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2019 Budget Request for the DOE Computational Science Graduate Fellowship (CSGF) Grant

Final Technical Report

Shelly Olsan, Principal Investigator, Krell Institute[1]

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Administrative Point of Contact: Shelly Olsan, (515) 956-3696, shelly@krellinst.org

[1] Krell Institute, 1609 Golden Aspen Drive, Suite 101, Ames, IA 50010, 515.956.3696, shelly@krellinst.org

Overview

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) takes 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-SC0020347.

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.

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.

HPC Training

Under this award, the fellowship introduced an innovative approach to integrating first-year Fellows into the HPC community by inviting them to attend the 2019 Supercomputing Conference (SC) in Denver, CO. This opportunity allowed the Fellows to access more comprehensive HPC training than what is typically offered at the annual meeting.

At SC, the Fellows participated in a variety of workshops and tutorials led by leading experts in the HPC research community. Additionally, they benefited from networking opportunities, including receptions and meetings with HPC leaders, which were thoughtfully organized by Krell.

Of the 26 first-year Fellows, 20 were able to attend, and their feedback was overwhelmingly positive, highlighting the value of this experience in fostering connections and expanding their understanding of the HPC landscape.

Cohort Information and Results

The cohort funded under this award included 26 fellows, 18 men and eight women. They represented 18 unique universities and completed practicums at 10 DOE Laboratories. These fellows entered the program representing 25 distinct and diverse undergraduate institutions including Florida International University, Mississippi State University, Bloomburg University, Union College, University of the Pacific, University of Hawaii at Hilo, and University of Delaware 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.

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: Sandia National Laboratories, Lawrence Livermore National Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, Brookhaven National Laboratory, Pacific Northwest National Laboratory, Oak Ridge National Laboratory, National Renewable Energy Laboratory, and the SLAC National Accelerator Laboratory.

Based on self-reported data, Fellows are working in a variety of areas or remain in graduate school: 15% of the cohort reports working in academia; 19% work in DOE laboratories; and

19% are employed in industry. Approximately one-fourth of the cohort continues work on their respective PhD degrees and the remaining members of the cohort have not reported status at the writing of this report.

Dissemination Plan

Fellows' research outcomes were shared via multiple outlets. The primary vehicle is *DEIXIS* magazine that highlights Fellows' accomplishments during their time in the fellowship. Additionally, a sister *DEIXIS* online webzine, social media platforms (X, Facebook, 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.

The participants in the fellowship continue to make impacts in their fields, produce papers, and win awards well into their careers.

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.