2021: A Milestone Year

Join us in celebrating:

- 30 years of the DOE CSGF
  - www.krellinst.org/csgf/anniversary
- 20 years of the Howes Scholar Award and 30 recipients
- A community of 450+ alumni as of September 1, 2021
- 2021-22: 107 fellows representing 48 institutions
- Our largest incoming fellow class: 32!

Share your memories via social media (#DOECSGF30):

Fellows & Alumni: Front & Center

Celebrating the program's impact, success and legacy by telling the stories of fellows, alumni and friends in their research and work environments

Then…

1995, Baltimore, MD

Fellows & Alumni: Front & Center

…and now

2019, Arlington, Virginia

DEIXIS 2021


DEPARTMENT OF ENERGY COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP
THE DOE CSGF ANNUAL
2021
DEIXIS
TOUR DE FORCE
Final-year fellow Quentarius Moore looks at how mechanical stress alters chemical reactions.
PAGE 16
STARS ARE BORN
Of galaxies, quantum control and climate change – other fellows share their stories.
PAGE 10
WHAT THEY'RE DOING NOW
Program alumni search for ways to put germs to work, store renewable energy and optimize simulations.
PAGE 22
PLUS: A conversation about NERSC's next big machine, dual Howes winners and more.


INVITED TALK
BIGGER COMPUTING CHALLENGES
A DOE CSGF alumnus reflects on how Perlmutter and other new supercomputers will help researchers tackle larger science problems.
Jack Deslippe leads the Application Performance Group at the National Energy Research Scientific Computing Center (NERSC) and chemistry and materials applications portion of the Department of Energy's (DOE's) Exascale Computing Project (ECP). He was a DOE Computational Science Graduate Fellowship (CSGF) recipient from 2006 to 2010.
Jack Deslippe
DEIXIS: CAN YOU TELL ME ABOUT YOUR EARLY SCIENCE INTERESTS?
Deslippe: As a kid, I dreamed of being an astronaut, and during high school, I became interested in physics – all the cool and weird things that happen at really big scales and really small ones. While majoring in physics at Clemson University, I fell in love with the idea that you could try to discover things as a career. For my Ph.D. I worked in a computational theory group at the University of California, Berkeley, trying to understand how materials work or how to design new ones from the ground up with unique properties for batteries, photovoltaics, energy conversion devices and more.
WHAT ABOUT COMPUTING?
I've always been a gadget guy. I fondly remember programming Texas Instruments TI-82 calculators in middle school and high school. I did web development in high school and became passionate about open-source software and Linux as a young adult.
But my current position is largely because of the CSGF. The scientific problems in my Ph.D. presented a serious computational challenge that requires high-performance computing (HPC) systems with tens to thousands of nodes and hours to days of calculation time. I discovered that I really loved algorithmic development and parallel programming. I wanted to tackle the HPC application development challenge within the scientific community.
HOW DID YOUR GRADUATE RESEARCH LEAD INTO YOUR WORK AT NERSC?
I was calculating the nanoscale properties of materials such as graphene sheets, some of the largest calculations ever with these methods. The codes that I needed just didn't exist or weren't meant to scale to very large systems. So I started developing the codes that could solve the problem. I led a team that produced our public release of a massively parallel HPC code, BerkeleyGW, that could take advantage of the country's biggest HPC systems. When I applied for my original position at NERSC in 2011, as a materials science consultant, I kept one foot in the science domain and had one foot in the computational science and HPC space.
WHAT DOES THAT WORK LOOK LIKE?
We're focused on the delivery and successful deployment of the Perlmutter system, the biggest, most powerful system ever at NERSC, up to four times that of Cori (previously NERSC's most powerful system). Much of its capability comes from graphics processing unit (GPU) accelerators that are embedded within a significant fraction of the system's nodes. We're partnering with different research teams around the country to prepare their applications for those GPU accelerators. We communicate regularly as a team, but we also have hackathon events, where we sit together and look at code, optimizing it and then recompiling it to see the difference. We want teams to be able to execute more challenging science problems on this system ones that take advantage of both the added computational power and our applications work.
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ALUMNI NEWS: NOTABLES
ASCENDING TO EXASCALE AND OTHER HEIGHTS
For the fellowship's graduates, the program's 30th was a very good year.
The Department of Energy's (DOE's) Exascale Computing Project (ECP) named Daniel Martin (1993-1996) the team lead for application development in earth and space science. Martin will help oversee and develop exascale-capable projects to explore the universe's structure and astrophysical phenomena and to better model earthquakes and clouds. Martin is a computational scientist and leader of the Applied Numerical Algorithms Group at Lawrence Berkeley National Laboratory.
DOE's Princeton Plasma Physics Laboratory touted Noah Mandell's work to improve a model of the plasma edge in tokamak fusion reactors. Mandell (2015-2019) extended the Gkeyll code to handle magnetic fluctuations. The simulations may help physicists understand and avoid machine-damaging heat bursts.
Giskit interviewed Sukin (Hannah) Sim (2016-2020) on its YouTube channel for a four-part series on her career and quantum circuits research. Sim, then a Harvard University doctoral candidate, also spoke about optimizing parameter-heavy circuits at QHack's 2021 Quantum Machine Learning Hackathon. She is now a research scientist with Zapata Computing.
Columbia University biomedical engineering professor Tal Danino (2006-2010) was among seven researchers who received the 2020 Pershing Square Sohn Prize for Young Investigators in Cancer Research. The award provides $200,000 a year for up to three years. Danino's lab programs probiotic bacteria to target tumors and deliver lung cancer therapeutics. Danino also was chosen by the Cancer Research Institute for its Lloyd J. Old STAR (Scientists Taking Risks) award, providing $1.25 million in project support over five years.
Amanda Randles (2010-2013), a Duke University biomedical sciences professor, delivered the virtual keynote talk at the 2021 Rocky Mountain Advanced Computing Consortium's High-Performance Computing (HPC) Symposium. Her group received a DOE INCITE grant of 290,000 hours on Summit, the HPC system at the Oak Ridge Leadership Computing Facility (OLCF), to model how cancer cells circulate. And the team's HARVEY code, which models the circulatory system, will be among the first to run on Aurora, the exascale computer planned for the Argonne Leadership Computing Facility (ALCF).
The Duke Arts website featured Clay Sanders (2016-2020) and his artwork, focusing on a commissioned painting that the campus arts center exhibited. He's now a mechanical engineer at Sandia National Laboratories, California.
Hannah De Jong (2014-2018) and her Stanford University colleagues developed a high-throughput, scalable method for sequencing the coronavirus genome while collecting DNA data about the human host.
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DEIXIS 2021

The DOE CSGF's annual publication – the 19th issue

- Available for download
  - https://www.krellinst.org/outreach/deixis-magazine
- Feature: NERSC's Perlmutter deployment
- Profiles: Fellows' research and alumni careers
- 2021 Howes Scholar Award winners
- Communicating Your Science and Engineering (CYSE) contest winning essay
- Fellows and alumni in the news
- Incoming and outgoing class summaries

DEIXIS 2021: Fellows

Read more about this week's presenters

- Alicia Magann
- Claire Kopenhafer
- Quentarius Moore
- Priya Donti
- …plus, other fellows in brief form

DEIXIS 2021: Alumni

Alumni reads

- Stefan Wild, Argonne
- Sarah Richardson, MicroByre
- Zachary Ulissi, Carnegie Mellon
- Jack Deslippe, NERSC

ALUMNI PROFILES

OPTIMIZED FOR DISCOVERY

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

By Jacob Berkowitz

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

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

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

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

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

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

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

ALUMNI PROFILES

MINDING THE STORAGE

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

By Andy Boyles

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

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

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

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

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

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

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

ALUMNI PROFILES

GERM WRANGLER

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

By Thomas R. O'Donnell

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

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

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

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

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

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

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

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

With that knowledge, researchers align bacterial functions with human needs. With an understanding of a bacterium's quirks,

CYSE Contest Winner

Congratulations, Ellis Torrance!

- The Communicate Your Science & Engineering (CYSE) Contest accepts (fellow and alumni) essay entries that explain scientific work with a broad, non-technical audience in mind. The competition's goal is to convey information, excitement and enthusiasm about computational science and engineering.
- Read her essay, "Sex Isn't Everything," in DEIXIS 2021

Podcast Launch

Science In Parallel

- Debuting two episodes in conjunction with program review
- First season to focus on the DOE CSGF's 30th anniversary
- Additional episodes will roll out between Labor Day and Thanksgiving 2021
- Hosted by Krell's associate science media editor, Sarah Webb
- Theme music teased this week

Podcast Launch

Science In Parallel:
People and Projects in Computational Science

www.krellinst.org/csgf/outreach/science-in-parallel

- First two episodes released this week
  - Jeff Hittinger: Leading by Example
  - Artificial Intelligence and Climate Change:
    Do the Work and Meet the People
    (Priya Donti, Kelly Kochanski and Benjamin Toms)

Share Your News & Accomplishments

- Facebook (public page & private group)
- Linked In (private group)
- Twitter

- Email csgf@krellinst.org
- Or reach out to a member of the Krell staff

- Images are always encouraged

Looking Ahead to In-Person Events

- Supercomputing Conference (SC21) – November 14-19, 2021
  - America's Center, St. Louis, Missouri (w/remote option)
  - DOE CSGF advisory committee-curated programming for first-year fellows
  - Attendance support for all fellows
- DOE CSGF Annual Program Review – July 18-21, 2022
  - Crystal Gateway Marriott, Arlington, Virginia
- A hopeful return to on-site practicums in 2022

What To Expect Today

Daily 10 a.m. to 4 p.m. CENTRAL

- Welcomes/notable information
- Howes Scholar talk
- Outgoing fellow talks
- Third-year fellow poster presentations

Recordings/content posted daily: ***www.krellinst.org/csgf/conf/2021***