HIGH-PERFORMANCE POSTDOCS

Fernbach Fellows Bring Fresh Insights to Computing

As the field of high-performance computing grows, so does the need for the steady input of fresh ideas provided by newly trained scientists. Lawrence Livermore National Laboratory has always been able to attract computer scientists with cutting-edge projects, colleagues, and computers, but in recent years, the Laboratory has boosted its recruiting profile even further—by offering the prestigious Sidney Fernbach Postdoctoral Fellowship in the Computing Sciences. The fellowship fosters creative partnerships between new and experienced scientists. In short, it ensures an annual cycle that refreshes advanced research in computer sciences at the Laboratory.

"The fellowship program has succeeded in attracting top talent to the Laboratory and provides them a unique opportunity to develop their computing research goals using our world-class computing facilities, with access to our cross-disciplinary expertise in computing, mathematics, and physics," says Bob Anderson, of Livermore's Center for Applied Scientific Computing (CASC). Anderson notes that the fellowship offers a very unusual level of autonomy for postdoctoral researchers. In addition, Anderson emphasizes, "The fellowship experience is not only about independence but also about collaboration. Our Fernbach fellows have done an excellent job capitalizing on the opportunity. With each of them, the Laboratory benefits—growing our internal capabilities as well as our external networks to scientific leaders elsewhere."

"Scientific computing is very broad and rapidly changing, and the Fernbach Fellowship reflects this," explains Jeff Hittinger, director of CASC, which is the programmatic home for the fellows. "The fellowship committee accepts applications from researchers across the computing sciences, including applied mathematics, computer science, data science, and computational science. This breadth and flexibility allows us to tap into the latest ideas."

Accelerating the Laboratory's Computing

Hittinger notes that for CASC—the Laboratory's window on computational research communities—"The Fernbach provides us the opportunities to augment existing areas of strength in our research portfolio and to build out new areas with the fellows' help." Anderson adds that the fellowship brings to the Laboratory opportunities to explore new, higher-risk approaches in computing. According to Tzanio Kolev, a CASC researcher who has served as a Fernbach mentor, "The fellows bring in new ideas, enthusiasm, and hard work that propel our teams further and ultimately help us deliver better insights and algorithms for the Laboratory's mission areas." Kolev continues to collaborate closely with the 2018 fellow, Will Pazner, who remained at the Laboratory after his fellowship term and in 2022 joined the faculty of Portland State University.

"Will and I published multiple papers together, which I think are some of the best papers I've been a part of," says Kolev. "His impact on my research and the MFEM (Modular Finite Element Methods software library) team cannot be overstated. We solved some really hard problems together that I previously didn't have any idea how we would overcome," Kolev says. "In addition to the research, Will also excelled in his team and code contributions. We were very happy to have him be a part of our team here and are looking forward to continuing to work together."

Finding Fernbachs

To create a good fit, the selection of Fernbach fellows is a multistage process. Anderson heads a Laboratory committee that represents a range of computing-related fields. "We invite three or four finalists to give talks on their research and interview with staff members," he says. "With the advice of the staff subject-matter experts, the committee chooses a fellow who we believe is best positioned to thrive in the environment here, provide excellent leadership, and ultimately impact the work of the Laboratory." The fellowship is a success partly by drawing on a wide range of mathematical and computational fields and by remaining specific to the Computing Directorate. The Laboratory also has the Lawrence Fellowship, open to postdoctoral researchers in all technical disciplines. Fernbach's name, however, stamps the newer fellowship with a focused prestige. For the same reason that the Institute of Electrical and Electronics Engineers (IEEE) Computer Society

CHEN WANG • 2022 Fernbach Fellow

Wang has been working toward "a paradigm shift in high-performance computing," away from the current consistency-centric input–output (I/O) programming model and into a synchronization-centric I/O model. His work is enabling the parallel computing field to "ditch" a standard (POSIX) that was first formulated decades ago for single-node computing: "POSIX suffers from scalability limitations and is not fit for high-performance computing storage systems. The storage consistency is stronger than needed. For today's parallel processing, we need a standard synchronization interface with custom consistency models."

STEVEN ROBERTS • 2021 Fernbach Fellow

"In graduate school, I first developed a hybrid technique to combine machine-learning models with traditional time-stepping methods used for solving the differential equations of typical science models. The method could achieve excellent speedups (700x in the best results), but it had several practical limitations and could be difficult to implement. During the fellowship, I developed a new approach, which overcomes these limitations. Notably it allows black-box machine learning and time-steppers to be combined in a nonobtrusive way."

STEFANIE GUENTHER • 2020 Fernbach Fellow

"During the fellowship, I developed numerical optimal-control methods to improve and accelerate current scientific machine-learning models. My research introduced new neural network architectures for improved network stability and training robustness, while leveraging high-performance computing. The fellowship provided me with the opportunity to collaborate with researchers from diverse areas, such that I was able to apply these ideas in a different context, which eventually led me to a new Laboratory Directed Research and Development project to explore advanced quantum control techniques."

WILL PAZNER • 2018 Fernbach Fellow

"As a fellow, I had the opportunity to focus on the development of computational physics methods that are specifically designed for high-performance computing architectures with GPUs (graphics processing units). One of the main challenges posed by numerical methods for computational physics is the solution to the large systems of equations that arise from the simulation of large-scale physics problems. These systems require large amounts of memory, and while GPUs excel at performing huge numbers of calculations quickly, they typically have relatively little memory. Furthermore, the amount of time spent reading and writing the data associated with these systems can dwarf the amount of time actually spent performing computational operations."

has its Sidney Fernbach Award for "outstanding contributions in the application of high-performance computers using innovative approaches," the Laboratory's Fernbach Fellowship has had the instant prestige to attract top computer science candidates who also might win postdoctoral research positions named for other giants in their field, such as the Wilkinson, Householder, and Von Neumann fellowships at other national laboratories.

Hittinger says, "We purposely named the fellowship after Sidney Fernbach, a pioneer in scientific computing and the original head of the Laboratory's Computation Department, to recognize his legacy and our commitment to expand the limits of what we can achieve through simulation and data science." Fernbach made Lawrence Livermore synonymous with advanced supercomputers and is widely acknowledged for his role in creating the world of scientific computing as we know it. He ensured the Laboratory had the best computers and built a multidisciplinary computing team known also for working closely with scientists and engineers across the site and beyond.

Degrees of Freedom

Along with the valuable opportunity to pursue their own research agenda, Fernbach fellows benefit from the mentorship of a Lawrence Livermore staff scientist. They arrive with the research momentum of their doctoral degree and build on it at the Laboratory. The initial fellowship year is typically renewed for a second year.

"The Fernbach Fellowship attracts the best and the brightest graduate students to the Laboratory because it gives them an opportunity to pursue their own research interests right out of the gate," says Kathryn Mohror, who is the Laboratory mentor to the 2022 fellow, Chen Wang. "Most people do not get this opportunity in their first job out of school and need to work towards someone else's goals for years before they can obtain their own funding. So, this opportunity is very attractive."

Recent Fernbach fellows have already gotten to know the Laboratory through internships or collaborations. In Wang's case, he had already coauthored papers with Mohror, including developing a tracing tool for tracking input–output (I/O) activity in parallel computing. High-performance computing started to be a primary interest of Wang's in undergraduate studies, long before his dissertation at the University of Illinois, where he focused on improving I/O efficiencies. "Here at the Laboratory, I get to do research I want to do: to pursue ideas that are interesting to me in high-performance computing storage systems. The fellowship gives me the flexibility to follow what I was trying to do in my dissertation."

The competitive process ensures selection of candidates with special potential to make the most of this research opportunity. Hittinger says, "Regardless of the specific project, it is always valuable to have an outside perspective, and the Fernbach fellows have the confidence to provide that perspective, which isn't always the case with postdoctoral researchers." For example, Hittinger points out that Stefanie Guenther (the 2020 fellow) has been an important contributor

The First Computing Hire

Sidney Fernbach (left), with Harold Brown (then Laboratory director), Edward Teller (right), and a newly developed computer in 1960.

The Lawrence Livermore tradition of finding early-career scientists to advance computational research started in 1952, when the new Radiation Laboratory branch had not yet opened. Edward Teller had just agreed to purchase a UNIVAC-1, that era's supercomputer, and realized he needed someone to run the machine, so he reached out to a newly minted Berkeley Ph.D. physicist named Sidney Fernbach, who had no computer experience. Teller laid down a challenge: "You are going to run the computer," but promised no title. Nonetheless, Fernbach jumped at the postdoctoral research opportunity and went on to be a legend in the development of supercomputers and a creator of the field of scientific computing.

As Fernbach later admitted, "When you are young, you will attempt anything!" Indeed, among early achievements, Fernbach's early computation department developed its own time-sharing software and performed its own maintenance to protect a classified environment. They worked closely with industry to design better computers. Fernbach immediately began his decades-long quest for more speed and power: "I was always looking for new machines." Teamwork was the key to his department's approach to scientific computing: "We assigned a mathematician to every physicist who had a problem."

Jeff Hittinger, director of the Laboratory's Center for Applied Scientific Computing, says, "Thanks to Fernbach and the team he assembled, Lawrence Livermore has long been renowned for our expertise in scientific computing and our use of high-performance computing to solve challenging problems in the national interest. The Fernbach Fellowship in the Computing Sciences provides an opportunity for the rising stars in scientific computing to join and to influence a first-class research environment that embraces the power of computing."

to the new quantum control effort she and Anders Petersson have developed. During her fellowship years, Guenther, Petersson, and Laboratory colleague Jonathan L. DuBois published an award-winning paper in *AVS Quantum Science* aimed at relieving a "major bottleneck" in quantum computing that arises from establishing the qubits into a well-defined initial state for computation.

Meanwhile, Steven Roberts, the 2021 fellow, works closely with the SUNDIALS team and is developing new, machine-learning inspired time integrators. SUNDIALS (the Suite of Nonlinear and Differential/Algebraic Equation Solvers) is an open-source library led by Carol Woodward, who serves as Roberts's Laboratory mentor. Roberts's work improves methods in solving fundamental computational problems in engineering and scientific modeling, and inclusion of his work in SUNDIALS helps illustrate a mutual benefit of the fellowship: furthering a Laboratory project, while enhancing exposure and applications for Roberts's work. This year, SUNDIALS won a prestigious honor from the Association of Computing Machinery.

Wang describes similar advantages of exposing his work to the real-world situations at the Laboratory. As his plan for work on a new I/O paradigm for parallel computing builds from the I/O tracing tool and moves in stages of deeper integration with Livermore colleagues. Wang sees his fellowship term as "starting small," in a stage of benchmarking with sets of code—a small-scale abstraction for test situations developed with other computer scientists at the Laboratory. Wang's plan then progresses to a stage of large-scale testing with thousands of nodes on Livermore's high-performance parallel computing machinery. These larger tests would involve problems formulated by other kinds of scientists working at the Laboratory.

Working at the Laboratory has also clearly benefitted Guenther's research. "Having access to Lawrence Livermore's supercomputing platforms throughout my fellowship greatly contributed to demonstrating the potential of the approach I was taking and enabled me to apply the ideas on relevant scientific machine-learning applications, rather than purely mathematical model problems," she says.

Integration of Experiences

The Fernbach Fellowship represents the latest evolution of Lawrence Livermore's deep tradition of matching postdoctoral talent with the staff experienced in related computational research. The fellows and their mentors say this relationship is among the great advantages of the fellowship.

"I worked with Chen for years, while he was a Ph.D. student, before he was awarded a Fernbach Fellowship. Being able to have him on our team, self-funded, is a big win for us," Mohror says. "Because we worked together so long before he came here, Chen's research goals are well-aligned with what our team is doing, so there is a lot of great synergy."

In counting the many benefits of the Fernbach Fellowship, Wang also emphasizes the mentor–mentee alignment. The mentorship helps shape the combination of research independence bundled with the intense staff interaction. Wang points out that this combination is difficult to find in research positions in big technology firms and in academia. "Kathryn Mohror is a really wonderful mentor, and she helps me make connections a student would not have pursuing their own research in other postdoctoral positions."

Roberts says, "The fellowship and my time at at the Laboratory have exposed me to so many new ideas, projects, and top-notch researchers. It has certainly helped to broaden my expertise and research directions. I've been very fortunate to be mentored by Carol Woodward, a world-renowned expert in solvers for differential and nonlinear equations. I've picked up a lot of practical knowledge and skills from her, especially with project and team management."

Unscripted Steps

Guenther recommends that future fellows reach out and connect with other researchers at the Laboratory and to continually look for collaboration opportunities. She found the interaction, particularly with a good mentor, invaluable to keeping research focused, inspired, and productive. "This fellowship provided me with the unique opportunity to define my own research plan early in my career, while providing the flexibility to adapt and change research directions when necessary. I got a chance to explore new and emerging ideas freely and develop them into research publications and software."

Roberts found during the initial year and a half of his fellowship that the scope of his work expanded well outside of the research he initially proposed. He joined forces with others to develop new time integration methods that can avoid the order reduction phenomenon: a troublesome loss of accuracy seen when solving certain types of stiff problems. "I am working with researchers at Lawrence Berkeley Laboratory to enhance the time-stepping capabilities of BISICLES, a code for ice-sheet modeling. Outside of the fellowship scope, I also have been involved in a feasibility study of how to best utilize cutting-edge machine-learning hardware, such as the Cerebras wafer-scale engine, for time integration."

Fernbach himself benefitted from this traditional Livermore scientific flexibility. He started as a theoretical physicist—work he continued on top of serving as Director of Computation. As Kolev points out, "we have important applications, challenging research problems, some of the most powerful supercomputers in the world, and amazing colleagues with which to collaborate. If new graduates like a challenge and working hard on problems that matter, they should consider applying to be a Fernbach fellow."

—Jeffrey Rosenfeld

Key Words: Center for Applied Scientific Computing (CASC), Fernbach Fellowship, input-output (I/O), Modular Finite Element Methods software library (MFEM), postdoctoral researchers, quantum computing, Suite of Nonlinear and Differential/Algebraic Equation Solvers (SUNDIALS).

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