Response to the ASCAC Charge to Review the Computational Science Graduate Fellowship Program

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Introduction

In response to a charge letter dated July 26, 2024, from then Acting Director of the Office of Science, Dr. Harriet Kung, to Dr. Martin Berzins, Chair of the Advanced Scientific Computing Advisory Committee (ASCAC), Dr. Berzins and the designated federal official, Dr. Ceren Susut-Bennett, formed a subcommittee to review the Department of Energy (DOE) Computational Science Graduate Fellowship (CSGF) Program.

The subcommittee was constituted in September of 2024 and consists of the following membership:

Prasanna Balaprakash	Oak Ridge National Laboratory
Tina Brower-Thomas (ASCAC)	Howard University
Jennifer Gaudioso	Sandia National Laboratories
Susan Gregurick (ASCAC)	National Institutes of Health (NIH)
William D. Gropp	University of Illinois, Urbana-Champaign
Arthur “Barney” Maccabe	University of Arizona
Irene Qualters (ASCAC) chair	Los Alamos National Laboratory (retired)
Mark E. Segal	National Security Agency (NSA)
Valerie Taylor (ASCAC) co-chair	Argonne National Laboratory
David Torres (ASCAC)	Northern New Mexico College
Stefan Wild	Lawrence Berkeley National Laboratory

The following report summarizes the findings and recommendations of the subcommittee. The executive summary provides an overall response to the charge. The executive summary is organized into a program overview followed by five themes within which we address the eight charge questions (labelled Q1-Q8). In a few cases, a theme responds to multiple related charge questions which were more easily addressed collectively. Subcommittee findings are summarized within each theme followed by a recommendation associated with the theme. Thus, there are five key recommendations identified in the Executive Summary.

Following the Executive Summary, subsequent sections of the report address the eight specific charges in more detail, identify significant data, and provide accompanying analysis and discussion of recommendations. The content of the report was informed by data provided by DOE CSGF Program Managers (PMs) and the Krell Institute. In addition, the subcommittee held interviews and discussions with the CSGF Principal Investigator (PI) and the two technical co-PIs. Additional expertise and supplemental public material were provided by subcommittee members. Prior to this review, the CSGF program was last reviewed by ASCAC in 2011 [1].

The charge to ASCAC [2] requested an examination of "the effectiveness and impact of CSGF and the quality and breadth of the program over the past decade". Among topics identified in the charge, the subcommittee was asked to address "the projected need for trained computational scientists in the DOE laboratories" and "continued U.S. leadership in computational science". In addition, the subcommittee was asked to address eight specific charge questions:

Q1. Does CSGF provide students with an effective and impactful program of appropriate quality and breadth?
Q2. Is there a unique role for CSGF in the landscape of federal graduate fellowship programs?
Q3. Is the program attracting diverse applicants and making awards to diverse cohorts?
Q4. How can CSGF reach a broader applicant pool?
Q5. Is the program appropriately tailored to support the computational scientist workforce needed at the DOE laboratories?
Q6. What is the most effective governance model for the program?
Q7. How should the CSGF evolve to ensure the best experience for students?
Q8. Is the program appropriately supporting students at institutions historically underrepresented in the federal research landscape?

[1] Response to the ASCAC Charge to Review the Computational Science Graduate Fellowship Program, 2011, https://science.osti.gov/-/media/ascr/ascac/pdf/reports/ASCAC_CSGF_Report_2011-Final.pdf

[2] U.S. Department of Energy Charge Letter from Acting Director of the Office of Science to ASCAC Chair, Dated July 26, 2024. https://science.osti.gov/-/media/ascr/ascac/pdf/charges/2024/revised-ASCAC-CSGF-Charge-Letter-07-2024_clean.pdf

Executive Summary

Program Overview

The DOE CSGF provides up to four years of fellowship funding to competitively selected U.S. citizen or permanent resident full-time students pursuing doctoral studies in computational science research within fields relevant to DOE missions.

The CSGF program has four objectives [1]:

1. *To help ensure an adequate supply of scientists and engineers appropriately trained to meet national workforce needs, including those of the DOE, in computational sciences.*
2. *To raise the visibility of careers in the computational sciences and to encourage talented students to pursue such careers, thus building the next generation of leaders in the field.*
3. *To provide practical work experiences for the fellows that allow them to encounter the cross-disciplinary, team-based, scientific research environment of the DOE National Laboratories.*
4. *To strengthen collaborative ties between the academic community and DOE National Laboratories so the fellowship's multidisciplinary nature builds the national community of scientists*

A distinguishing characteristic of the program includes its focus on helping to build DOE-relevant capability and capacity in the nation's next generation of computational scientists. The fellowship ensures a multidisciplinary computational science program of study and includes a research practicum at one of 21 DOE facilities, which includes 17 DOE labs. The DOE Office of Science, in partnership with the National Nuclear Security Administration (NNSA), administers the program through a grant to the Krell Institute. The program began in 1991 and continues to evolve in response to the expanding and changing role of computational science in science and engineering essential to DOE laboratories. Currently, 146 graduate students at 45 universities are supported by the CSGF program. Additional information on the program can be found at https://science.osti.gov/ascr/CSGF and https://www.krellinst.org/csgf/.

Effectiveness, Impact, Quality, and Breadth over the Last Decade

Computational science sits at the intersection of mathematics, computer science, and applied disciplines. For DOE laboratories, the applied disciplines are primarily based in engineering and physics. In the last decade, less than half of U.S. research PhDs in physics, mathematics, computer science, and engineering have been granted to U.S. citizens or permanent residents, the population eligible for the fellowship [2]. CSGF has both anticipated and adapted to workforce needs at DOE labs for computational scientists deeply skilled in cross-disciplinary, team-based science and engineering (e.g. exascale modeling, quantum information sciences, artificial intelligence, data science). The CSGF program of multidisciplinary study and the team-based practicum at a DOE lab effectively address training of the student while fostering long standing professional bonds among current and former fellows. The program's enduring community building promotes excellence and cohesion among the

nation's research workforce across industry, DOE labs, federal agencies, and academia in support of DOE and the nation's economic security.

CSGF leadership has implemented and maintained a rigorous process of applicant screening, fellow selection, student mentoring, and engagement. The resulting success of CSGF is evident in longitudinal studies and surveys that document the quality of fellows' publications, recognition received by fellows, subsequent career growth, and fellow satisfaction with the program. This program has demonstrated agility in responding to the need for a math/computer science track and inclusion of a broad set of considerations in candidate selection. The program selection processes have also demonstrated scalability as the number of applicants from across the U.S. has significantly increased along with the number of distinct colleges and universities from which fellows received their undergraduate degrees. Importantly, CSGF is building both capability and capacity in the computational research workforce needed by DOE labs and the nation. The subcommittee concludes that CSGF quality and breadth in the last decade have been excellent, both effective and efficient. Further, considering DOE cross-cutting priorities, such as quantum information science (QIS) (National QIS Research Centers) and artificial intelligence (FASST), as well as numerous national computational science priorities (e.g., [4,5,6]), the subcommittee views continued U.S. computational science leadership as critical for both DOE and the nation. The subcommittee applauds CSGF effectiveness, impact, quality and breadth over the past decade.

Nonetheless, with rising fellowship interest among students and growing demand from DOE labs, the program must continue to evolve its strategic approaches to maximize stakeholder impact in the next decade. The additional funding as recommended in the 2011 CSGF program review has resulted in growth in the number of new fellows: from 23 in 2014 to 40 fellows in 2024. However, single digit acceptance of applicants has become the norm.

Recommendation (R1)

The subcommittee recommends that the DOE Advanced Scientific Computing Research Program (ASCR) foster growth of CSGF. This growth can occur through encouraging the program to develop deeper strategic engagement, alignment, and coordination with the DOE labs to both prioritize needs and secure additional collaborative funding. Other opportunities for growth (e.g. via collaboration with agencies similarly dependent on use-inspired and applied research from a multidisciplinary scientific workforce), should be explored by ASCR in partnership with NNSA/ASC.

Uniqueness in the Federal Landscape (Q2)

Many federal agencies support graduate fellowships, including the National Science Foundation, National Institutes of Health, the Department of Defense, National Oceanic and Atmospheric Administration, and the National Aeronautics and Space Administration. Like the CSGF, these programs are focused on STEM disciplines and require citizenship/permanent residency. Four characteristics collectively define the uniqueness of CSGF: 1) CSGF is dedicated to multidisciplinary large-scale scientific computing,2) CSGF includes a four-year stipend, 3) CSGF includes a hands-on, 12-week practicum experience within a national laboratory, and 4) CSGF includes a strong mentoring element. The DOE laboratory practicum provides fellows with access to a wide range of advanced computing systems, instruments, data, and expertise. The mentoring network and support for conference attendance is

unique among computing-related fellowship programs. In materials provided through surveys of CSGF cohorts, the Annual Program Review meeting was cited as a primary venue for fellows to network and build lasting career bridges. Most fellows ultimately pursue career opportunities in industry but value both the skills and the professional ties formed as a CSGF Fellow. This cultivation of an enduring sense of community across academic, industry, and federal computational scientists delivers lasting value to the DOE and the nation. As a result, the CSGF fellowship program produces the largest cohort of multidisciplinary computational science graduate fellows per year.

Recommendation (R2)

ASCR, in partnership with NNSA/ASC, should continue to support the CSGF program given its uniqueness within the federal landscape and its demonstrated success in making significant and lasting contributions to the development of the nation's multidisciplinary computational scientists.

Increasing Program Excellence by Expanding Capacity (Q3, Q4, Q8)

Over the last decade, the CSGF program has strategically expanded and strengthened excellence in the national talent pipeline for scientific and technological domains essential to the future of DOE missions. Its efforts benefit not only the DOE labs but the economic and national security of the United States. CSGF has maintained high quality in the cohorts and has taken a holistic approach to meeting the gap in U.S. multidisciplinary computational scientists. Geographic, institutional, field of study, and individual applicant qualities are considered and tracked. Broadening the fields of study within the CSGF applicants has improved, with the addition of a mathematics/computer science track in 2018, in anticipation of the growing importance of these disciplines for the workforce of DOE labs and the nation's economic competitiveness. The fellow selection process is comprehensive, including, for example, first-in-family to attain college degree and veteran/military status. Over the last decade, CSGF has successfully undertaken actions to attract high-quality applicants from a much wider range of public and private universities across the nation. In the past five years, as a result of targeted outreach by CSGF, the number of undergraduate schools that are producing fellows has increased to 200, encompasses more states, includes more R2 institutions, and exhibits greater balance between public and private institutions. As noted in the recent CSGF longitudinal study, faculty engagement is an essential element in successfully identifying and cultivating promising graduate student talent across differing fields of study. The program acknowledges the challenges and the value in successfully expanding its recruitment efforts (e.g., universities within EPSCoR states). It is playing a pivotal role in building a versatile U.S. workforce capable of addressing complex national challenges and maintaining U.S. technology leadership.

Recommendation (R3)

As part of an overall strategic plan (see R4 on page 8), in support of CSGF mission objectives 1 and 2, the program should develop a comprehensive talent outreach strategy to efficiently expand the fellowship's pipeline across the U.S. Development and implementation of that strategy should leverage the outreach strategies and academic partnerships of DOE labs.

Meeting the DOE Laboratory Need for Computational Scientists/Effective Governance (Q5, Q6)

The demand for highly capable computational scientists within the DOE laboratories remains both acute and enduring. The precise emphasis in required skills continues to evolve in response to DOE mission challenges and the new opportunities brought with a disruptive technology landscape. Recent changes in the focus of student research choices emphasize data science, machine learning, artificial intelligence, and quantum information sciences. In anticipation of these emerging needs, the program introduced a new mathematics/computer science track.

The CSGF program has implemented operational governance and processes that convincingly demonstrate robust and consistent quality for program objectives 2 and 3. Adaptability and scalability in governing the fellow selection process has been successfully demonstrated over the last decade. Progress towards increasing both capability and capacity in the nation's multidisciplinary computational workforce has resulted from the CSGF governance model. Notably, the makeup of core governance bodies include not only lab but also university, industry, and other federal agency members. The program is ideally poised to further increase its strategic collaborative engagement with the academic community, industry, and the DOE labs. Greater flexibility and agility in the makeup of CSGF governing teams may be needed to help meet the nation's, and DOE's, future workforce needs in computational science leadership.

Recommendation (R4)

The subcommittee recommends that the CSGF program, with guidance from ASCR and with greater input and participation from DOE labs, develop a five-to-ten-year strategic plan that addresses all four program objectives, including specific and measurable outcomes. The program should revise its governance bodies accordingly to prioritize greater stakeholder engagement while maintaining/improving efficiency and effectiveness of operations.

Quality and Breadth of Student Impact/Evolving to Meet Student Needs (Q1, Q7)

Over the past decade, CSGF alumni report increasing satisfaction in the accrued benefits of the fellowship. The survey of alumni examines satisfaction in topics such as computational skill development, improved research quality, new skills acquired, and access to new opportunities. Importantly, nearly 100% agree that this fellowship was "the right career decision". Even during the COVID pandemic, virtual practicums maintained high levels of satisfaction.

The program's unique strengths in providing computational science education and multidisciplinary training provide an excellent foundation for development of the next decade of leaders in computational science. Continued program agility and responsiveness will ensure excellence in attracting and developing future fellows. Likewise, the program's demonstrated rigor in measurement and evaluation of results will be essential to ensuring effective and efficient strategic evolution.

The subcommittee concludes that CSGF is "providing students with an effective and impactful program of appropriate quality and breadth." Moreover, the CSGF model of evolutionary change paired with robust evaluation of results is key to both past and future success.

Recommendation (R5)

As CSGF looks to the future, we recommend that the program consider evolving student needs in the following areas: emerging technologies integration, professional skills development, academic institutional reach, building community, fellowship support services, and program evaluation.

[1] DOE Computational Science Graduate Fellowship website, https://www.krellinst.org/csgf/about-doe-csgf.

[2] Survey of Earned Doctorates (SED) 2023, National Center for Science and Engineering Statistics, Table 1-6, Research doctorate recipients by trend broad field of doctorate and citizen status, 1978-2023. https://ncses.nsf.gov/pubs/nsf24336/table/1-6

[3] Review of DOE Computational Science Graduate Fellowship, November 23, 2011. Submitted to the Office of Science, DOE, by the Subcommittee of the Advanced Scientific Computing Advisory Committee. https://science.osti.gov/-/media/ascr/ascac/pdf/reports/ASCAC_CSGF_Report_2011-Final.pdf

[4] SIAM Task Force Report : The Future of Computational Sciences, 2024, The Society for Industrial and Applied Mathematics. https://www.siam.org/media/cfufuosh/siam-report-on-the-future-of-computational-science.pdf

[5] National Academies of Sciences, Engineering, and Medicine, 2023. Charting a Path in a Shifting Technical and Geopolitical Landscape: Post-Exascale Computing for the National Nuclear Security Administration, Chapter 4, p. 82-90, Workforce Needs. https://nap.nationalacademies.org/catalog/26916/charting-a-path-in-a-shifting-technical-and-geopolitical-landscape

[6] National Academies of Sciences, Engineering, and Medecins, 2024. Foundational Research Gaps and Future Directions for Digital Twins, Chapter 7, p.109-13, Preparing an Interdisciplinary Workforce for Digital Twins. https://nap.nationalacademies.org/catalog/26894/foundational-research-gaps-and-future-directions-for-digital-twins

Supporting Detail for Specific Charge Questions (Q1-Q8)

The subsequent sections of the report provide more detailed data, discussion and analysis of the eight specific charge questions. These sections provide the basis for the five recommendations identified in the Executive Summary. To improve readability, charge questions Q3, Q4, and Q8 have been combined under the Theme of Increasing Program Excellence by Expanding Capacity.

Effectiveness and Impact for Students (Q1)

The subcommittee finds that the CSGF program has had a significant and sustained impact on filling critical workforce needs in computational science. CSGF has increased the number and quality of computational scientists through its support of graduate students over the past decade, and indeed, since its inception. The 2022 [1] and 2017 [2] longitudinal studies of CSGF recipients highlight benefits that students received from their participation. Significantly, the percentage of alumni who report that CSGF participation played a major role in each of the top benefits of the program increased – beyond already lofty numbers – from the 2017 to 2022 studies as shown in Figure F1.

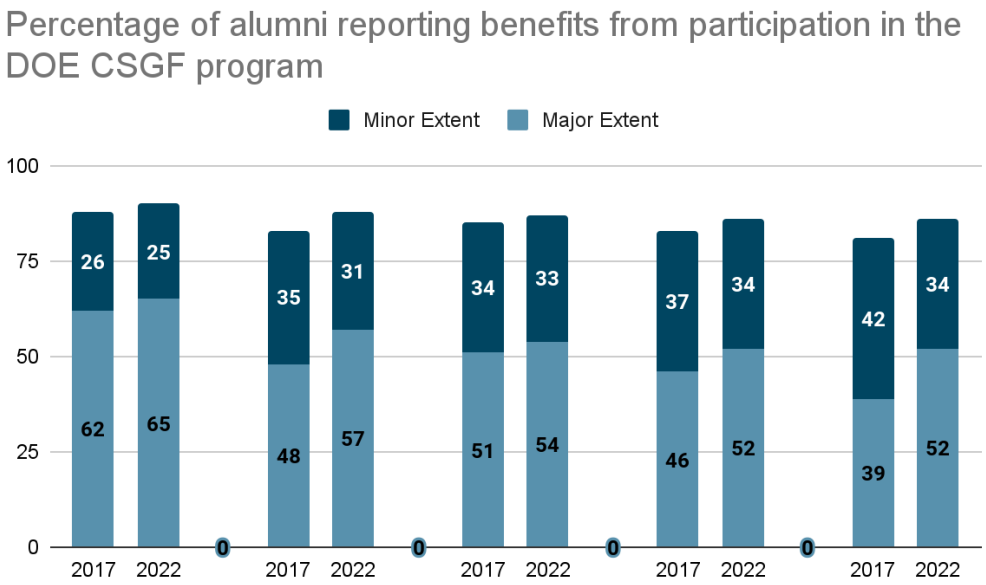


Figure F1: The five major benefits perceived by students (from L to R): (i) Enhanced their knowledge of HPC; (ii) Improved overall quality of their research; (iii) Enhanced their computing capabilities; (iv) Increased their subject matter knowledge/expertise in other areas (i.e., other than computing capabilities); (v) Improved their research skills and/or techniques. [Data is from [1] & Figure 1 of abbreviated 2022 study and April 19, 2017 ASCAC presentation of John Wells and Tara Dunderdale, Westat]

Students have reported a broad set of career impacts from their participation in the CSGF program. For example, in the 2022 Longitudinal study [Figure 4-24, 1], 93% and 60% of students strongly agreed that accepting the DOE CSGF was the right decision for their career and that their experience as a Fellow continues to help achieve their career goals, respectively. Similarly, 90% of students agreed that the experience provided them with professional knowledge and skills that they would not have developed otherwise, and that because of this experience, they have encouraged others to pursue computational science and engineering as a field of study. Consequently, the program has influenced individuals'

career goals and direction, and enhanced students' skills and expertise, communication skills, and degree of self-confidence in their field.

The Fellowship has also accelerated or otherwise transformed the rising trajectories of many students. The subcommittee found a breadth of impacts to specific individuals noted over the past decade; for brevity, we include two such anecdotes. In his 2017 presentation to ASCAC [4], Jeff Hammond (then Intel, now NVidia) noted that the CSGF program "is the single most important thing that has happened to me in my professional life." Ariel Kellison (from Cornell University/Sandia National Laboratories) notes that a key impact of the CSGF program was the pairing with Laboratories "that are currently in need of tools that can be deployed… I get to hear about how formal methods are used in the lab and outside my wheelhouse, which is really cool" [5].

The Fellowship has also grown the national ecosystem developing software for science and engineering. In part through structural elements (e.g., the program of study, practicum, training opportunities at the annual program review) of the CSGF program, a growing number of alumni reported leading such development during the Fellowship. Figure F2 also highlights that this increase has been largely sustained since the Fellowship, which is an important hallmark given the attrition sometimes seen for contribution to scientific codes, software suites, and open-source software.

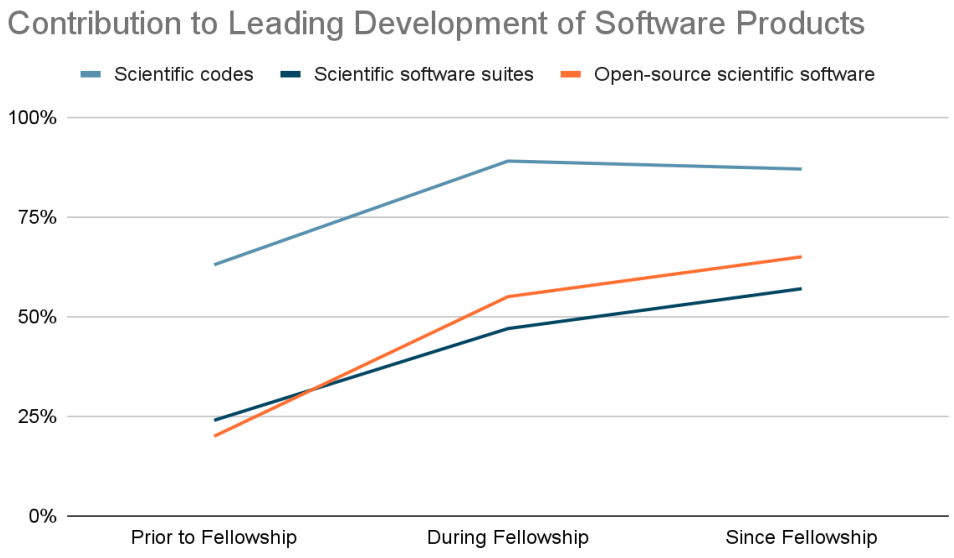


Figure F2: Percent of CSGF alumni leading development of software products before, during, and after the Fellowship. (Created from data in Figure 4-14 of [2])

One of the key benefits to students is that the CSGF Fellowship significantly frees them to select their research topics (as opposed to having topics dictated from other drivers such as advisor funding in the area). One evident benefit of this flexibility is that the resulting research topics pursued under the CSGF are often harbingers of emerging research and technology areas of national importance. For example, a

recent ASCAC subcommittee examining U.S. competitiveness in HPC noted [3]: "The CSGF program provides a barometer for disciplines that will be of interest to future DOE computing. Computational biology, machine learning, and quantum computing are among the subjects that began to swell in the ranks of CSGF applicants before the labs were hiring as high a percentage of employees in these categories."

Effectiveness and Impact of the Fellowship Elements

The CSGF structure has five primary elements designed to help impact and breadth for students

1. An interdisciplinary program of study
2. At least one 12-week practicum at a DOE Laboratory
3. Participation in the CSGF Annual Program Review
4. Community building
5. Close tracking and agile response to changes

The program of study is a key differentiation from other federally funded fellowships and includes courses in science & engineering, mathematics/statistics, computer science, and high-performance computing. Krell staff and the CSGF steering committee closely track a student's progress through all phases of their individual program of study. Although the program of study requires students to take additional courses beyond those required to satisfy their doctoral requirements, the 2022 longitudinal study [1] reports that alumni find that taking courses outside of their degree field enhances their ability to perform interdisciplinary research. For example, one alum stated [1]: "*The program of study is one of the most underrated features of the CSGF… this is a fellowship that makes you take classes outside of your main field, and one such class was quantum computing, which probably was one of the earliest classes that was offered in the field. Now I do a lot of research on quantum computation and other forms of computation… The fact that I took a course in alternative computing, like quantum computing, early on was very formative and enabled me to do a lot of other types of computing research that I do now. That's been very key for my research.*"

The 12-week practicum at a DOE Laboratory is intended as a broadening experience, where a Fellow performs research in an area distinct from their current thesis topic. In many cases, the practicum has furthered the growth of students as independent researchers. Over the course of the CSGF program, a growing number of students have performed an additional practicum, often at a second Laboratory. The 2022 longitudinal study noted significant student satisfaction along many fronts with the practicum. As indicated in Figure 4-1 of [1], over 68% of students were satisfied with support received from their practicum supervisor and Laboratory staff along a broad array of criteria, including generating ideas about research, direction during practicum research, obtaining access to specialized equipment for research, gaining a better understanding of continued opportunities for collaboration, increased awareness of professional development opportunities, expanding career networks, and finding employment opportunities.

The CSGF Annual Program Review brings together students (and their academic advisors) to share research (through presentations, poster sessions, and casual conversation), network with other

students, alumni scientists (from Labs, industry, and academia) and Federal program managers, and provide professional development activities. The 2022 longitudinal study [1] notes that an overwhelming majority of students reported significant benefits from the program review in facilitating interaction with researchers in other fields, intellectual stimulation and exchange, and insight into current and/or future big picture problems. Other key benefits were in terms of professional development and networking. For example, the 2024 program review included elements such as:

- A focused gathering of the incoming cohort of students
- A pre-reception aimed at making connections among students and attendees
- A lunch & civics talk
- A showcase of all DOE labs for learning about individual DOE labs, practicum shopping, employment, etc.
- A professional development workshop
- A science communication panel
- Additional programming curated/facilitated by and for students and alumni.

The 2022 longitudinal study [1] also noted that recent cohorts were far more likely to find that aspects of the program review were useful in obtaining employment and developing mentoring relationships.

In terms of community building, a common refrain in the documents and data provided was the significant "cohort" nature of the CSGF, especially relative to other interdisciplinary doctoral fellowship programs. In addition to the program review and practicum, this community aspect is engineered in ways such as an annual Communicate Your Science & Engineering (CYSE) essay contest, a Slack space managed by and for students and alumni, and the establishment of an alumni association (independent of Krell and the PIs). According to the 2022 longitudinal study [1], over half of alumni report that they have stayed in touch with other CSGF recipients and over 40% report that they have stayed in touch with their Laboratory practicum supervisor. Additionally, over 80% of alumni reported that the CSGF program actively took steps to make them feel included as a member of the CSGF community. A contributing factor to the benefits of this cohort nature is the increased breadth of students. For example, over the past five years, the 170 fellowships awarded reflect 101 distinct undergraduate institutions, a key signal of the breadth of perspectives contributing to the CSGF cohort. This breadth is mirrored by the breadth of research topics pursued by current students, ranging from the study of crop traits in corn to the understanding of exoplanets to developing state-level digital twins for the spread of epidemics.

A final structural benefit to students is the close tracking and agile response to changes over the course of their fellowship. Krell staff hold regular office hours for students and are continuously available – via slack, email, phone, etc. – to support students with concerns and issues. Krell staff and steering committee members also leverage their significant experience across many doctoral programs to direct students to appropriate resources and effective solutions. For example, when students encounter interpersonal challenges with their academic advisor or research group, the fellowship PIs and Krell staff, in consultation with the steering committee, work with the fellow to find resolution, from reaching out to the fellow's department and advisor to helping the student find a new research group at that or

another university. A key advantage of the fellowship being connected to the student, and not the institution or advisor, is that it provides flexibility for the student to change advisors or institutions if that is in their best interest. It is also noteworthy that the Fellowship agilely transitioned to virtual practicums at the onset of the COVID 19 pandemic, with most students noting that they were "able to establish and maintain important connections and receive mentoring from their advisor and others that led to enhancements in their skills and knowledge" [1]. The Fellowship routinely solicits feedback from students annually following the program review meeting, and surveys alumni annually on employment, achievements, and contact information.

As the fellowship continues to grow and evolve over time, it is important that the CSGF program continues to re-evaluate, augment, and substitute these structural elements to maximize the impact and cohort/community nature of high value to students. The committee identified six areas of evolution for consideration by the program. These are identified in recommendation (R5) in the Executive Summary and discussed in detail within the report section responding to Q7.

[1] DOE CSGF: 1991-2021, A follow-up study of recipients and programmatic outcomes, December 2021, https://www.krellinst.org/doecsgf/docs/2022_DOE_CSGF_Longitudinal_Study-Web.pdf

[2] DOE CSGF: 1991-2016, A follow-up study of recipients and programmatic outcomes, February 2017, https://www.krellinst.org/doecsgf/docs/2017_DOE_CSGF_Longitudinal_%20Study-Web.pdf

[3] DOE ASCAC Subcommittee report, Can the United States maintain its leadership in high-performance computing?, 2023 https://science.osti.gov/-/media/ascr/ascac/pdf/meetings/202306/ASCAC_Subcommittee_on_American_Competitiveness_202306.pdf

[4] Jeff Hammond. Down the rabbit hole: From B3LYP to x86, ASCAC presentation, April 2017. https://science.osti.gov/-/media/ascr/ascac/pdf/meetings/201704/Hammond_ASCAC2017_final.pdf

[5] Sarah Webb. Subduing software surprises. DEIXIS. August 2024. https://deixismagazine.org/2024/08/subduing-software-surprises/

Uniqueness in the Federal Landscape (Q2)

There are at least 38 graduate fellowship programs that are focused in computer science fields of study that are spread across academic, non-profit, industry, and federal agencies [1]. The National Science Foundation's Graduate Fellowships in Computer and Information Science and Engineering (CSGrad4US) is dedicated to computer and information science and engineering research rather than a focus on cross-disciplinary computational science.

The DOE offers two fellowship opportunities for computational graduate students to receive funding for their studies: the Office of Science Graduate Student Research (SCGSR) program and CSGF.

The SCGSR program provides stipend support for students to collaborate with a DOE national laboratory, working with national laboratory scientists and using state-of-the-art facilities and cutting-edge scientific instrumentation. In 2024, DOE selected 62 graduate students representing 25 states and Puerto Rico. However, only four students were from a computer science field of study as represented by ASCR [2]. Moreover, the SCGSR emphasis is neither multidisciplinary nor computational science.

The DOE CSGF provides opportunities to students pursuing doctoral degrees in fields that require advanced computational methods and high-performance computing to solve complex science and engineering problems of relevance to DOE. The subcommittee finds that the CSGF program remains unique among federal graduate student fellowship programs. Graduate programs, such as those offered by the National Science Foundation and National Institutes of Health, or DOE SCGSR do not target multidisciplinary computational sciences. Similarly, the Department of Defense, National Aeronautics and Space Administration and National Oceanic and Atmospheric Administration have agency-specific graduate fellowships that may encompass multidisciplinary use-inspired or applied research but do not include the breadth of career development components within CSGF.

The CSGF program offers four full years of cross-disciplinary training, which is best illustrated by a strong specific program of study and a practicum within one of the DOE national laboratories. In addition, this program offers an annual program review held each summer in the Washington, D.C. area and is the main venue for fellows to network and build bridges. CSGF cohorts attend the annual International Conference for High Performance Computing, Networking, Storage, and Analysis (colloquially known as Supercomputing) and are encouraged to present posters at this meeting. The CSGF Executive Committee, with counsel from the Steering Committee, provides oversight, technical guidance, and expertise for the fellowship program.

The impact of this fellowship includes a broader reach to universities, colleagues, and other fellows from industry and government. The focus on outreach to a wide set of public/private institutions is evident in the 2023 cohort. This serves to engage university faculty and departments that may not currently offer multidisciplinary programs of computational science study.

Recognition of scientific impact is readily evident in prize-winning teams at international conferences (see Team Including Fellow and Alumnus Wins HPC Prize for COVID-19 Research | DOE CSGF; Fellow on COVID-19 Bell Prize-Winning Team).

Based on the Westat review [3], the primary reason students apply for this fellowship is the level of stipend support. However, the most valuable experience for participants of this program, as indicated in

the fellows' survey, is the networking opportunities and exposure to the national laboratory's capabilities and resources. Importantly, alumni who have gone through this program seem to have continued in computational science and 46% continue to use DOE supercomputers. The number of alumni who remain in the DOE national laboratory system is at 15% (current data provided by DOE ASCR). While this may appear to be a low percentage, it is more positive when viewed in the U.S. landscape where more than 80% of the nation's researchers are funded by industry and fewer than 10% are federally funded [4].

As noted in the Executive Summary, the subcommittee finds that the program is unique in the federal landscape and strongly recommends (R2) that ASCR continue its support of CSGF in partnership with NNSA/ASC.

[1] Profellow online resource and free database for information on professional and academic fellowships. https://www.profellow.com/

[2] SCGSR Awrad and Publications 2024 WDTS SCGSR Offer Accepted https://science.osti.gov/wdts/scgsr/SCGSR-Awards-and-Publications

[3] US DOE: Computational Science Graduate Fellowship 1991-2021 December 2021 by Westat, accessed 11/2024 https://www.krellinst.org/doecsgf/docs/2022_DOE_CSGF_Longitudinal_Study-Web.pdf

[4] U.S. R&D and Innovation in a Global Context: The 2024 Data Update, AAAS, Figure 3.3. https://www.aaas.org/sites/default/files/2024-04/AAAS%20Global%20RD%20Update%202024.pdf

Increasing Program Excellence by Expanding Capacity (Q3, Q4, Q8)

The CSGF program has implemented strategic approaches to expand and strengthen the national talent pipeline in critical scientific and technological domains. These approaches directly benefit DOE scientific and nuclear security programs and potentially improve the economic and national security of the United States. This section of the report addresses the following three charge questions:

Q3. Is the program attracting diverse applicants and making awards to diverse cohorts?
Q4. How can CSGF reach a broader applicant pool?
Q8. Is the program appropriately supporting students at institutions historically underrepresented in the federal research landscape?

Given the overlap in these questions, we combine the three charge questions in our response and discuss the following three areas (1) Current CSGF Strategies to Broaden the Applicant Pool, (2) Broadening the Awardee Cohort, and (3) Recommendation to strengthen the strategies to broaden the applicant pool.

CSGF Strategies to Broaden the Applicant Pool

According to [8], CSGF engaged in numerous types of recruitment activities, including direct mail, follow-up postcards and emails, print ads, digital/online ads, in-person recruitment, online recruitment meetings, social media promotion, informational sessions/webinars, Science in Parallel podcasts, McNair Scholars Outreach, and DOE Lab Student Programs Outreach. The CSGF program has thereby increased the demographic reach of the applicant pool along four dimensions.

First, there is the dimension of the disciplines represented in computational science, recognizing the need for additional mathematics and computer science expertise in anticipation of new technology capable of solving complex national challenges. A significant milestone was the introduction of a Mathematics/Computer Science track in 2018, which has helped broaden the traditional engineering-dominated landscape. Prior to 2018, engineering disciplines dominated the program. The addition of the Mathematics/Computer Science track [1] has helped rebalance this, attracting 75 applicants for 10 available fellowships in 2021, making up approximately one-third of that incoming cohort. By 2021, mathematics/computer science fellows represented one-quarter of all program participants (28 individuals), demonstrating successful expansion of disciplines. In 2024, out of 40 total fellows, the mathematics/computer science track represented about 28% (11 fellows) [2], supporting the continued success of cultivating a more comprehensive and adaptable computational science workforce.

Second, the CSGF program has prioritized recruiting high-quality candidates from a wider range of academic experiences, with particular emphasis on:

- First-generation college students (currently 12-18% of applicants)
- Active-duty military personnel, reserve military personnel, and veterans (currently ~1% of applicants)

In 2022, 2023, and 2024, 16%, 16%, and 12% of applicants were first-generation, respectively [8]. In 2024, while applicant home addresses remain clustered in the states of Colorado, Illinois, New York, Texas and Seattle, more than 40 states had at least one applicant.

Third, with guidance from DOE and the CSGF Steering Committee, the program improved national awareness of the fellowship, resulting in expansion in the number of high-quality applicants from across the U.S. Krell recruits at national conferences, career fairs, and virtual information sessions of varying size, focus, and venue.

Fourth, the CSGF program has extended the reach of the fellowship to institutions within states/territories previously overlooked in the federal research landscape. Institutions previously with less representation in the federal landscape are defined as institutions located in Experimental Program to Stimulate Competitive Research (EPSCoR) designated states. States or territories participating in EPSCoR receive less than 0.75% of total federal R&D funding over a three-year average. Of the 50 US states and 16 territories, 25 states and 3 territories qualify as EPSCoR. A significant number of non-R1 institutions exist within EPSCoR states.

Since the most frequent source of information was an academic advisor or professor, the program "has focused on increasing the visibility of the fellowship with individual faculty" [5]. In 2023, there were 513 applicants to the program for across the US and its territories. A promising outcome of the recruitment efforts is described in the 2024 evaluation report. It was noted that in 2024, the applicant pool included 199 unique undergraduate institutions, of which 141 are non-R1 institutions.

Broadening the Awardee Cohort

Selection data from 2024 demonstrates the program's commitment to identifying and supporting exceptional talent across various backgrounds. For instance:

- In Science and Engineering, the selection process has focused on identifying top-performing candidates from different educational backgrounds
- Selection rates show a deliberate approach to recognizing outstanding potential across different student populations

The program maintains extremely high standards while expanding its reach [1]. In 2021, 484 applicants competed for 32 fellowships, demonstrating both the program's prestige and the substantial pool of qualified candidates. Selection committees include experts from academia, DOE, other government agencies, and industry, including former CSGF recipients. The program maintains a rigorous approach to talent selection, ensuring that:

- Only the most qualified candidates are selected by an experienced cross-disciplinary selection process of industry, academic and laboratory scientific experts
- Selection processes prioritize academic excellence and potential impact
- Recruitment strategies align with national scientific and technological needs

From 1991-2021, six institutions accounted for more than 40% of all recipients (MIT, Stanford University, University of California, Berkeley, Harvard University, University of Illinois Urbana-Champaign, and Caltech). However, from 2015 to 2024, the same six institutions accounted for 20.4% of recipients.

The program selected recipients from 76 universities representing 33 states and the District of Columbia (1991–2021). The ratio of recipients from public (49%) and private institutions (51%) seems balanced in the most recent cohort (2018-2021) [2].

The DOE CSGF program is very competitive. According to [1], in 2021, 484 applicants competed for only 32 fellowships (6.6%) that were awarded that year. "Over the past 15 years, from 349 to 729 students have applied annually for an average of 21 awarded fellowships" [9].

Recommendations to Strengthen CSGF Strategies to Broaden the Applicant Pool

The subcommittee commends the CSFG program for its impact in building the nation's awareness of, and capacity in, multidisciplinary computational science. As specified in (R4) of the Executive Summary, the subcommittee recommends that the program "develop a comprehensive talent outreach strategy to efficiently expand the fellowship's pipeline across the U.S. Development and implementation of that strategy should leverage the outreach strategies and academic partnerships of DOE labs. As noted in the recent CSGF longitudinal study, faculty engagement is an essential element in successfully identifying and cultivating promising graduate student talent across diverse fields of study."

The DOE CSGF program stands at the forefront of developing critical national scientific talent serving as a key strategic investment in the United States' technological capabilities. By implementing the recommended comprehensive national talent outreach strategy, the CSGF can further strengthen its pivotal role in expanding the pool of U.S. citizens pursuing advanced computational sciences, building a versatile workforce capable of addressing complex national challenges and maintaining the U.S. competitive edge in emerging technological domains.

[1] U.S. DOE CSGF: 1991-2021, A follow-up study of recipients and programmatic outcomes, December 2021, John Wells, Holly Bozeman, Brad Keller, Atsushi Miyaoka, Vasiliy Sergueev, Adrienne von Glatz, Kerri Wills, Westat . Report accessed 11/2024. https://www.krellinst.org/csgf/study

[2] DOE CSGF, FY 2024 Cohort Report, Christine Chalk, SC Program Manager for CSGF, May 17, 2024

[3] 2020 Budget Request for the DOE Computational Science Graduate Fellowship, Shelly Olsan, 09/01/2020 - 08/31/2024

[4] 2023 Computational Science Graduate Fellowship Program, Shelley Olsan, 09/01/2023-08/31/2027

[5] 2024 Computational Science Graduate Fellowship Program, Proposal #0000279814, Krell Institute, Inc., Ames, Iowa, P.I. Olsan, Shelley

[6] DOE CSGF Review of the DOE CSGF Program, Responses to ASCAC Committee October 18, 2024

[7] Department of Energy Computational Science Graduate Fellowship: A Briefing for DOE NNSA and Office of Science, March 1, 2024

[8] DOE CSGF Recruitment Summary; Correspondence: Response to ASCAC subcommittee questions, David Brown (LBL), Jeff Hittinger (LLNL), Shelly Olsan (Krell Institute) October 10, 2024

[9] The Early Years and Evolution of the DOE Computational Science Graduate Fellowship Program, DOE Computational Science Graduate Fellowship Research Showcase, David Brown, James Hack, and Robert Voight, 2021

Meeting the DOE Laboratory Need for Computational Scientist (Q5)

The first of four objectives of the DOE CSGF program is the following: *To help ensure an adequate supply of scientists and engineers appropriately trained to meet national workforce needs, including those of the DOE, in computational sciences* [1]. From inception, the DOE CSGF program was tailored to support the national needs for computational scientist workforce, including that of the DOE National Laboratories. As noted previously, some of the unique program requirements that support this objective include the following:

- a multidisciplinary program of study for a future in computational science.
- at least one 12-week practicum at an approved DOE National Laboratory.
- participation in an annual scientific program review.

These three requirements provide the fellow with the program of study focused on computational science, along with an opportunity to put into practice the program of study, via the practicum, and an opportunity to engage with other computational scientists via the annual scientific program review. All components are important to establishing a computational scientist workforce.

The 12-week practicum is unique to the DOE CSGF program. Fellows pursue research outside of their thesis studies, thereby expanding their research capabilities. Fellows choose from 21 DOE facilities and 22 physical locations. The practicum may be completed any time during the first two years of the fellowship, with the summer months serving as the common time frame. An additional financial allowance is provided to cover extra expenses during the 12-week practicum. Figure F3 identifies the distribution of completed practicums, 1992-2020. The data indicates an opportunity for the different DOE facilities to better engage with the fellows about practicum opportunities.

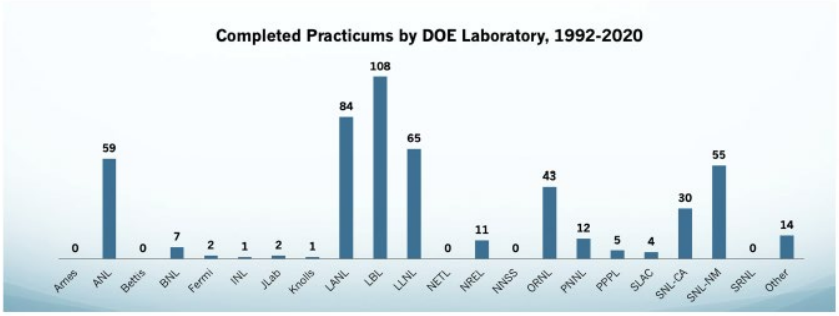


Figure F3: Distribution of completed practicums by DOE Laboratory, for the time period of 1992-2020 [4].

The 2022 DOE CSGF Longitudinal Study included a survey as well as interviews with CSGF alumni from 1991 (the program inception) through 2021 [2]. The response rate among alumni was 50 percent, with 213 alumni out of 422 completing the survey. In the interviews, the alumni were asked about the extent

to which the CSGF program, based on their perceptions, has been successful in meeting the DOE's workforce needs in computational science and engineering. The study indicated that "Most of the alumni indicated that the program had been effective in this respect." Below is one of the quotes from an alumni expressed on this topic:

> *I work with other CSGF fellows at [DOE National Laboratory name], and I think it's pretty universal that we feel the fellowship prepared us very well for what the Department of Energy workforce needs are. I think a lot of us have said, 'The fellowship really helped us to hit the ground running when we got to the labs.'*

Figure 4-36 from the 2022 DOE CSGF Longitudinal Study identified the professional interest of current fellows, for which 88% noted the DOE Laboratory as a professional setting in which they planned to apply. Next was industry at 65%, followed by academia at 61%. In terms of the current employment data for 487 alumni, only 15% (or 71) are at the DOE Labs [3]. The remote location of many DOE Labs was identified as a deterrent for a professional job [2].

Findings

Based upon the data from the longitudinal study and other references, we have the following findings:

- The DOE CSGF program does an excellent job of providing essential program components (e.g., multidisciplinary program of study, practicum, annual meeting) to prepare the Fellows for a successful career in computational science.
- The DOE CSFG is an important program to meet the national computational scientist workforce needs, including that of DOE Labs.
- The current acceptance rate of applicants is less than 10%. Moreover, computational scientist workforce needs are expected to grow, with the use of AI in many engineering and science disciplines.

Recommendations

- Given the value of the DOE CSGF program in meeting the computational scientist workforce needs, it is important to maintain the program per Recommendation (R1) of the Executive Summary: *The subcommittee recommends that the DOE ASCR foster growth of CSGF……*
    - Growth of the DOE CSGF program will better meet workforce needs.
    - The different DOE laboratories should take advantage of lessons learned in engaging the CSGF Fellows in practicum opportunities.

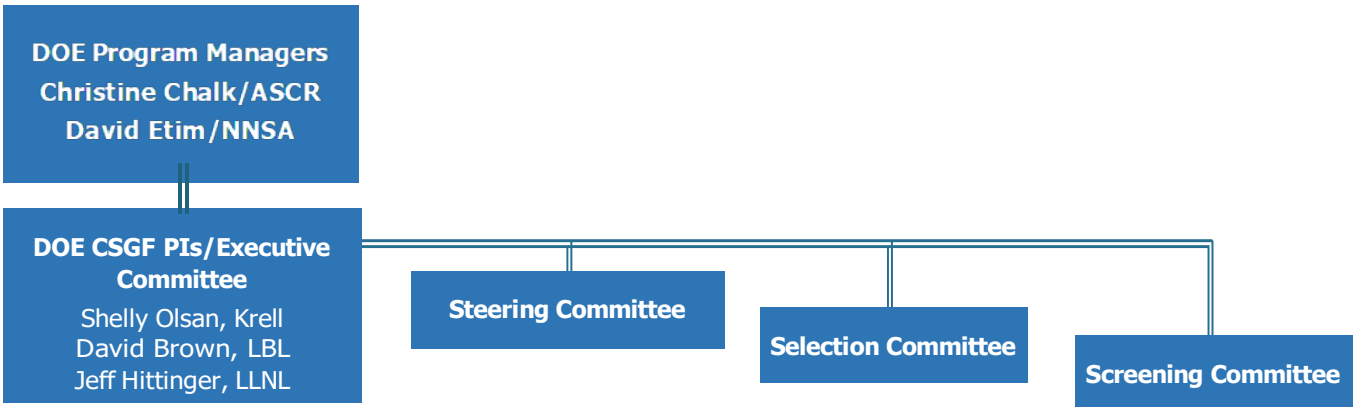
[1] DOE Computational Science Graduate Fellowship website, accessed 11/2024. https://www.krellinst.org/csgf/about-doe-csgf

[2] 2022 DOE CSGF Longitudinal Study, accessed 11/2024. https://www.krellinst.org/doecsgf/docs/2022_DOE_CSGF_Longitudinal_Study-Web.pdf

[3] Materials from the 2024 DOE CSGF Briefing Slides for ASCAC CSGF Subcommittee.
Brown, D., Hack, J., and R. Voight, "The Early Years and Evolution of the DOE Computational Science Graduate Fellowship Program," *IEEE Computing in Science & Engineering Magazine*, Vol. 23, No. 6, 2021.

Effective Governance (Q6)

In this section we examine the CSGF Governance Model. Specific aspects considered are its contributions to the quality of the outcomes for the fellows, its overall decision-making effectiveness, its inclusiveness and transparency to stakeholders, and its adaptability. The description of the program governance and current membership was provided by the CSGF PIs in documents, presentations, and discussions with the subcommittee.



The Executive Committee is the decision-making body for the program. It is composed of the PI and the two technical co-PIs. The Executive Committee selects members of the Steering Committee and sets the agenda for meetings of the Steering Committee, which occur at least twice per year at the discretion of the Executive Committee. The two technical co-PIs are also members of the Steering Committee along with seven additional experts. The membership and expertise of the Steering Committee includes DOE lab stakeholders as well as industry and academia.

The Governance model has been consistent for the past seven years after a modest adjustment following the death of the original PI in 2017. Steering Committee terms are three years renewable at the discretion of the Executive Committee. As a practical matter, membership in the Steering Committee, and indeed Selection and Screening Committees, tends to be enduring with a strong bias for new members drawn from those who have previous deep involvement in the program. Among the nine Steering Committee members, five members come from four DOE laboratories (three from NNSA laboratories, 2 from Office of Science laboratories). Geographically, the Steering Committee member institutions are predominantly based in the West Coast (six of nine).

The DOE CSGF Governance model is well established. As noted in documentation submitted to the committee, the Steering Committee has clearly defined functions which encompass both strategic and operational aspects of the program. The Steering Committee is responsible for defining criteria for fellow selection. In addition, the Steering Committee members are directly involved in fellow onboarding and transition. Moreover, Steering Committee individuals participate in the fellow screening and selection process, reinforcing excellence and consistency in the process. The Screening Committee has three tracks: Science/Engineering, Mathematics/Computer Science, and overall fit evaluation. The composition of the Screening Committee is large with significant institutional and disciplinary breadth, including more than sixty experts in total across DOE laboratories, other federal agencies, academia, and industry. The screening process is rigorous, well-documented, and transparent

to applicants and stakeholders. Similarly, the Selection Committee (18 experts across two tracks) and process is impressive in its makeup and effectiveness. The Mathematics/Computer Science track has been integrated flawlessly. The growth in applicants and attendant reviews has been managed with unrelenting quality in fellow selection and unwavering attention to ensuring successful fellows.

As noted above, the oversight, transparency, and effectiveness of CSGF operations is excellent, providing an extremely effective introductory experience for prospective fellows. The mission of CSGF is well defined and visible on the CSGF website [1].

Pursuit of the four mission objectives is evident in the achievements of the program operations documented in the longitudinal study [2]. For example, the expanded reach to a larger and broader population of potential fellows is demonstrated by the growing number and geographic breadth of applicants as well as the increasing number of academic institutions. Excellence in governance of the program operations is strongly evident in the caliber of fellows, including not only screening, selection, and onboarding but also the fostering of an enduring computational science community. Importantly, both annual and longitudinal program trends are well documented, measuring impact and quality well beyond the term of the fellowship.

Two areas of improvement in governance were considered by the subcommittee in developing its recommendation (R4) defined in the Executive Summary:

> The subcommittee recommends that the CSGF program, with guidance from ASCR and with greater input and participation from DOE labs, develop a five-to-ten-year strategic plan that addresses all four program objectives, including specific and measurable outcomes. The program should revise its governance bodies accordingly to prioritize greater stakeholder engagement while maintaining/improving efficiency and effectiveness of operations.

The first improvement concerns stakeholder engagement. While the fellows are strongly engaged as strategic stakeholders, the strategic engagement of DOE laboratories is not as robust. The CSGF governance model is well-defined but not externally visible. More importantly, it is not evident how strategic engagement of DOE laboratories occurs beyond those few represented on the CSGF Steering Committee. Solid laboratory operational engagement occurs during the screening and selection process, continuing through the practicum process. Measures of satisfaction and impact of the program across the set of DOE laboratories would reinforce/guide program direction.

The second related improvement shows in the lack of visible strategic goals (e.g. on a five-year horizon). Given the highly successful past 30 years, setting ambitious, measurable 5-to-10-year goals aligned with ASCR strategies and with input from a broader set of stakeholders (e.g. DOE laboratories, DOE/non-DOE programs) seems to be a natural next step. The mechanism(s) for developing and communicating such strategic goals need not be organizational but could, for example, leverage existing program planning processes within DOE and its laboratories.

[1] DOE Computational Science Graduate Fellowship website, https://www.krellinst.org/csgf/about-doe-csgf.

[2] 2022 DOE CSGF Longitudinal Study, accessed 11/2024. https://www.krellinst.org/csgf/study

Evolving to Meet Student Needs (Q7)

Over the last decade, the CSGF program has demonstrated remarkable success in developing computational science leaders. This conclusion by the subcommittee is based on comprehensive longitudinal data analysis of the past decade. Our assessment is detailed in the previous Effectiveness and Impact for Students (Q1) section. Alumni achievements demonstrate the program's effectiveness in preparing fellows for impactful careers: 90% of alumni are employed in computational science and engineering fields across industry (37%), academia (27%), and DOE laboratories/government positions (20%). The program's research impact is evidenced by alumni scholarly productivity, with CV analysis documenting 4,925 journal articles published predominantly in highly influential journals. The program has maintained outstanding academic outcomes, with 89% of alumni completing their PhDs and another 10% in progress toward completion. Beyond academic and research excellence, the program has fostered a vibrant professional community. Alumni report high satisfaction with their practicum experiences and research collaborations at DOE laboratories. The strength of the CSGF network is demonstrated by 62% of alumni maintaining active connections with other recipients. These outcomes have been achieved through an efficient administrative structure that channels the vast majority of program funds directly to fellowship support, making the CSGF program a model for maximizing impact while minimizing overhead costs.

Executive Summary recommendation (R5) notes six specific areas for program evolution:

> As CSGF looks to the future we recommend that the program consider evolving student needs in the following areas: emerging technologies integration, professional skills development, academic institutional reach, building community, fellowship support services, and program evaluation.

Each area builds on existing program strengths while introducing approaches to leverage DOE laboratory resources more effectively, particularly in emerging technologies, professional development, and community building. Special emphasis is placed on creating clear pathways for fellows to access laboratory expertise, workshops, and mentorship opportunities, ensuring they benefit fully from the extensive resources available across the DOE laboratory complex. These improvements would maintain the program's high standards for scientific excellence while expanding support for fellows' comprehensive development as computational scientists.

Emerging technologies integration: The CSGF program could enhance its focus on emerging technologies by increasing its leverage of the extensive resources and expertise available at DOE laboratories. The program's emphasis on computational science excellence would be strengthened through structured engagement with artificial intelligence, machine learning, and quantum information sciences, areas where DOE laboratories maintain significant research programs, industry partnerships, and specialized facilities. Through coordination with DOE laboratories, fellows would gain access to established workshop series that cover both fundamental principles and advanced applications in these fields. The laboratories' existing training programs, which regularly update their content to reflect new developments in quantum methods, neural networks, and high-performance computing, would provide fellows with practical, hands-on experience using cutting-edge technologies. These learning opportunities would be carefully integrated with the program's core computational science curriculum,

ensuring that fellows develop both foundational knowledge and expertise with emerging tools. The laboratories' proven track record in delivering effective technical training, combined with their regular workshop offerings in advanced computing technologies, would create a natural pathway for fellows to engage with these essential areas while maintaining the program's high standards for scientific excellence.

Professional development: The CSGF program could strengthen its fellows' professional development through a comprehensive approach to communication skills training and career advancement opportunities. Through structured research presentations, participation in the annual essay contest, and targeted workshops in grant writing, poster design, and science policy engagement, fellows would develop essential skills in conveying complex computational concepts to audiences with a wide variety of technical breadths and depths. The program could leverage the DOE laboratories' established professional development workshops and training programs, which have successfully prepared generations of scientists in these crucial skills. The program could provide hands-on learning experiences where fellows receive constructive feedback from experienced DOE laboratory mentors, while encouraging them to share their research insights through contributions to the program's magazine and participation in thoughtfully designed outreach activities. DOE laboratories' existing communication and policy workshops could be made available to fellows, providing them access to proven training approaches and experienced mentors who understand both technical depth and effective communication. Regular engagement in major conferences and industry events would create valuable networking opportunities, helping fellows explore various career paths and build lasting professional connections within the broader computational science community. These professional development activities would be carefully integrated into the fellows' existing research commitments, ensuring they complement rather than compete with their primary scientific work.

Community building: The CSGF program could strengthen its community and professional network through a comprehensive engagement strategy that leverages both digital offerings and in-person connections. The program could facilitate informal mentorship opportunities that connect current fellows with experienced alumni through online platforms like Slack and LinkedIn, facilitating knowledge exchange and professional development. A matching system could pair fellows with mentors during program reviews, considering research interests, and career goals to create meaningful, lasting relationships. The DOE laboratories' established mentorship programs and professional networks could allow a more formal mechanism initiated through the Lab points of contact (POCs), providing fellows access to experienced scientists and proven mentoring approaches. The program would enhance laboratory engagement through expanded practicum opportunities, particularly in emerging areas, while offering flexible participation options to accommodate fellows' schedules and locations. This approach would combine traditional strengths in computational science with new connection opportunities, allowing fellows to benefit from both established expertise and emerging research directions at DOE laboratories. Regular assessment of these initiatives will ensure they effectively serve fellows' needs while maintaining the program's high standards for scientific excellence.

Academic institutional reach: The CSGF program can increase its student impact by building strong partnerships with additional schools throughout the U.S. (e.g. EPSCoR institutions) and developing clear pathways for students into computational science across the country. In prepared slides, the program provided strong evidence that they are reaching an expanded set of institutions both at the

undergraduate and graduate level., The program is not yet fully benefitting from the breadth of the U.S. academic community. The program can accelerate and further strengthen connections with EPSCoR schools through targeted efforts, working closely with faculty to identify promising students with computational interests. By establishing formal partnerships with EPSCoR institutions, the program can create structured opportunities for students to learn about computational science careers and to develop relevant skills before applying. The program can also provide support resources for fellows from EPSCoR institutions, ensuring they have the tools and mentoring needed to succeed in computational science research. This support would include access to computational training resources, regular check-ins with program mentors, and connections to other fellows with similar backgrounds. The DOE laboratories could play an important role in this effort through their established outreach programs and partnerships with EPSCoR institutions and by providing computational science workshops tailored for students. Through careful monitoring of these initiatives and regular feedback from participants, the program would contribute to building the nation's capacity in computational science while maintaining the program's high standards for technical excellence.

Student support resources: The CSGF program could enhance its existing support for fellows' overall well-being through coordination and communication of support resources available to fellows. The program, through institutional liaisons and laboratory POCs, would ensure fellows can easily locate information on support services at their host institutions and DOE laboratories (e.g. health insurance, work-life balance programs). To accommodate varying personal circumstances, the program can provide flexibility in completion timelines and workload arrangements, allowing fellows to maintain research progress while addressing health or other needs. The program could coordinate with DOE Laboratory POCs to connect fellows with existing wellness programs and support services during their practicum experiences. Clear guidelines can be established for fellows who desire to change research groups or advisors, with defined steps to enlist support from program staff to help maintain research continuity during transitions. A dedicated information resource can provide fellows with straightforward information about what support services are available from the program and contact information for academic and practicum support questions. This comprehensive support framework would help fellows balance their research commitments with personal well-being, encouraging long-term career commitment to the field. Regular check-ins with program staff would help identify and address any challenges early, creating an environment where fellows can thrive both personally and professionally. Given the high value student surveys place on the program's existing support services, the intent is to leverage institutional and lab contacts to ensure fellows have a comprehensive view of available services.

Program evaluation: The CSGF program measures and improves its effectiveness through a clear evaluation approach that tracks key indicators of success while gathering detailed feedback from participants. The program can leverage and adapt this proven approach to focus on data and evaluation, which ensure informed decisions about program priorities and improvements while maintaining the high standards that make CSGF a leader in computational science training.