its administrative aspects, joining an initiative to involve graduate students in hiring professors. "Faculty, especially your advisor, can have such a large impact on your experience, personally and professionally," she says. A student committee joined interviews to understand candidates' approaches to mentoring, teaching, diversity and equity. She eventually coordinated the program, ensuring committees considered graduate student input.

Jasrasaria will surely find herself on the other side of the faculty hiring table someday. She's eager to coach students and build relationships while probing significant questions. "That's something I love about the DOE CSGF and scientific environments that I've been part of and that I hope to bring to scientific communities in the future."



Calculated densities of the electron (red) and hole (blue) wave functions of a cadmium-selenide nanocrystal shows that they mirror atomic orbitals, as expected. *Credit: Dipti Jasrasaria.*

TAKING THE HELM AND OTHER HIGHLIGHTS

Former fellows make their mark with prestigious awards, research funding and communication about their work.

Lawrence Berkeley National Laboratory chose **Stefan Wild** (2005-2008) to head its Applied Mathematics and Computational Research Division. Wild moved from Argonne National Laboratory.

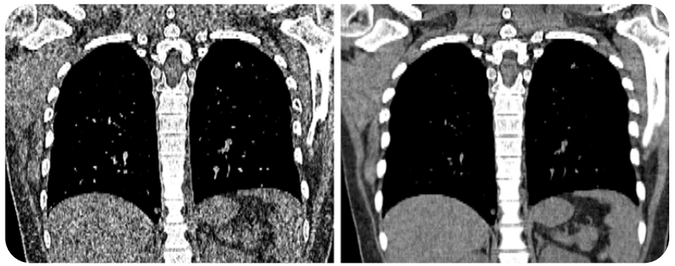
Devin Matthews (2010-2014), a Southern Methodist University assistant professor of chemistry, and Field G. Van Zee of the University of Texas at Austin received the 2023 James H. Wilkinson Prize for Numerical Software. The Society for Industrial and Applied Mathematics (SIAM) presents the award every four years for outstanding software creation or contribution. Matthews and Van Zee developed BLIS (BLAS-like library installation software), a portable open-source framework for mathematical operations that separates architecture-dependent components from algorithmic-dependent ones. The innovation allows rapid library deployment across modern CPU architectures.

Matthews also earned a five-year Department of Energy Early Career Research Program grant to develop mathematical methods for computationally approximating complex quantum-mechanical interactions of light and matter. The project has implications in semiconductor design, chemical reactivity and photosynthesis.

The National Science Foundation (NSF) named **Asegun Henry** (2005-2009), Massachusetts Institute of Technology mechanical engineering associate professor, one of three recipients of the 2023 Alan T. Waterman Award, the NSF's highest honor for early-career researchers. Henry was recognized for his advances in nanoscale heat transfer and high-temperature energy systems and technologies that could mitigate climate change. He will receive $1 million in grant support over five years.

A rendering of human vascular system forces calculated with Amanda Randles' algorithms. *Credit: Liam Krauss, Lawrence Livermore National Laboratory, and Cyrus Tanade, Randles Lab.*

The Association for Computing Machinery special interest group on energy systems and informatics awarded its Doctoral Dissertation Award to **Priya Donti** (2017-2021) for her thesis, "Bridging Deep Learning and Electric Power Systems." Donti earned a computer science and public policy Ph.D. from Carnegie Mellon University in 2022 and is an MIT electrical engineering and computer science assistant professor.



A medical computed tomography coronal image as reconstructed with clinical software. Right: The same image as reconstructed by the model-based iterative reconstruction (MBIR) method that Matthew Norman developed with ORNL and Purdue University researchers. The MBIR image has better quality, clearer lesion detection and less noise. *Credit: Xiao Wang, ORNL.*

William Moses (2018-2022) won Best Student Paper at the SC22 supercomputing conference for work on parallel computing and compilers, tools that translate code from one programming language to another. The team's Enzyme framework helps users optimize their programs for parallel processing, freeing them to concentrate on research instead of rewriting code.

Intersphere Inc., a weather and climate technology startup founded by **Ben Toms** (2017-2021), received $1 million in commercialization funding from America's Seed Fund, the NSF's Small Business Innovation Research program. In 2021, the company received $256,000 from the program. Intersphere's forecasts range from two weeks to two years. The firm recently released worldwide wind- and solar-energy production forecasts.

The Oppenheimer Science and Energy Leadership Program chose Lawrence Livermore National Laboratory's **Teresa Bailey** (2002-2006) as a fellow. Oppenheimer fellows spend a year visiting labs and meeting with senior leaders on organizational, policy, scientific and other challenges facing the national laboratory system and DOE.

Los Alamos National Laboratory's **Aric Hagberg** (1992-1994) was named a 2023 SIAM fellow for his contributions to network science and dynamical systems. As an applied mathematician, he primarily focuses on nonlinear dynamics, pattern formation and complex systems.

The American Institute of Chemical Engineers presented **Ashlee Ford Versypt** (2006-2010), a University at Buffalo chemical and biological engineering professor, the 2022 David Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education.

Three alumni earned time on DOE supercomputers via the 2023 INCITE (Innovative and Novel Computational Impact on Theory and Experiment) program. Oak Ridge National Laboratory (ORNL) computational climate scientist **Matthew Norman** (2008-2011) and researchers from multiple other labs will use 450,000 node-hours on Oak Ridge's Summit to develop a next-generation Earth system model tailored to machines at the DOE's Leadership Computing Facilities. Duke University's **Amanda Randles** (2010-2013) is principal investigator for a project using 800,000 Summit node-hours to create digital models of microfluidic devices to measure blood-cell properties. Brown University's **Brenda Rubenstein** (2008-2012) and a team of university and national lab researchers will tap 100,000 node-hours on Argonne's Polaris to develop exascale simulations of quantum materials.

In 2022, **Randles** received a five-year, $3.5 million Director's Pioneer Award from the National Institutes of Health to support innovative, risky research. Randles and her team will create physics-based artificial intelligence models of blood flow dynamics using input from smart watches and other wearable monitoring devices.

Norman, meanwhile, was part of an Oak Ridge and Purdue University team that won the Truth-Based CT Reconstruction Challenge organized by the American Association of Physicists in Medicine. Each team used simulated, raw computed tomography scanner data to reconstruct the highest possible resolution medical images to diagnose clinical disease with minimal radiation. The ORNL/Purdue team's tool integrated three separate models that simulate scanner physics, statistical noise for unknown errors, and image correction and artifact suppression.

Tim Germann (1992-1995) was among nine scientists named Los Alamos National Laboratory Fellows for 2022. The lab recognized Germann for "making seminal scientific contributions in a number of computational areas and serving in a number of leadership roles." Germann works in computational materials science, computational epidemiology and computational co-design.

Jarrod McClean (2011-2015) of Google Quantum AI is coauthor of a *Science* paper that touted substantial advantages in using quantum computers for specific tasks, including predicting properties of physical systems and learning models of physical dynamics.

Ethan Coon and fellow Oak Ridge scientists created a high-performance Arctic tundra simulation, finding that soil subsidence due to permafrost thaw would be self-limited in the decades ahead. *Credit: David Graham, ORNL.*

Among four centers that shared $56 million in five-year DOE awards for mathematical multifaceted integration capability centers, two include program alumni. **Jeffrey Hittinger** (1996-2000), director of Lawrence Livermore National Laboratory's Center for Applied Scientific Computing, will work with experts from three other labs and two universities on the Center for Hierarchical and Robust Modeling of Non-Equilibrium Transport (CHaRMNET) to devise long-term models of plasmas for fusion energy and national security. **Edgar Solomonik** (2010-2014), a University of Illinois Urbana-Champaign computer science professor, will join researchers from two DOE laboratories and three other universities on Sparsitute, which will build methods to solve big problems using sparsity, in which connections between data and other elements grow slowly with calculation size.

Ethan Coon (2005-2009) is a member of ORNL teams that will use computer modeling and data to help devise climate change mitigation for two urban areas. The multi-instiutional DOE Urban Integrated Field Laboratories (IFL) program gathers data and builds models predicting local climate change effects, particularly in disadvantaged neighborhoods. One IFL will focus on Beaumont and Port Arthur, Texas coastal communities; the other will simulate Baltimore's urban environment.

Coon also is on an ORNL team that used the lab's Advanced Terrestrial Simulator code to model how permafrost will respond to gradual land-surface sinking as climate change warms the Artic tundra. The study found that although the ground will continue to subside as major ice deposits melt, releasing greenhouse gases, its uneven progress could lead to a drier landscape, slowing the process through the end of the century, an ORNL release said. The simulation results were published in the *Proceedings of the National Academy of Sciences*.

The New York Times featured **Jordan Hoffmann** (2014-2018) and colleagues' study examining how cricket embryo cells organize and differentiate. They used geometric modeling and machine learning to reconstruct cell nuclei movement through cytoplasm. Their results could help researchers predict early development in other insect species. Hoffmann works at Inflection, an artificial-intelligence startup.

The India-based magazine and website *Mint Lounge* highlighted **Mala Radhakrishnan** (2004-2007), who has compiled her science-based poetry in two books. Radhakrishnan, a chemistry professor at Wellesley College, often tweets her poetry at @atomicromances.

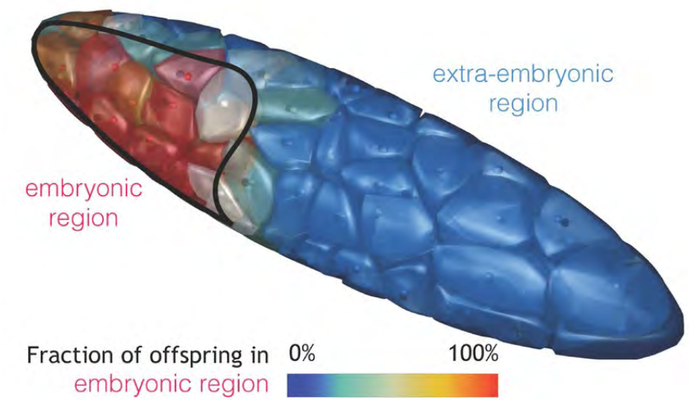
Alicia Magann (2017-2021) led Sandia National Laboratories' quantum computing research that could help avoid supply chain issues and maintain order during global unrest. The team's proposed feedback-based algorithms, described in papers published in *Physical Review Letters* and *Physical Review A*, could tackle complex optimization problems with multiple variables when medium-to-large-scale quantum computers are available.

ORNL's **Steven Hamilton** (2007-2011) leads ExaSMR, an Exascale Computing Project effort to integrate and optimize existing neutron transport, reactor depletion, thermodynamics and other codes to run on the newest, fastest DOE machines, including ORNL's Frontier and Argonne's Aurora. ExaSMR will give nuclear engineers the highest-resolution reactor simulations to date, letting them design the next generation of nuclear plants, including small modular reactors, with fewer full-scale physical experiments. The project aims to make large-scale reactor simulations easier to access, cheaper to run and more accurate than the current state of the art.

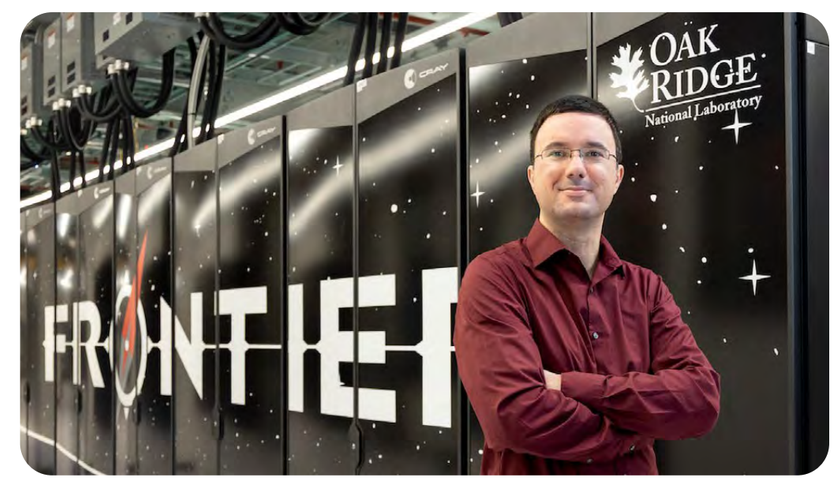
The Gladstone Institutes featured **Isha Jain's** (2013-2016) research into the possible beneficial effects of hypoxia, or chronically low oxygen. Scientists have long noted that people living at high elevations have lower rates of metabolic conditions such as diabetes, coronary artery disease and obesity. Her studies in mice with graduate student Ayush Midha found that hypoxia's effects varied between organs. The project could help lead to drugs that mimic the phenomenon's benefits.

A Harvard University group including **Malia Wenny** (2017-2021) described in *Nature* a way to transport gases in porous liquids, a new material class. Using experiments and simulations, the group identified microporous nanocrystals that can absorb gas molecules, letting water-based liquids store much higher oxygen and carbon dioxide concentrations than normal aqueous solutions. The technology could lead to artificial blood and related medical applications.

Loyola University Chicago's Stritch School of Medicine named **Peter Kekenes-Huskey** (2004-2007) as 2022 Senior Scientist of the Year for his innovative research and commitment to improving the health of communities. Aiming to develop new drug targets, Kekenes-Huskey's group uses computer algorithms to examine how cellular processes lead to immune and cardiovascular diseases.



A rendering of a computational model describing nuclei movement inside an egg from the cricket *Gryllus bimaculatus*. Color coding is based on how nuclei are distributed as a cricket develops. *Credit: Jordan Hoffmann and Seth Donoughe, with input from Cassandra Extavour and Chris Rycroft.*



Steven Hamilton has led a team for the past six years in the development of ExaSMR, which integrates and optimizes codes needed to simulate nuclear reactor designs on exascale supercomputers. *Credit: Genevieve Martin, ORNL.*

CLASS OF 2023

Christopher Balzer
Chemical Engineering
California Institute of Technology
Advisor: Zhen-Gang Wang
Practicum: Sandia National Laboratories, New Mexico (2021)

Thomas Blommel
Physics
University of Michigan
Advisor: Emanuel Gull
Practicum: SLAC National Accelerator Laboratory (2021)

Kyle Bushick
Materials Science
University of Michigan
Advisor: Emmanouil Kioupakis
Practicum: Lawrence Livermore National Laboratory (2021)

Lindsey Byrne
Astronomy
Northwestern University
Advisor: Claude-André Faucher-Giguère
Practicum: Lawrence Berkeley National Laboratory (2021)

Madelyn Cain
Physics
Harvard University
Advisor: Mikhail Lukin
Practicum: Lawrence Berkeley National Laboratory (2021)

Gabriel Casabona
Theoretical Astrophysics
Northwestern University
Advisor: Shane Larson
Practicum: Los Alamos National Laboratory (2022)

Scott Emmons
Computer Science
University of California, Berkeley
Advisor: Stuart Russell
Practicum: Argonne National Laboratory (2021)

Nicholas Ezzell
Physics
University of Southern California
Advisor: Daniel Lidar
Practicum: Los Alamos National Laboratory (2021)

Koby Hayashi
Computer Science
Georgia Institute of Technology
Advisor: Haesun Park
Practicum: Lawrence Berkeley National Laboratory (2021)

Louis Jenkins
Computer Science
University of Rochester
Advisor: Sreepathi Pai
Practicum: Sandia National Laboratories, New Mexico (2021)

Christopher Kane
Physics
University of Arizona
Advisor: Stefan Meinel
Practicum: Lawrence Berkeley National Laboratory (2021)

Arianna Krinos
Biological Oceanography
Massachusetts Institute of Technology
Advisor: Michael Follows
Practicum: Lawrence Berkeley National Laboratory (2021)

Peter Lalor
Nuclear Engineering
Massachusetts Institute of Technology
Advisor: Areg Danagoulian
Practicum: Los Alamos National Laboratory (2021)

Kyle Lennon
Chemical Engineering
Massachusetts Institute of Technology
Advisor: Patrick Doyle
Practicum: Sandia National Laboratories, New Mexico (2021)

Jack Lindsey
Computational Neuroscience
Columbia University
Advisor: Ashok Litwin-Kumar
Practicum: Sandia National Laboratories, New Mexico (2021)

Rebekah Loving
Computational Biology
California Institute of Technology
Advisor: Lior Pachter
Practicum: Brookhaven National Laboratory (2021)

Guy Moore
Materials Science and Engineering
University of California, Berkeley
Advisor: Kristin Persson
Practicum: Lawrence Livermore National Laboratory (2021)

Jamin Rader
Climate Dynamics
Colorado State University
Advisor: Elizabeth Barnes
Practicum: Pacific Northwest National Laboratory (2021)

Jason Torchinsky
Computational Mathematics
University of Wisconsin-Madison
Advisor: Samuel Stechmann
Practicum: Sandia National Laboratories, New Mexico (2021)

Michael Toriyama
Computational Materials Science
Northwestern University
Advisor: Jeffrey Snyder
Practicum: National Renewable Energy Laboratory (2021)

Amalee Wilson
Computer Science
Stanford University
Advisor: Clark Barrett
Practicum: Pacific Northwest National Laboratory (2021)

Boyan Xu
Computational Biology
University of California, Berkeley
Advisor: Ksenia Krasileva
Practicum: Oak Ridge National Laboratory (2021)

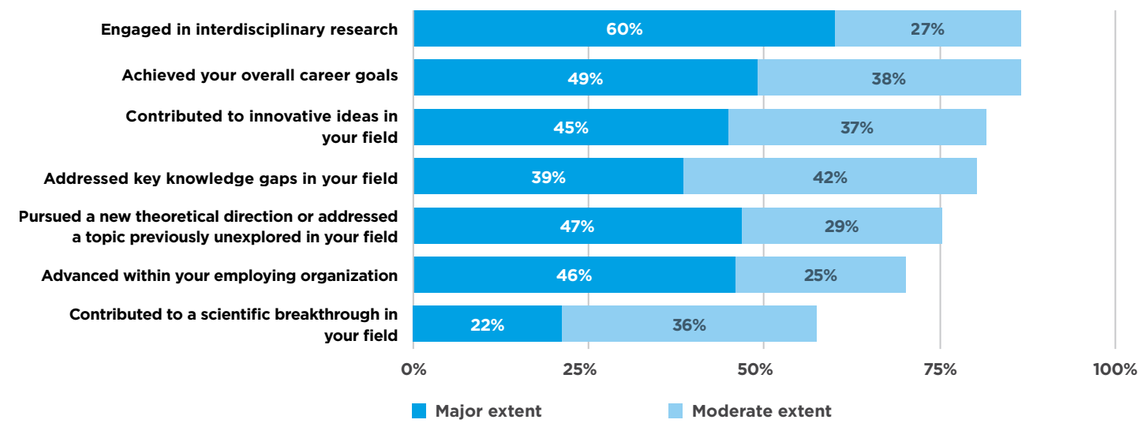
Claire Zarakas
Atmospheric Sciences
University of Washington
Advisor: Abigail Swann
Practicum: Lawrence Berkeley National Laboratory (2021)

Lauren Zundel
Physics
University of New Mexico
Advisor: Alejandro Manjavacas
Practicum: Brookhaven National Laboratory (2021)

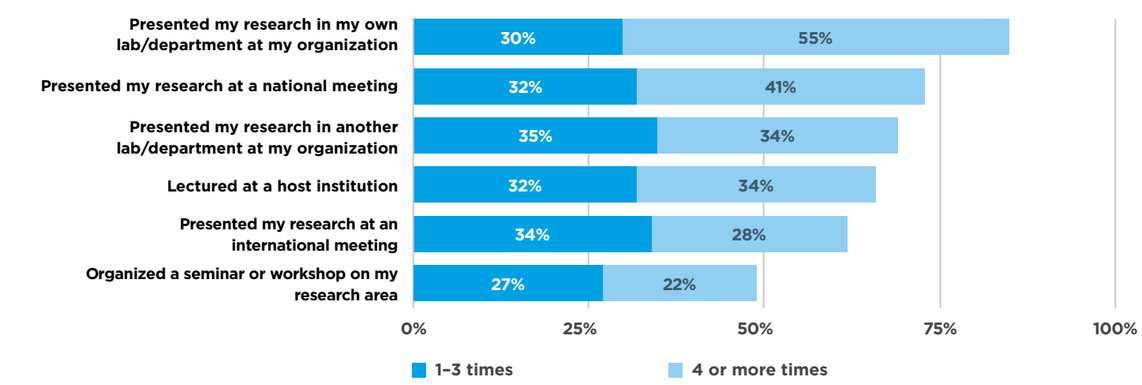
DOE CSGF: ALUMNI ACCOMPLISHMENTS

The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) trains leaders who are ready to plunge into their fields, instilling high-performance computing as a tool for discovery across government, academia and industry. A survey of 213 program alumni found an overwhelming majority engaged in interdisciplinary research, achieved career goals and contributed innovative ideas to their subject areas. Almost all have presented their ideas at their home institutions, national meetings and other venues, most of them multiple times. *Source: U.S. Department of Energy Computational Science Graduate Fellowship 1991-2021: A Follow-up Study of Recipients and Programmatic Outcomes.*

Percent of alumni reporting the extent to which they engaged in professional activities



Percent of alumni reporting how often they made professional accomplishments



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