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# 2020 Budget Request for the DOE Computational Science Graduate Fellowship (CSGF) Grant

## Final Technical Report

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## Overview

Workforce development in computing is critical to maintaining the nation's scientific and economic leadership. As computing becomes the foundation of innovation across every sector — from energy and quantum computing to national security and artificial intelligence — training a skilled, diverse, and adaptable computing workforce ensures that the United States remains at the forefront of discovery, competitiveness, and technological resilience.

As a nationally recognized program since its 1991 formation, the DOE CSGF continues to be considered a model of a successful program that addresses the challenging national workforce needs in computational science and engineering. The DOE CSGF has a particular emphasis on high performance computing (HPC) that enables advancements in computational science and engineering (CSE) relative to areas of national importance.

The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) is essential for addressing the increasingly complex national workforce demands stemming from the growth of computational science and engineering challenges. Computational science and engineering (CSE) take a multidisciplinary approach that utilizes scientific computing to tackle practical problems and provides technical tools across the spectrum of scientific discovery. The DOE CSGF specifically highlights high-performance computing (HPC) as a critical CSE enabling technology, driving advancements in science and engineering that are vital to both the DOE and the broader economy. This report will highlight the cohort funded under award DE-SC0021110.

Since its inception, the DOE CSGF program has selected and trained graduate students to apply advanced scientific computing to critical areas of science and engineering for the nation. For nearly three decades, the Krell Institute, in collaboration with committees of prominent scientists, has led the development of a diverse computational science workforce that supports the DOE's mission. This workforce development has been the primary focus of the highly effective DOE CSGF program, which is supported by the DOE Office of Science and the DOE National Nuclear Security Administration (NNSA).

## Program Goals and Objectives

The specific goals of the DOE CSGF program are:

- To help ensure an adequate supply of scientists and engineers appropriately trained to meet national workforce needs, including those of the DOE, in computational science.
- To raise the visibility of careers in the computational sciences and encourage talented students from diverse backgrounds and institutions to pursue such

careers, thus building the next generation of leaders in the field.

- To foster the development of a community of computational scientists that spans all the disciplines of science and engineering as well as professionals across academia, the federal government laboratories, and the commercial sector.
- To provide practical work experiences for the Fellows that introduce them to the multidisciplinary, team-based scientific research environment of the DOE National Laboratories.
- To strengthen collaborative ties between the academic community and DOE National Laboratories so the fellowship's multi-disciplinary nature builds the national community of scientists.
- To continue to evolve the program to address the changing needs of the DOE and the broader scientific community in computational science.

The DOE CSGF program supports talented graduate students in their studies and research at American colleges and universities, focusing on areas where computation is essential for scientific and engineering understanding and discovery. The program's ongoing success is driven by two key factors: the extensive participation of the technical community and effective execution of the program.

The following sections detail the unique elements of the DOE CSGF Program and outline the components and tasks involved in its management and execution plans.

**The Program of Study**

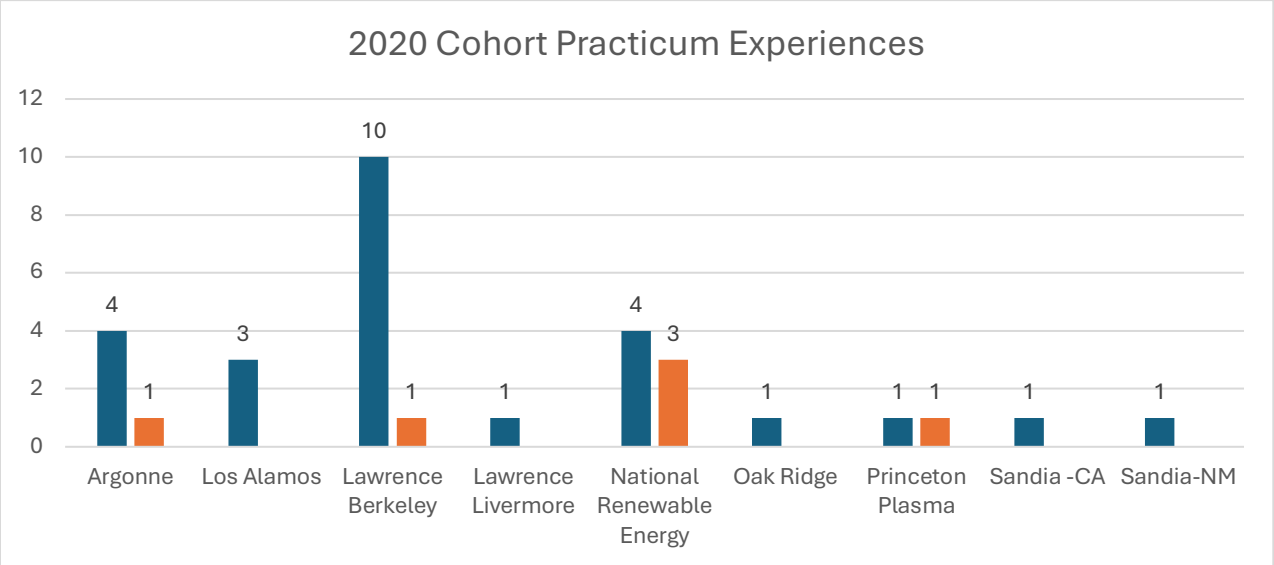
The hallmark of the DOE CSGF is its cross-disciplinary training, which is best illustrated by a strong Program of Study (POS) requirement. The fellowship mandates a POS that will provide a solid background in a scientific or engineering discipline and in computer science/engineering and applied mathematics/statistics. The major field must fall in one of these categories and the program of study must demonstrate breadth through substantial academic achievement in at least one year of courses in the other two. In addition, recognizing the essential need for technical computing expertise, the POS must include a course in high-performance computing. The coursework must be completed within the fellowship's first two years (or three in the case of Fellows who applied to the program as undergraduate seniors). This unique and essential element gives students the opportunity to explore other disciplines intrinsic in the practice of computational science and requires Fellows to become comfortable working across disciplines. The Krell Institute coordinates and monitors all POS requirements throughout a Fellow's tenure in the program, obtaining approval from the Technical Co-PIs — or members of the Steering Committee for novel cases — for any changes, and ensuring all necessary coursework is completed in a timely fashion.

**The Research Practicum**

An unmatched opportunity to experience the breadth, quality, and excitement at a DOE National Laboratory is an important benefit of the DOE CSGF that the Krell Institute will continue to administer in detail for the Program. This experience offers the Fellows insight into how their scientific interests can translate to research areas important to the nation.

The Research Practicum requirement specifies that Fellows spend a significant period working with a DOE Laboratory to broaden their intellectual experience and to learn about scientific research from some of the nation's top practitioners. The practicum is intended as a broadening experience, distinct from the students' academic requirements to perform thesis research. Nevertheless, in many instances, the practicum has impacted the Fellow's thesis substantially. This practicum requirement ensures that Fellows complete a research project at one of the numerous DOE-approved laboratory sites for a minimum of 12 weeks. The combination of graduate study, research at academic institutions and practical experience with DOE facilities ensures that the program produces individuals capable of significantly contributing to research and development in computational science with a strong understanding of HPC.

The chart below illustrates the number of fellows who completed practicums and at which DOE laboratories. The blue bar represents first practicum experiences, which are required, and the orange bar represents second practicum experiences which are optional. This cohort attended nine different laboratories with six fellows choosing additional laboratory experiences. Due to the pandemic, students were allowed to complete first practicums virtually. However, second practicum experiences were on-site when the facilities were allowed to re-open.



**Annual Program Review**

The DOE CSGF Annual Program Review held each summer in the Washington, D.C. area, provides one of the main opportunities for the Fellows to interact with each other, Fellowship alumni, laboratory staff, and DOE program management. The annual meeting is one of the most appreciated features of the fellowship, and the most productive to connect and develop life-long relationships.

Attendance at the program review is a DOE CSGF benefit and a requirement. The review provides a forum for fourth-year Fellows and any other departing Fellows to present plenary lectures on their research. These talks are the meeting's focus. Krell staff records these presentations, edits, processes, and posts them on the fellowship website. Additionally, the Fellows' recordings are promoted on social media to gain more exposure for the Fellows' research, the Program itself, and the DOE sponsors.

Fellows in years one through three are required to present a poster, which provides a valuable mechanism for assessing Fellows' progress. To encourage effective communication and facilitate Fellow-alumni interaction, alumni work with the Krell Institute to offer peer feedback on Fellow posters after the session. Surveys indicate that the Fellows find this feedback extremely valuable. These presentations also provide an annual assessment of the program's progress and value.

A second goal of the program review is to acquaint Fellows with the DOE Laboratories and showcase practicum and employment opportunities. During the meeting, Fellows can learn more about the Laboratories and what they offer by attending a DOE Laboratory Poster Session. This session provides a direct entry point to connect with DOE Laboratory researchers, and oftentimes, future employers.

Fellows use the time together to meet informally with one another and with alumni, who often attend. The Fellows find this networking to be an important and valuable aspect of the review, with impact on their eventual career paths. It also is key to building a community of computational scientists, relationships that can span careers.

Due to the pandemic, the program hosted the 2020 and 2021 meetings virtually. The fellowship community was able to gather in person for the 2022 and 2023 meetings.

Over the course of their time as fellows, this cohort:

- Interacted with leadership from DOE including the Associate Director of Advanced Scientific Research in the Office of Science; the Assistant Deputy Administrator of Strategic Partnerships in the Office of Defense Programs, NNSA; the Director of the Office of Science; and the Deputy Administrator of Defense Programs, NNSA.
- Participated in professional development workshops on mental health and wellness as graduate students and communicating about research to a large audience.
- Attended program alumni panels on topics such as entering the workforce after graduation and managing mental health while in graduate school.
- Met and interacted with over 100 DOE CSGF fellows at each in-person meeting; over 15 DOE laboratory representatives each year; and numerous alumni and university representatives.

## Training and Professional Development

### HPC Training

***Supercomputing (SC)*** — Attending the SC Supercomputing Conference provides DOE CSGF fellows with an essential, immersive training experience in high-performance computing that goes far beyond what they can gain in a classroom or lab. At SC, students learn directly from the developers of cutting-edge architectures, programming models, and software tools, participate in hands-on tutorials and workshops, and see how HPC is applied to major scientific and engineering challenges across national laboratories, industry, and academia. The conference also exposes them to the latest trends shaping the future of supercomputing while giving them valuable opportunities to build professional networks, form collaborations, and connect with potential mentors and employers. In this way, SC accelerates students' technical development and prepares them to become effective contributors to the national HPC workforce.

The DOE CSGF provides an opportunity for fellows to attend SC every year and requires them in their first year of fellowship to attend workshops and tutorials in HPC. For this cohort, unfortunately, the pandemic forced SC20 to be held virtually, but 20 of the 26 first year fellows were able to attend workshops, tutorials and technical sessions online. For SC21, SC22 and

SC23, 45% of the members of this cohort attended and took advantage of the training and networking opportunities.

The feedback from the fellows was overwhelmingly positive, highlighting the value of this experience in fostering connections and expanding their understanding of the HPC landscape.

One fellow wrote in a post-event survey administrated by Krell:

> *This was a great way to get access to a border in scope, application, and sector within the HPC community. As an introduction to HPC methods, it was great. Since the conference has a variety of users (new, experts, and everything in between) the sessions are very much tailored to the audience's questions. This significantly helped me follow along without the worry of beginner sessions getting too advanced.*

**Practicum** — As discussed earlier in this report, a benefit and requirement of the DOE CSGF is that all fellows complete one 12-week practicum at a DOE national laboratory. Not only does this experience expose fellows to the national laboratory complex, it also provides critical training in their research areas and provides them access to world-class facilities and computing. A research practicum provides PhD students with structured, hands-on experience applying their skills to real scientific or technical problems, making it one of the most effective forms of advanced training. Unlike coursework or isolated research tasks, a practicum places students in a professional research environment—often a national laboratory, industry group, or specialized research center—where they work alongside experienced scientists and engineers on active, mission-relevant projects. And when positions open in the national laboratories, prior practicum students are often highly competitive candidates: they already understand the lab environment, have proven they can contribute effectively, and require less onboarding. Practicums therefore act as a natural pipeline to national lab careers, benefiting both the student and the laboratory.

## Professional Development and Leadership

***Professional Development Sessions*** — Fellows receive professional development opportunities at the annual program review meeting. Additionally, opportunities promoted on LinkedIn from various sources are shared with the fellows. This cohort attended two formal professional development sessions and were made aware of multiple opportunities for development provided by national laboratories and universities.

***Mentoring*** — The DOE CSGF recognizes the importance of reciprocal mentoring relationships among alumni and current fellows, and this kind of community building is considered by the

program as critical for knowledge sharing towards progress and innovation. Mentoring by alumni is a vital component of a fellow's professional growth because it connects students with individuals who have successfully navigated the very path they are now on. Alumni mentors offer practical guidance grounded in real experience—whether it's choosing research directions, preparing for internships, applying to postdoctoral positions, or transitioning into national labs, industry, or academia. Their insights help fellows understand how to translate their training into career opportunities and avoid common pitfalls. Alumni also broaden a fellow's professional network, providing introductions, collaborations, and visibility within the scientific community. Just as importantly, alumni serve as relatable role models who can offer encouragement, perspective, and strategic advice at key points in a fellow's development. In this way, alumni mentoring strengthens the fellowship community and creates a supportive pipeline that helps current fellows succeed and contribute meaningfully to the broader scientific workforce. Alumni mentoring is provided to each fellow by both the DOE CSGF Steering Committee and its broad alumni network.

***Leadership*** — Fellows are also given meaningful opportunities to develop and demonstrate leadership, an essential skill for advancing in today's scientific and technical fields. Roles are provided to fellows at the program review meeting by leading poster review sessions, social activities and informational panels. These experiences not only build confidence and professional maturity but also prepare fellows to become future leaders in academia, industry, and national laboratories.

## 2020 Cohort Information and Accomplishments

The cohort funded under this award included 26 fellows, 17 men and nine women. They represented 17 unique universities and completed practicums at nine DOE Laboratories. These fellows entered the program representing 25 distinct and diverse undergraduate institutions including University of North Carolina at Greensboro, University of Texas at Austin, University of Maryland at College Park, and University of Colorado at Boulder to name a few.

At the time of joining the fellowship, this cohort contained 12 first-year doctoral students, 11 senior undergraduate students, one employed individual, and two master's degree students matriculating into a new university. For a full listing of the 2020 cohort, see below.

## 2020 Cohort Listing

| Name | University | Field | Practicum Location |
|---|---|---|---|
| **Alexandra Baumgart** | California Institute of Technology | Mechanical Engineering | Los Alamos National Laboratory |
| **Marc Davis** | Massachusetts Institute of Technology | Electrical Engineering and Computer Science | Argonne National Laboratory |
| **Emily de Jong** | California Institute of Technology | Mechanical Engineering | National Renewable Energy Laboratory |
| **Anthony Degleris** | Stanford University | Electrical Engineering | Argonne National Laboratory |
| **Ian DesJardin** | University of Maryland, College Park | Aerospace Engineering | Princeton Plasma Physics Laboratory |
| **Kiran Eiden** | University of California, Berkeley | Astrophysics | National Renewable Energy Laboratory |
| **Ethan Epperly** | California Institute of Technology | Applied and Computational Mathematics | Lawrence Berkeley National Laboratory |
| **Margot Fitz Axen** | University of Texas at Austin | Astronomy | Lawrence Berkeley National Laboratory |
| **Grant Johnson** | Princeton University | Plasma Physics | Lawrence Berkeley National Laboratory and Los Alamos National Laboratory |
| **Ariel Kellison** | Cornell University | Computer Science | Sandia National Laboratories, CA |
| **Nikita Kozak** | Stanford University | Mechanical Engineering | Lawrence Berkeley National Laboratory |
| **Mary LaPorte** | University of California, David | Plant Biology | National Renewable Energy Laboratory |
| **Nishad Maskara** | Harvard University | Physics | Lawrence Berkeley National Laboratory |
| **Kaishu Mason** | University of Pennsylvania | Statistics | Lawrence Berkeley National Laboratory |
| **Albert Musaelian** | Harvard University | Applied Mathematics | Lawrence Berkeley National Laboratory |
| **Laura Nichols** | Vanderbilt University | Computational Solid State Physics | Lawrence Berkeley National Laboratory |
| **Graham Pash** | University of Texas at Austin | Computational Science, Engineering and Mathematics | National Renewable Energy Laboratory |

| | | | |
|---|---|---|---|
| **Danilo Perez Jr** | New York University | Neural Science | Argonne National Laboratory |
| **Justin Porter** | Rice University | Mechanical Engineering | National Renewable Energy Laboratory and Lawrence Livermore National Laboratory |
| **Luis Rangel DaCosta** | University of California, Berkeley | Materials Science | Argonne National Laboratory |
| **Rachel Robey** | University of Colorado Boulder | Applied Mathematics | Oak Ridge National Laboratory |
| **David Rogers** | Stanford University | Earth System Science | Los Alamos National Laboratory |
| **Benjamin Sepanski** | University of Texas at Austin | Computer Science | Lawrence Berkeley National Laboratory |
| **Ellis Torrance** | University of North Carolina at Greensboro | Environmental Health Science | Lawrence Berkeley National Laboratory |
| **Margaret Trautner** | California Institute of Technology | Computing and Mathematical Sciences | Sandia National Laboratories, NM |
| **Santiago Vargas** | University of California, Los Angeles | Theoretical and Computational Chemistry | Lawrence Berkeley National Laboratory |

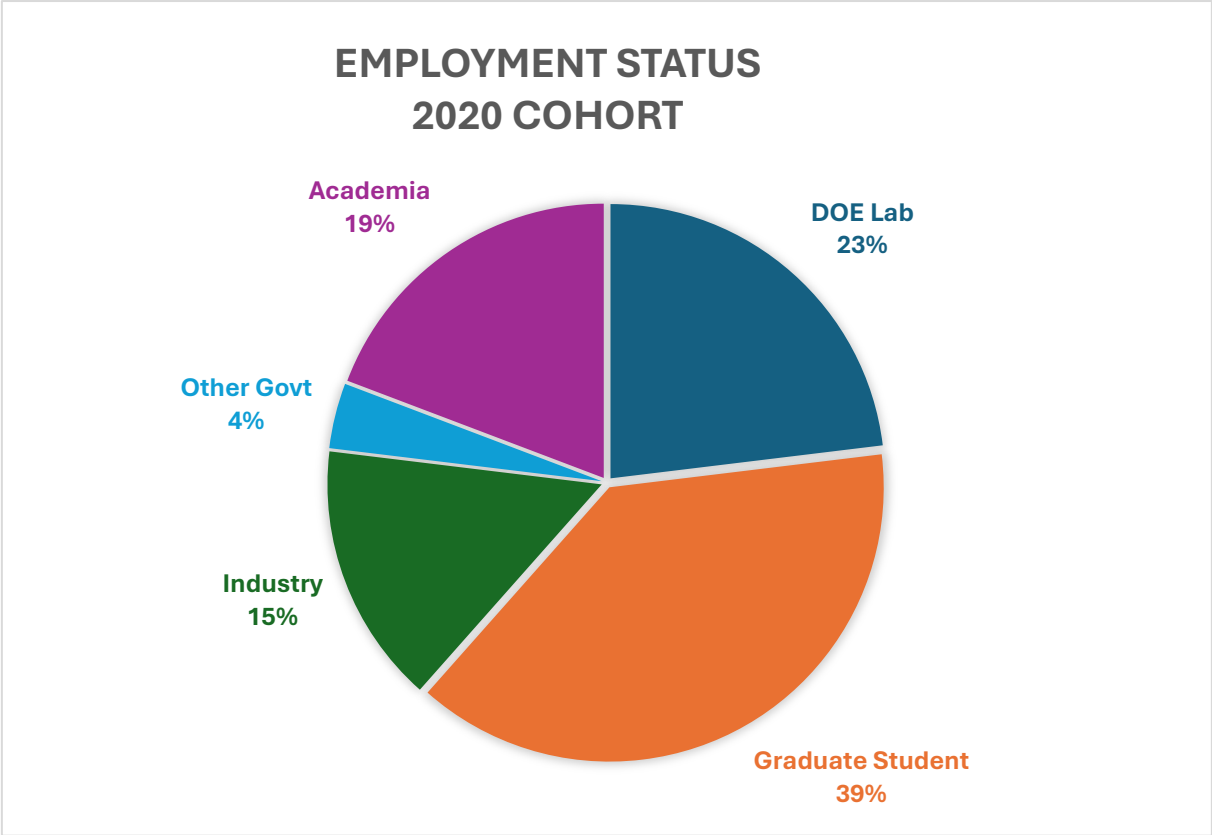
**Practicum** — During the award's duration, each fellow completed at least one practicum experience, while five fellows completed two practicums. A variety of DOE Laboratories hosted this cohort for practicums: Argonne National Laboratory, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Sandia National Laboratories, and the Princeton Plasma Physics Laboratory.

**Publications** — Graduate students are in a learning phase while in school, which means their primary focus is on developing research skills, learning methodology, and contributing to long-term projects. Because of this, it's common that they don't publish frequently during grad school – their work often takes several years to develop into publishable outcomes. However, after they graduate and become independent research, the produce publications and innovation at a higher rate. The investment made in them during graduate training pays off later, because the expertise, data, and foundational work developed in graduate school lead to contributions once they're in postdoctoral, academic, national laboratory, or industry positions.

As a result of their fellowship research, ten individuals from this cohort now have been published in peer-reviewed journals such as, *Journal of Plasma Physics, Nature, Nature Physics, Nature Chemistry, Journal of Chemical Physics, Physical Review E, The Astrophysical Journal, Journal of Computational Physics, and Microscopy and Microanalysis, G3: Genes|Genomes|Genetics, Frontiers in Microbiology, and Atmospheric Measurement Techniques*. This diverse range of publications illustrates the multi-disciplinary aspect of the DOE CSGF.

**Employment** — The DOE CSGF plays a critical role in strengthening the nation's scientific and technical workforce. Fellows go on to hold key positions across sectors – becoming faculty, researchers, and innovators. Their work contributes directly to national priorities in science and technology. Fellows often finish their PhD research outside of the four-year funding provided by the DOE CSGF. However, over half of this cohort is employed currently.

Based on self-reported data, Fellows are working in a variety of areas or remain in graduate school: 19% of the cohort reports working in academia; 23% work in DOE laboratories; and 15% are employed in industry. Nearly 40% of the cohort continues work on their respective PhD degrees.



## Dissemination Plan

The fellowship program's outcomes were widely disseminated through Krell-produced publications, conference presentations, and targeted communications such as newsletters, webinars, and social media. Career tracking demonstrated fellows' contributions to the scientific and technical workforce, while engagement with academic institutions, industry, and national laboratories shared best practices in mentorship and professional development. These dissemination efforts highlighted the program's impact and provided a model for cultivating the next generation of scientists and engineers.

The primary dissemination vehicle is DEIXIS magazine that highlights Fellows' accomplishments during their time in the fellowship. Additionally, a sister DEIXIS online webzine, LinkedIn, and podcasts (Science in Parallel), and pertinent press releases shared via the program's website (www.krellinst.org/csgf). The Fellows also presented their research progress during their time in the fellowship at the annual program review meetings. In their first three years, they presented research posters to the attendees which included DOE HQ, DOE Laboratory staff, colleagues and advisors. In their final year of the program, each Fellow presented a research talk to the attendees discussing their accomplishments and outcomes during the time of the award's support.


## Impact Statement

The real-world benefits of this program can be seen by the alumni contributions. As the cohort funded by the award move through their careers, they can be expected to join the career activities and accomplishments of their alumni peers. In general alumni of the DOE CSGF are employed in industry, academia and DOE laboratories where they make a range of professional contributions to computational science. Alumni have received many professional awards, grants and patents and have published research at an impressive rate.

Although the DOE CSGF has achieved remarkable success, the demand for highly trained researchers who utilize high-performance computing (HPC) across various disciplines continues to exceed available resources. To maintain its competitive advantage, the U.S. must enhance its investment in scientific computing and in the training and retention of computational scientists. The need for an adequate supply of these professionals — across National Laboratories, academia, and industry — has never been more critical. The DOE CSGF makes an important contribution to this demand.

To date, the DOE CSGF program has produced over 500 alumni — each an American citizen or legal permanent resident with a Ph.D. — guaranteeing a steady supply of scientists and engineers working in the public interest. Many DOE CSGF alumni are employed with the DOE National Laboratories; roughly 20 percent are employed in support of the U.S. government. Other alumni have pursued academic careers in which they contribute to the development of the next generation of computational scientists. In addition, the DOE CSGF has extended its reach far beyond the labs, emerging as an important factor in helping the U.S. maintain its edge in the multibillion-dollar technology sector. Together and individually, these computational scientists are critical links in our nation's innovation chain; the human capital that is helping ensure that the enormous potential benefits of advanced computational science are applied to solving our nation's most complex scientific and engineering challenges.