DOE CSGF

The U.S. Department of Energy Computational Science Graduate Fellowship

1991-2011

Recipient Outcomes and Programmatic Impacts

Submitted by the Krell Institute

The U.S. Department of Energy
Computational Science Graduate Fellowship
1991-2011

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Table of Contents

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Executive Summary

A strategic priority of the United States (U.S.) Department of Energy (DOE) involves contributing to national progress through scientific and technological discovery and innovation. To that end, DOE has instituted special initiatives aimed at developing and maintaining a pool of talented, highly qualified, and motivated scientists and engineers for service in government laboratories and in academia and industry. Especially notable among these initiatives is the DOE Computational Science Graduate Fellowship (DOE CSGF).

Established in 1991 and administered since 1997 by the Krell Institute, DOE CSGF is especially on target since computational science has been described as essential to advances throughout society and deemed one of the most important technical fields of the 21st century. Computational science — or, more inclusively, computational science and engineering (CSE) — is a multidisciplinary field involving "the innovative and essential use of high-performance computation, and/or the development of high-performance computational technologies, to advance knowledge or capabilities in a scientific or engineering discipline."[1] The DOE CSGF includes a required program of study, research practicum, and annual conference, among other features. It was launched specifically to provide education and training for the development of CSE skills and techniques in promising doctoral students within and across science, technology, engineering, and mathematics (STEM) fields.

This report presents a study of DOE CSGF recipient outcomes and programmatic impacts, focusing on the 1991-2011 Fellow cohorts. The

[1] From the DOE CSGF application.

three-pronged research strategy is based on data collection via 1) a general survey of former and current Fellows and 2) reviews of Fellow curricula vitae, and supplemented by 3) in-depth interviews.

Survey

The survey instrument was designed to capture a broad range of information about the Fellowship recipients, with particular reference to their DOE CSGF experiences, educational effects, and employment issues. Reflecting an overall 70% response rate (236 respondents), the survey respondents constituted a generally representative sample across DOE CSGF cohorts and doctoral fields.

Fellowship Experience: Positive Fellowship experiences and high levels of satisfaction were found to be the rule. Virtually all Fellows found the Fellowship useful and indicated high levels of satisfaction with the Fellowship program in general, and found it useful in a variety of ways beyond the financial support provided, particularly as regards intellectual stimulation and exchange, interaction with other researchers, and professional growth. In particular, 96% reported the usefulness of the annual conference, especially in regard to intellectual stimulation and exchange, followed by cross-disciplinary interaction, and networking opportunities. Along the same lines, the generation of a DOE CSGF community of scholars and the building of collaborative networks — notably, often across generational and disciplinary lines — were found to be critical outcomes of the Fellowship experience. Moreover, enduring professional relationships and personal friendships were not unusual and the idea of "giving something back" was prominent among alumni Fellows. Mentoring also, in terms of both giving and receiving, was especially valued, as was the practicum experience, which offered Fellows work in national laboratories. Interestingly, virtually no actual substantively negative statements were offered about the Fellowship experience in any of the survey responses or related comments, even though opportunities to provide them were presented as a matter of course.

Education Effects and Attainment: Over 98% of the respondents indicated a direct impact of the DOE CSGF on their research, not only in the methods they used to pursue it in light of their exposure and

training in computational techniques and expanded computing capabilities, but also their scientific research focus. Comments by survey respondents consistently pointed to the DOE CSGF as critical to their academic success and development. While referencing the program of study and practicum requirements, they also repeatedly emphasized the importance of the conference and access to the DOE CSGF network and other researchers in their development as computational scientists and engineers and to broadening their scientific horizons.

Professional Direction and Employment: The majority of respondents (68.6%) indicated professional association membership, which is typically employed to signal professional participation and involvement. Furthermore, in reference to the multidisciplinary nature of CSE, 30% reported membership in professional associations outside of their doctoral disciplinary fields. Also, when involved in professional associations, Fellows tended to be engaged in special roles (e.g., organizational officer, board member, committee chair, etc.). Of Fellows with completed doctorates, 28% were in government, 38% in education, and 34% in the private sector. Moreover, 89% indicated CSE-related employment. In fact, 71 Fellows reported DOE employment, of which 44, or 62%, indicated employment in the very same DOE laboratory in which they had carried out their DOE CSGF research practicum, arguably showing a direct Fellowship effect. Also, 97% of the Fellows indicated that, besides their own personal motivation, the quality of their education and training was the most important factor affecting career advancement in their positions, followed by mentoring cited by 71%.

Curricula Vitae Analysis

Curricula vitae (CVs) obtained from 170 Fellows also were used as a research device, providing information on awards, careers, productivity, collaborations, and service, particularly in regard to scientific community development and participation.

Awards and Honors: For excellence in their work and for outstanding service, 145 Fellows reported receiving some 387 special recognition awards conferred from a variety of sources, including private

foundations and government agencies. Also, 40 Fellows reported winning 92 relevant grants and contracts, again from a variety of private and public sources (including DOE). Also striking were the 113 Fellows indicating the award of other types of fellowships; counts of fellowships came to 186 across the CVs. In addition, 8 individuals reported patents, both awarded (8) and pending (6).

Public Intellectual and Service Activity: Some 32 Fellows indicated contributions to the media and public sphere through, among other things, writing reviews, providing special topic interviews, acting as experts and advisors, and developing and contributing to special informational programs and websites. Also, Fellows performed a wide range of secondary and optional unpaid service activity roles, such as volunteer instructors and tutors, Service as academic and professional mentors was specifically indicated by 54 Fellows, and referee and reviewer service was mentioned by 63 Fellows. In general, assistance to various groups in numerous principal and supportive positions were notable among alumni Fellows.

Leadership Positions: With some reporting multiple positions, 17 Fellows reported having held leadership positions across various sectors. These ranged from team leaders, directors, and managers to organizational presidents and executives, and were, as might be expected, especially apparent among Fellows from the earlier DOE CSGF cohorts — including leadership positions in DOE and other government agencies.

Collaborations: Research and publication collaborations reflect relational structures through which scientists and engineers are linked to wider professional communities. Examining the CVs for indicators of possible DOE CSGF-influenced co-authorships and research projects after Fellowship completion, 31 Fellows were found to have collaborative relationships with practicum laboratory members and 41 reported collaboration with other Fellows, indicating a growing community and network among DOE CSGF participants.

Publications: Number of publications often is used as an indicator of productivity and of participation and position in professional communities. Although the high and low counts of publications for

individuals were quite variable, the median number of publications for 142 Fellows since DOE CSGF completion has ranged from 18 to 33. Also, peer-reviewed publications in top-ranked journals are treated as a major indicator of scientific productivity and of contributions to research and knowledge creation. In that regard, at least 96 alumni Fellows have published in the top-ranked journals for STEM in general and for their specific fields.

Interviews

In-depth semi-structured interviews were conducted with 20 Fellows, selected across cohorts and fields, to complement the survey and CV findings for a more detailed understanding of the DOE CSGF recipient outcomes and programmatic impacts. The interviews were transcribed and analyzed as text using both deductive and inductive approaches. These involved association and concordance analyses of primary themes and keywords determined based on conceptual relevance and textual mapping: *fellowship, computational science, laboratory, career, collaboration, network, conference, mentoring,* and *service*. Word associations, showing keywords and their significant one-to-one relationships with other words within the textual corpus, and concordances, involving the examination of actual occurrence contexts and specificity relative to explicit word usage, constituted the initial interpretive components for analyzing the interviews.

All of the interviewed Fellows spoke highly about their Fellowship experience, and almost all made similar mention of their practicum. Usually, they mentioned it by name and described the nature of their work and gave tribute to their advisor. Almost all — 19 of the 20 — also described what they considered other valuable features of the program, most commonly the course requirements and the funding. Furthermore, these comments also were used to draw points of comparison and to distinguish DOE CSGF — in very positive terms — from other fellowships. Most interviewees suggested that they are leaders in their respective fields and are working on projects that they described as innovative with the potential to impact the future in positive ways. Moreover, they cited DOE CSGF as a critical influence in this regard. Also, explicitly pointing to their scholarship as such, references to, for example, recognition and awards for groundbreaking

research, patents, and the establishment of cross-disciplinary projects were made by the Fellows. Interestingly, especially given concerns about recipient roles and Fellowship impacts, discussions of scholarship were framed largely in terms of practical applicability. Note that most discussions of service focused on dedication to mentoring and to recruitment of new talent to the DOE CSGF program. Also, while not typically discussed directly as such, community building was evidenced in references to recruitment, mentoring, collaboration, and networking activities with other Fellows.

Conclusion

The DOE CSGF has played a critical role in educating and training scientists for DOE and other government agencies, academia, and industry. Indeed, the DOE CSGF represents a major investment in STEM in service to the country. Managed by the Krell Institute, the DOE CSGF program has consistently garnered high praise by recipients. The superior benefits and opportunities that DOE CSGF offers have made it one of the most sought-after and effective fellowships available in terms of support, education, and training in related fields and otherwise. It also has operated to maximize contributions to knowledge creation and community building and to the broader DOE mission.

Taking all of the components of this study together, it is clear that DOE CSGF recipients can be characterized as playing important roles as computational scientists and engineers and as community builders and leaders. DOE CSGF recipients are arguably high achievers by nature and their successful outcomes and engagement of the Fellowship were to be expected, especially given the rigorous and competitive selection process and the continual evaluation and commitment required by the program. By linking individual elements with institutional and external realities and needs, the DOE CSGF program itself has operated to identify and involve individuals who might serve not only the field and their own professional goals, but also the national agenda and society more generally, both directly and indirectly. Accordingly, Fellows act as partners in providing support and assistance for fulfilling needs delineated in the DOE CSGF objectives and the DOE mission. This point was supported across the research platforms and strategies, and was reflected in both overall and individual Fellow profiles.

Introduction

The mission of the United States Department of Energy (DOE) involves contributing to national progress through scientific and technological discovery and innovation. As a strategic priority of the DOE, accomplishing this mandate requires a workforce with a range of expertise in science, technology, engineering, and mathematics (STEM). It refers, in particular, to expertise that includes high quality computational skills to meet the increasingly complex challenges and demands of today's innovation-driven knowledge society. Accordingly, DOE looks to develop the kinds of talent necessary to excel in this environment.

More specifically, recruiting, developing, and sustaining a STEM workforce with topnotch computational skills is a necessary goal for staffing and fulfilling the crucial roles of the DOE national laboratories, and for meeting increasing demands for such skills in other government agencies and in the private sector. To that end, DOE has developed special initiatives aimed at keeping "a steady stream of bright and motivated new talent flowing into the DOE workforce" to ensure to the scientific and technological success of the country.[1] Especially notable among these initiatives is the **DOE Computational Science Graduate Fellowship** (DOE CSGF).

Established in 1991, the DOE CSGF program is in keeping with government recommendations for creating and maintaining a qualified and competitive STEM workforce as a national planning activity that is sustained, ongoing, and coordinated for continuing progress (cf. Graham et al. 2004; Brody 2005; NAS 2005, 2010). In particular, DOE CSGF supports doctoral students in the pursuit of "novel scientific or engineering discoveries" using high performance computing (HPC) resources.[2] It advocates taking advantage of innovations in emerging computing technologies to advance knowledge and practical applications. More to the point, the necessity of HPC for scientific discovery and innovation is increasingly apparent in the face of the complex problems and needs of society today. DOE CSGF is especially

[1] http://jobs.energy.gov/entry-level-students
[2] From the CSGF application.

on target since computational science has been described as essential to advances throughout society and deemed one of the most important technical fields of the 21st century.[3]

Against this backdrop, this report presents a study of DOE CSGF recipient outcomes and programmatic impacts, focusing on the 1991-2011 Fellow cohorts. It addresses a variety of both general and specific questions to explore related issues and determine the effects of the Fellowship relative to the general DOE mission. For example, how successful has DOE CSGF been in contributing to the STEM workforce? What has been its impact, if any, on advancing computational science as a field? In practical terms, to what extent has the DOE CSGF helped to increase the pool of qualified computational scientists and engineers from which DOE can draw to staff it national laboratories and from which other government agencies, academia, and industry can benefit? In response to such questions, the Krell Institute which, on behalf of DOE, has administered the DOE CSGF program since 1997, called for the conduct of this independent study as part of its overall assessment and management efforts.

In this introductory section, a brief conceptual discussion of computational science itself is next provided as a foundation for understanding the role and broader implications of DOE CSGF relative to the purpose of this report and to the STEM workforce in general. An overview of the Fellowship program, with particular reference to its special features, is then offered as background, followed by a general description of the study assessment approach and research strategy. Various aspects of the DOE CSGF program and Fellowship recipients are identified and delineated as indicators for the later parts of the report in which the study findings are detailed. These include sections on the Fellowship experience itself, on Fellowship recipient education, on Fellowship recipient careers and accomplishments, and on Fellowship recipient demographic backgrounds. The concluding section consists of final comments and assessments.

[3] See Kiernan (2005); President's Information Technology Advisory Committee (PITAC) reports [http://www.nitrd.gov/pitac/reports]

The Field of Computational Science and Engineering

Computational science — or, more inclusively, computational science and engineering (CSE) — is an evolving field that entails "the innovative and essential use of high-performance computation, and/or the development of high-performance computational technologies, to advance knowledge or capabilities in a scientific or engineering discipline."[4] More to the point, CSE is a multidisciplinary area with connections across STEM fields. It focuses on the development of problem-solving methodologies and robust tools for the solution of scientific and engineering problems, and, arguably, will play an important — if not dominating — role for the future of the scientific discovery process and engineering design (SIAM 2006). CSE encompasses the systematic development and application of computing systems and computational solution techniques for modeling, simulation, and analysis of scientific and engineering phenomena.[5]

To model complex systems, scientists and engineers develop computer programs and application software necessitating massive amounts of calculations, the execution of which are possible only via distributed computing platforms or on high performance or super computers. As a multidisciplinary field, CSE can be engaged both to enable HPC applications to important domain-specific problems and to confront "grand-challenge" science and engineering applications. Accordingly, it can lead to insights that might not be possible if relying on more traditional theory or experimentation alone.

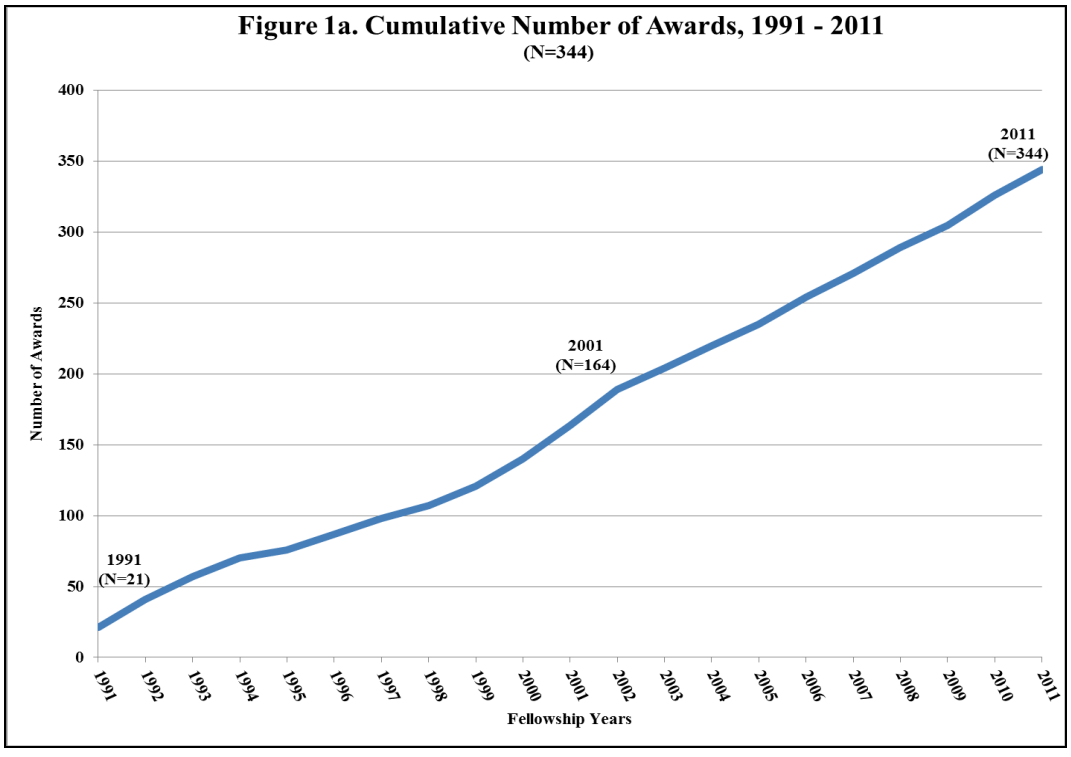
The role and purpose of CSE in this environment is one of next generation computing, supporting large-scale operations that cover "applications in science/engineering, applied mathematics, numerical analysis, and computer science. Computer models and computer simulations have become an important part of the research repertoire, supplementing (and in some cases replacing) experimentation. Going from application area to computational results requires domain expertise, mathematical modeling, numerical analysis, algorithm development, software implementation, program execution, analysis,

[4] From the DOE CSGF application.
[5] Cf. http://catalog.gmu.edu/preview_program.php?catoid=17&poid=6884&returnto=1307.

validation, and visualization of results. CSE involves all of this."[6] More to the point, the DOE CSGF program was launched specifically to develop related skills and techniques in individuals within and across STEM fields.

The Fellowship Program

The DOE CSGF is defined within the mission of DOE's Advanced Scientific Computing Research program to "discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the Department of Energy."[7] Sponsored by DOE's Office of Science and National Nuclear Security Administration, the Fellowship is aimed at training scientists and engineers to meet U.S. workforce needs in CSE, and at building a larger CSE-based community across STEM fields. Between 1991 and 2011, the DOE CSGF was awarded to 344 Fellows, as shown in Figure 1a.



[6] SIAM (2001).
[7] http://science.energy.gov/ascr/about

The DOE CSGF is highly competitive, with qualified applicants far exceeding the number of available awards. (For example, in 2011, 628 applicants vied for the 17 Fellowship awards that were afforded in the program.) Eligibility extended to senior undergraduate and first and second year graduate students pursuing STEM doctoral degrees.[8] The DOE CSGF is open to U.S. citizens or permanent resident aliens who are planning full-time, uninterrupted study toward a Ph.D. at an accredited U.S. university. Selected STEM doctoral students were provided support for up to four years of study, with funding provided through the DOE Office of Science and National Nuclear Security Administration. The Fellowship screening committees have been constituted by experts in related fields from academia, DOE and other government agencies, and industry, and by former DOE CSGF recipients who serve to "give back" to the community.

The DOE CSGF is a unique and innovative fellowship program with four principal objectives, as reported on its website[9]:

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 make national DOE laboratories available for practical work experiences for fellows ensuring cross-disciplinary experience in highly productive work teams.
3) To strengthen collaborative ties between the national academic community and DOE laboratories so that the multidisciplinary nature of the fellowship builds the national community of scientists.
4) 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 computational science.

Various fellowship features were put into place in pursuit of these objectives, most notably

[8] Beginning in 2013, only senior undergraduate and first year graduate students are eligible to apply.
[9] http://www.krellinst.org/csgf/about-doe-csgf

- a detailed interdisciplinary program of study providing a broad and encompassing education as a foundation for further CSE training and practice;
- a research practicum which provides experience working with experts in DOE laboratories on applicable CSE projects;
- an annual conference which offers knowledge exchange, career development, and networking opportunities; and
- various other Fellow interaction and community building activities.

Particularly unique to the DOE CSGF are the *program of study* and the *research practicum* as central requirements. While DOE CSGF recipients are pursuing doctoral degrees in STEM fields, the individualized programs of study that are required for the Fellowship typically must be completed prior to the third year of the Fellowship. The curricular requirements are meant to instruct STEM students in the use of advanced computational tools; the programs of study are developed to enhance the applicable knowledge and computational skills that the students will obtain relative to and beyond that typically required in their disciplines alone. CSE itself, as previously discussed, is approached as an integrated interdisciplinary field and the Fellowship's curricular requirements are aimed at providing a comprehensive "toolkit" of mathematical, scientific, and computational skills and techniques that can be brought to bear on relevant issues in government, academic, and industrial sectors today and in the future. Such skills are especially critical given projected needs for exascale computing capabilities for the scientific and technological modeling, simulation, and analysis required in today's innovation-driven world and — in keeping with DOE's overall mission — to meet the environmental, economic, and security challenges of the future.

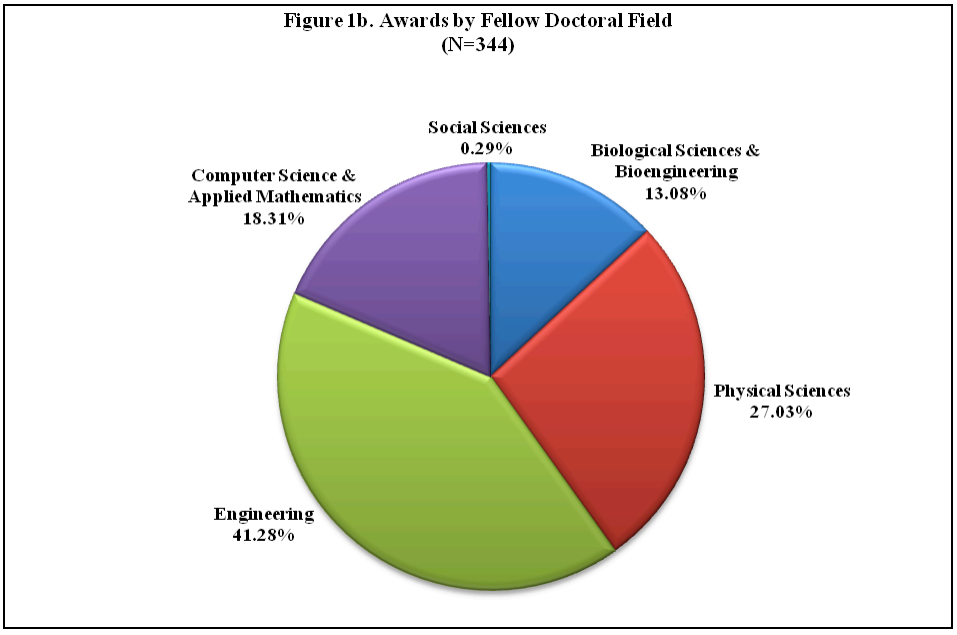
The Fellowship was designed specifically to expand understanding and develop skills to bring computational breadth and techniques to bear across STEM fields (and beyond). In particular, the DOE CSGF's program of study and practicum requirements ensure that recipients obtain the background and necessary skills to excel as computational scientists and to actively participate in related applications. Thus, for example, along with the required coursework in the program of study,

the practicum allows Fellows to gain relevant experience in various aspects of CSE.

Note that, while Fellows have represented diverse STEM disciplines,[10] reflecting the interdisciplinary nature of the CSE community, their doctoral fields have been broadly categorized for administrative purposes under four main headings:

- Biological Sciences and Bioengineering
- Computer Science and Applied Mathematics
- Physical Sciences
- Engineering

In addition, Social Sciences have been considered when relevant. As is apparent in Figure 1b, the majority of Fellows over time have been in Engineering. However, the twelve-week research practicum is deliberately set outside of the Fellow's formal field of study. This is a particularly defining feature and benefit of the Fellowship, operating to bridge gaps and cross boundaries to expand related knowledge and build a broader scientific community.



[10] Including, chemistry, computer science, earth sciences, engineering, environmental sciences, life sciences, mathematics, physics, space sciences, and statistics. [http://www.krellinst.org/csgf/about-doe-csgf/fields-study]

DOE CSGF programmatic aims include encouraging HPC use through related education and training, offering HPC-focused practica, and facilitating access to DOE systems. The DOE CSGF practicum opens doors to students and offers the DOE national laboratories as unique opportunities for education and training for the future. Moreover, the available practicum sites, as delineated in Table 1, are represented in the national laboratory system, offering "access to leading scientists; world-class scientific user facilities and instrumentation; and large-scale, multidisciplinary research programs unavailable in universities or industry."[11]

Table 1. Practicum Sites

Practicum Laboratory/Research Site	Short Form/Abbreviation
Ames Laboratory	Ames
Argonne National Laboratory	ANL
Bettis Atomic Power Laboratory	Bettis
Brookhaven National Laboratory	BNL
Fermi National Laboratory	Fermi
Idaho National Laboratory	INL
Knolls Atomic Power Laboratory	Knolls
Lawrence Berkeley National Laboratory	LBNL
Lawrence Livermore National Laboratory	LLNL
Los Alamos National Laboratory	LANL
National Renewable Energy Laboratory	NREL
Oak Ridge National Laboratory	ORNL
Pacific Northwest National Laboratory	PNNL
Princeton Plasma Physics Laboratory	PPPL
Sandia National Laboratories — CA	SNL—CA
Sandia National Laboratories — NM	SNL—NM
Savannah River National Laboratory	SRNL
SLAC National Accelerator Laboratory	SLAC
Supercomputer Computations Research Institute	SCRI

Again, the practicum turns on HPC — the heart of CSE — and access to DOE computing facilities provides the means by which related training and applications are pursued. Through the practicum requirement, Fellows have access to DOE laboratories where they build collaborative relationships through their participation on team projects and by pursuing cross-disciplinary research. Students are provided firsthand experience and opportunities to learn and better understand related techniques and tools and to pursue high-end operational skills and large-scale science. Based on cutting-edge computational projects and

[11] http://science.energy.gov/wdts

HPC access, it is the basis on which much scientific progress and technological advancement relies.

Another critical feature of the program is the *annual conference*, offering professional workshops, presentation opportunities, information on DOE resources, and exposure to and networking with CSE experts and scholars. Held in the Washington, DC, area each summer, the annual conference is a venue in which past and current Fellows, DOE staff, faculty, and other members of the CSE community come together to share ideas, support one another, and learn about DOE research and employment opportunities. Future employment and career development prospects are presented for planning and placement and the conferences also serve as important networking venues, as do DOE CSGF-supported regional events. Collaborative and mentoring relationships are often established through formal and informal means at the conferences, with past Fellows and other CSE experts interacting with each other and providing guidance to new Fellows.

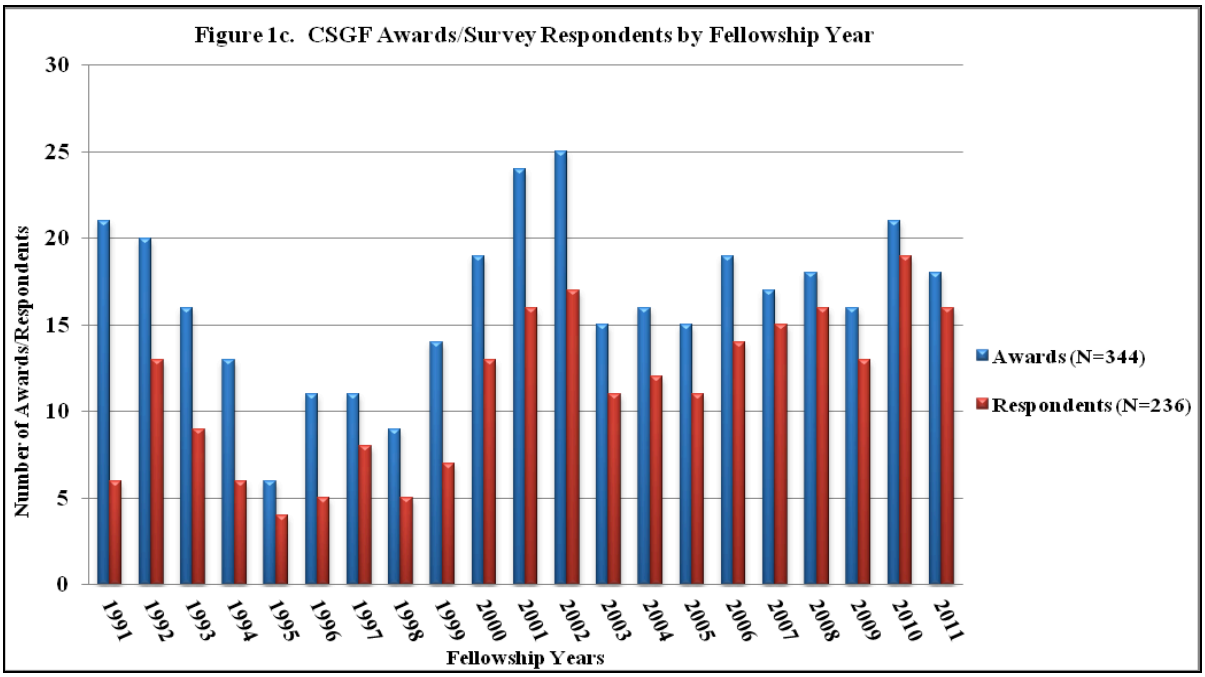
The DOE CSGF program demands excellence of its Fellows, making progress and accomplishment a requirement for continued participation. Offering up to four years of support, the award must be renewed each year, dependent on assessments of Fellow active involvement and progress. While continual feedback and evaluation are key elements of the program, they also provide information for the Fellows and serve as resources for further refinement of the program in keeping with its overall purpose.

Research Strategy

A multifaceted research strategy was engaged for this study. A mixed-method and multi-level approach in which both quantitative and qualitative data were collected and analyzed was used to provide an overall picture of DOE CSGF recipient outcomes and program effects. Primary data collection was conducted via 1) a general survey of former and current Fellows and 2) reviews of Fellow curricula vitae and resumés, and supplemented by 3) in-depth interviews. The research design was developed to capture and explore selected outcomes *vis à vis* the 1991-2011 Fellowship recipients, including, for example,

disciplinary preparation, doctoral degree completion, and employment sector. The data were used, in part, to build a set of measures to characterize fellowship participation in relation to program and degree completion and career trajectories. In addition, more focused examinations of selected DOE CSGF recipients and their contributions were conducted in consideration of program objectives emphasizing leadership and community building.[12]

The general survey was administered online, with 236 respondents (an overall 70% response rate) across Fellow cohorts, as can be seen in Figure 1c relative to the total 1991-2011 DOE CSGF awards.

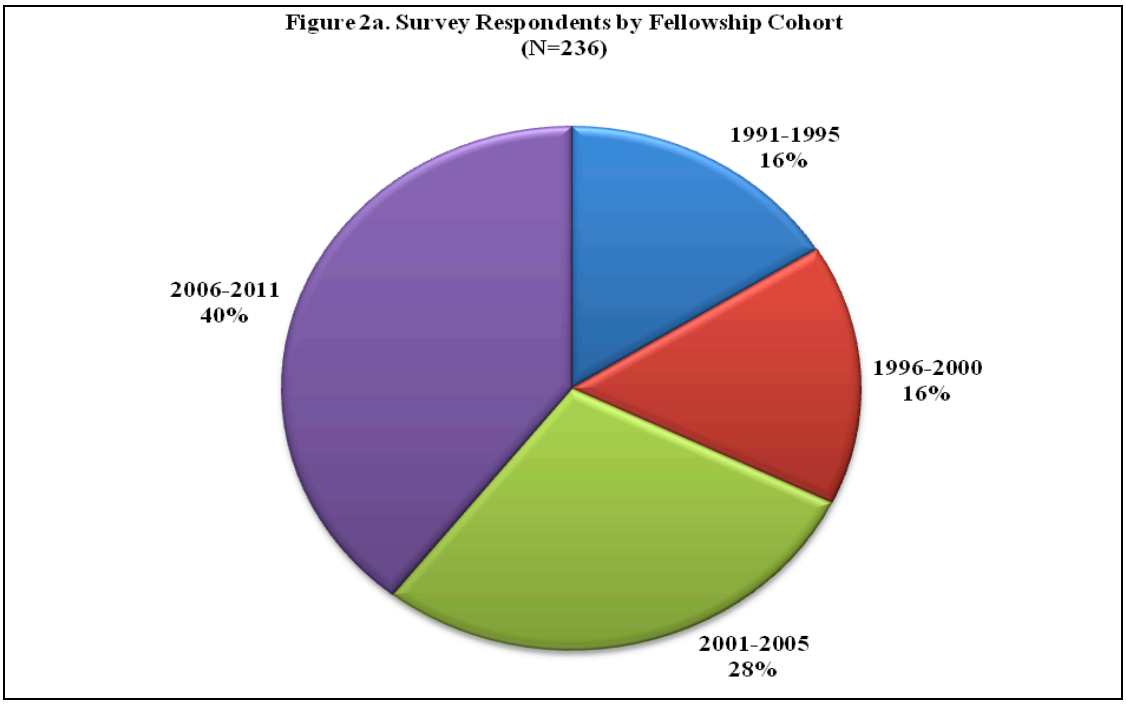


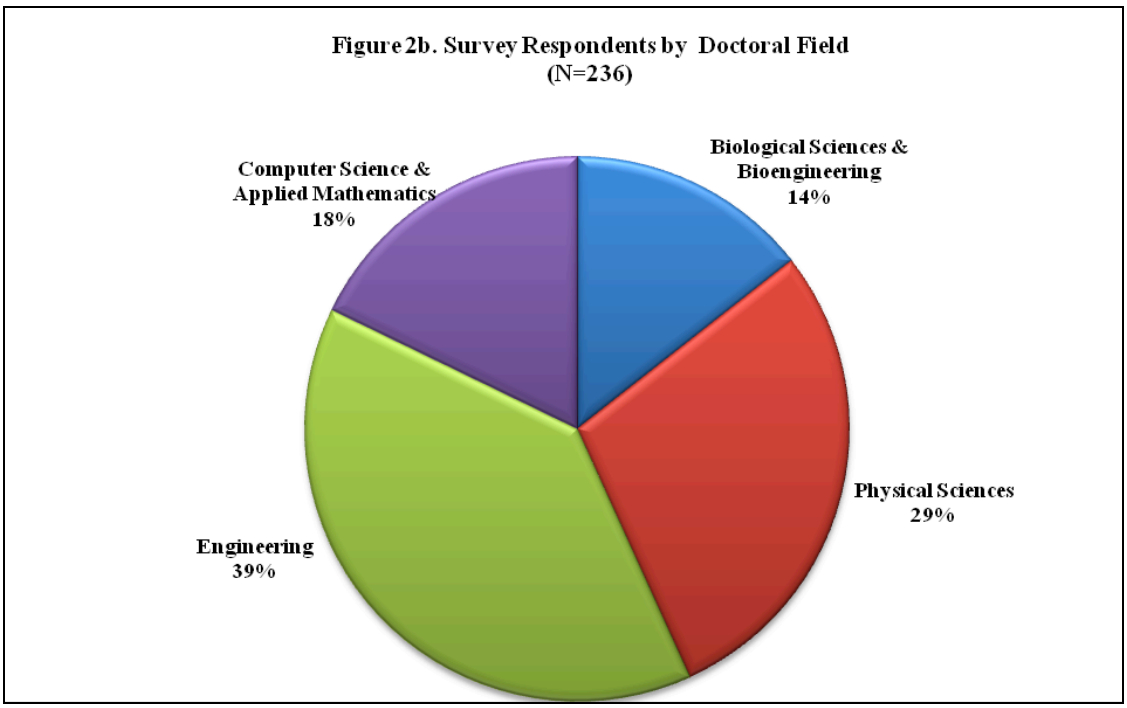
The survey was meant to gather data on Fellows relative to their CSE experience and degree and career outcomes and to provide general insight into DOE CSGF impact and effectiveness. Moreover, it offered Fellows an opportunity to evaluate Fellowship benefits and outcomes and for self-assessment. Accordingly, the survey instrument was designed to capture a broad range of information about the Fellowship recipients,[13] including

[12] See Appendix A for additional methodological notes.
[13] See Appendix B for a copy of the survey instrument.

- educational backgrounds, trajectories, and outcomes,
- demographic profiles,
- doctorate disciplinary fields,
- doctorate completion rates,
- career paths, expectations, and outcomes,
- occupation and employment characteristics, and
- Fellowship experiences.

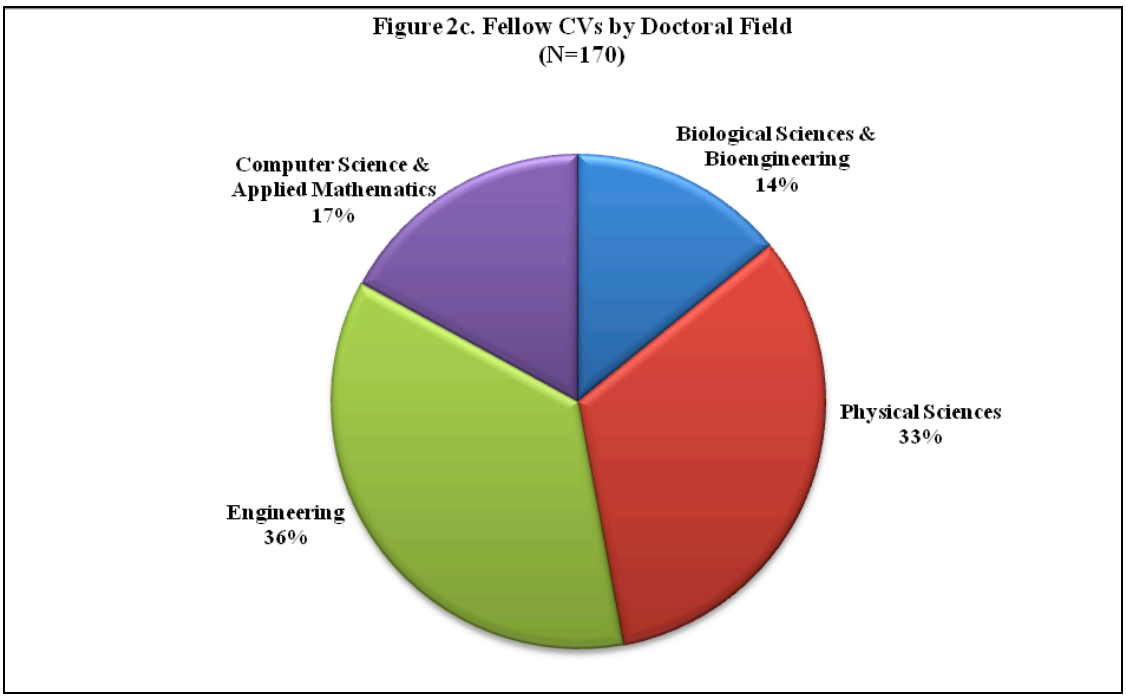
As can be seen in Figures 2a and 2b, survey respondents constituted a generally representative sample across Fellowship cohorts and doctoral fields.

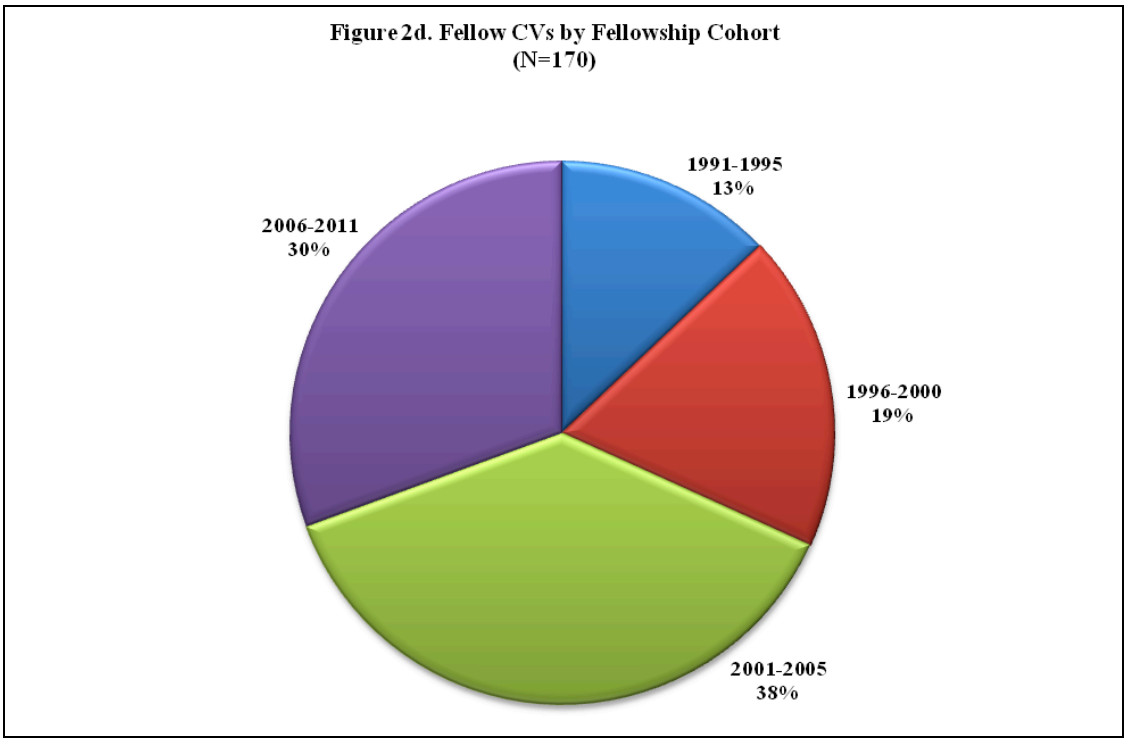




Also, curricula vitae (CVs) and resumés were collected and used as an additional data source. For purposes of this study, the CV is more than simply a list of credentials; it is a historical document that evolves over time, capturing changes in interests, jobs, and collaborations. Accordingly, it can be a rich source of longitudinal data, containing information on the timing, sequence, and duration of jobs, work products (e.g., articles, patents, papers, etc.), collaboration patterns, and scholarly lineage. Therefore, using the CV as a data source and research device, each Fellow was treated as "a walking set of knowledge, skills, technical know-how and, just as important, a set of sustained network communications" (Dietz et al. 2000, p. 420),[14] and a related coding protocol was developed to capture a wide range of relevant information.[15] CVs for 170 Fellows, as represented in Figures 2c and 2d, were collected.

[14] Much of the pioneering work using CVs as data sources and on CV analysis in this regard was sponsored by DOE's Office of Science (Dietz et al. 2000).
[15] See Appendix C.





Furthermore, in-depth, semi-structured interviews were conducted with 20 alumni Fellows, randomly selected across cohorts and fields

from an initial pool of 217, to augment and extend the other data collection activities. The interviews provided a means, on the one hand, to gather insights and learn more about the nuances that can be lost in surveys and, on the other hand, to gain a sense of the extent to which the Fellows view the findings as applicable or not and why, given their specific situations.

While common themes and elements were expected, discussions with Fellows were used to gain a clearer picture of how other conditions and structural features might affect Fellow outcomes and the overall efficacy of the program. Accordingly, an interview protocol was developed with an eye to further contextualizing and providing a more detailed understanding of the Fellowship experience and outcomes. To a certain extent, the survey and CV findings were used to inform the interview strategy, pointing toward certain dimensions as more critical than others. However, the interviews, which were conducted via telephone, were semi-structured, with an emphasis on drawing out the Fellows' own opinions, rather than forcing their ideas into narrow categories. Each interview was transcribed and then thematically coded and analyzed using individual review and discursive analytic techniques.[16]

In general, the surveys, CVs, and interviews provided data on the backgrounds, experiences, program participation, career trajectories, and contributions of individual fellows, along with other relevant data on their educational attainment, interdisciplinary research, laboratory projects and performance, and professional achievements and recognition. Also, where appropriate and possible, these data were supplemented with information from the Krell Institute database, with particular reference to disciplinary features, curricular background, and laboratory experience, and to information about program administration. Together, these data collection efforts provided means for developing broader integrated profiles on Fellow participation, productivity, and contributions and general Fellowship effects, as reported in the following sections.[17]

[16] Based on hand coding and also employing text mining and qualitative data analysis software (T-Lab and Nvivo). See Appendix D for thematic coding categories.
[17] See Appendix A for additional methodological notes.

Who Will Do (Computational) Science?: The Big Picture

"Innovation" and "discovery" are the watchwords of the day, and the relevance of science, technology, engineering, and mathematics (STEM) is front and center in addressing environmental, economic, and security issues not only in the United States (U.S.), but in countries around the world. However, just as when Pearson and Fechter (1994) posed the critical question in their landmark volume — *Who will Do Science? Educating the Next Generation* — it is perhaps even more pressing today and is particularly apt in reference to Computational Science and Engineering (CSE) as a growing field. While controversies and debates abound surrounding STEM workforce capacities in general, the need for computational scientists and engineers with knowledge and skills focused on high performance computing (HPC) goes without question. Moreover, as also noted by Pearson and Fechter in reference to STEM in general, the need for support during the lengthy training needed to pursue STEM careers must be addressed in response to calls for expanding the CSE workforce. It is in this vein that the U.S. Department of Energy's Computational Science Graduate Fellowship (DOE CSGF) is here assessed relative to recipient outcomes and effects on CSE capacity building efforts.

To derive an overall picture of this situation and the relevant structural issues and dynamics attending it, this part of the study relies primarily on findings obtained from responses to a survey of 1991-2011 DOE CSGF recipients. It looks especially to explore the Fellowship experience, education, employment, and demographic background of the Fellows in terms of the DOE CSGF objectives, as discussed in the previous section, aimed at CSE-related education and training, careers, and community building and participation.

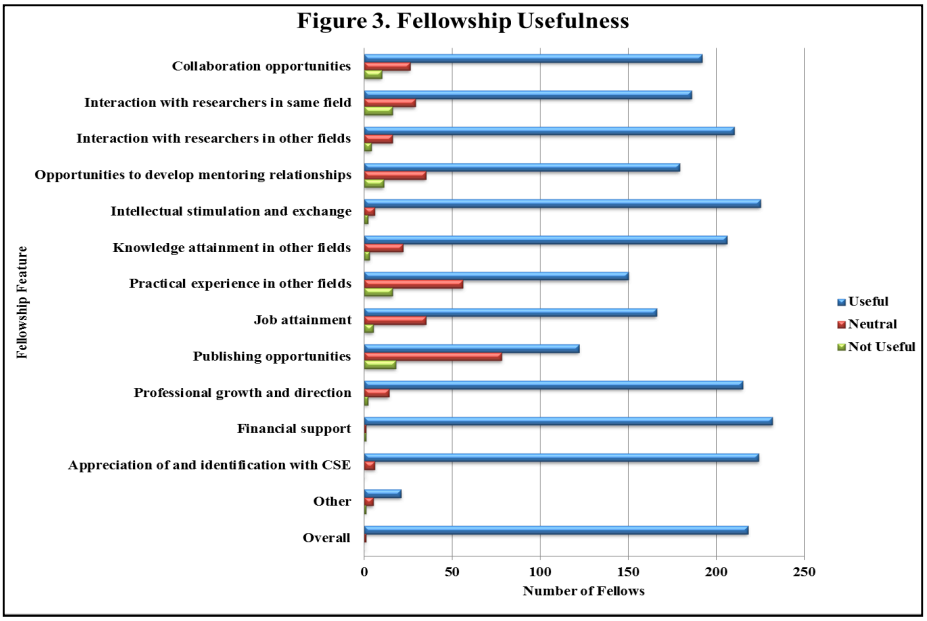
The Fellowship Experience

Employing a more comprehensive approach to the notion of support, a goal of the DOE CSGF has been to add value to the Fellowship experience of award recipients through programmatic elements aimed specifically at driving excellence in CSE and providing opportunities and resources for advancement. In addition to basic financial assistance, the DOE CSGF has included elements by which skills, knowledge,

opportunities, and other resources for navigating and succeeding in CSE and related employment could be imparted to Fellowship recipients. Accordingly, as previously discussed, the DOE CSGF program has included a variety of other features — such as the research practicum and the annual conference — to encourage and support individual efforts in completing their STEM doctoral education and attaining training and success in CSE and related careers.

As an initial point of reference, note that all — 100% — of survey respondents, across cohorts and disciplines, indicated satisfaction with the Fellowship and their experience. The multidimensional approach engaged in the CSGF program reflects an integrative model representing a well-defined plan developed to deliver a broad base of services and resources to Fellows for disciplinary and further professional socialization and development.[18] As shown in Figure 3, the vast majority of Fellows also reported not only the overall usefulness of the DOE CSGF program in their academic pursuits, they reported that it had been useful in a variety of ways beyond the financial support provided, especially as regards intellectual stimulation and exchange, interaction with other researchers, and professional growth. Indeed, virtually all respondents — 99.5% — were affirmative in indicating the program's usefulness.

Figure 3. Fellowship Usefulness



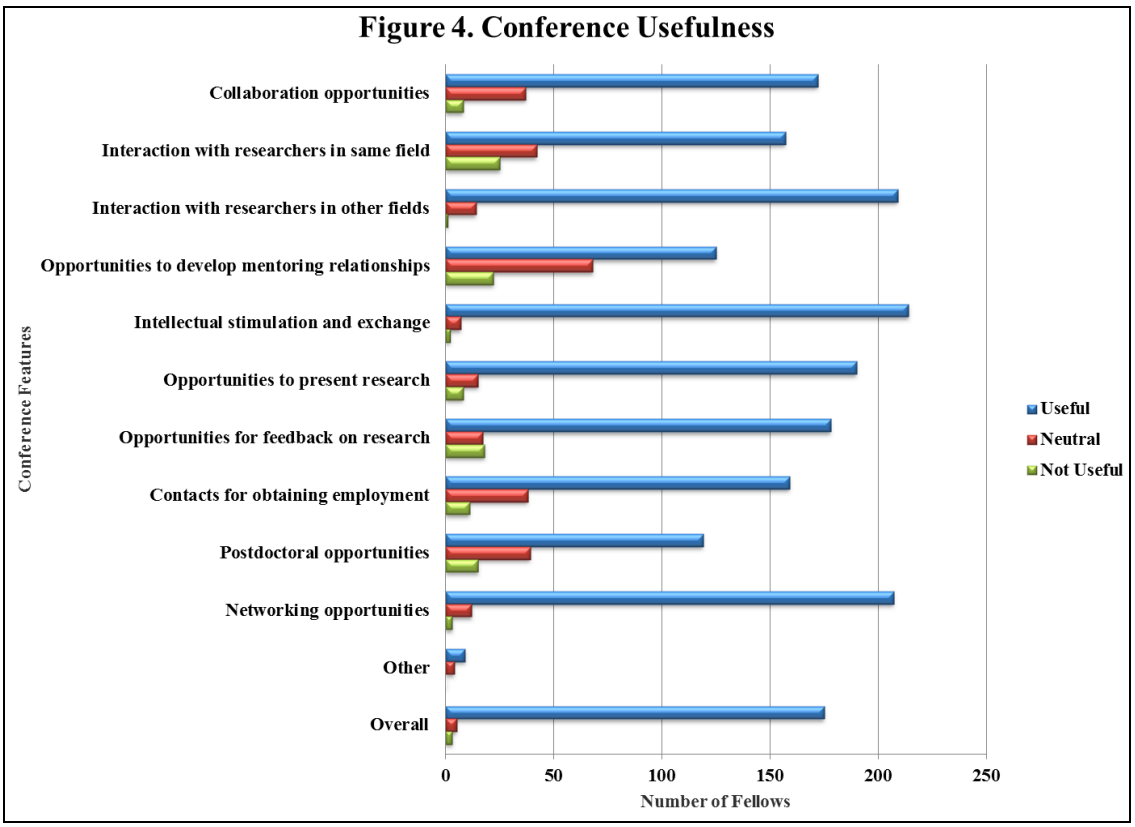
[18] Cf. Bowman and Stage (2002).

A central activity and resource provided by the Fellowship program has been the annual conference. As a principal DOE CSGF component, the conference serves various purposes for the individual Fellows, including providing opportunities for networking, mentoring, career guidance, and intellectual exchange. According to survey responses and individual comments, the conference has been a vital means for facilitating networking and fostering the mutual exchange of experiences and ideas. It especially provides opportunities for professional socialization, a process that involves learning and adapting to professional cultures, internalizing professional identities, and demonstrating professional membership.[19] Moreover, the conference has operated to encourage communication and information sharing among Fellows that extend far beyond the formal programmatic activities. Thus, the usefulness of the conference relative to the specific purposes for which it was established was a key issue explored in the survey.

As can be seen in Figure 4, an overwhelming number of Fellows found the conference useful along several dimensions. In particular, intellectual stimulation and exchange, followed by cross-disciplinary interaction, and networking opportunities were rated highly across all Fellows. Over 96% of 223 respondents found the conference especially useful in terms of intellectual stimulation. Of 224 respondents, 93% cited interaction with researchers in other fields as particularly useful, as did 93% of 222 respondents in regard to networking opportunities afforded by the conference. In fact, all of the specified aims of the conference received positive marks in general relative to their usefulness, with 96% of Fellows reporting positive ratings of its overall usefulness.[20]

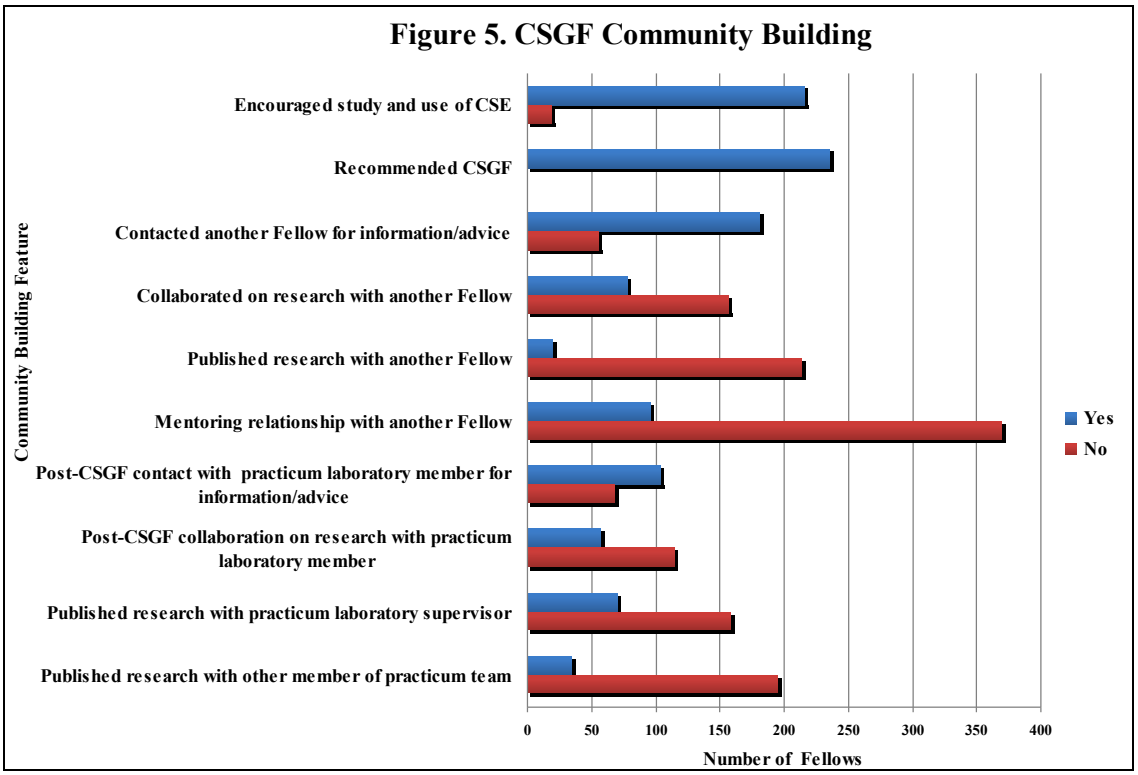
[19] Cf. Dryburgh (1999).

[20] The numbers reported here do not include counts for those respondents indicating "does not apply" for the specified Conference features.

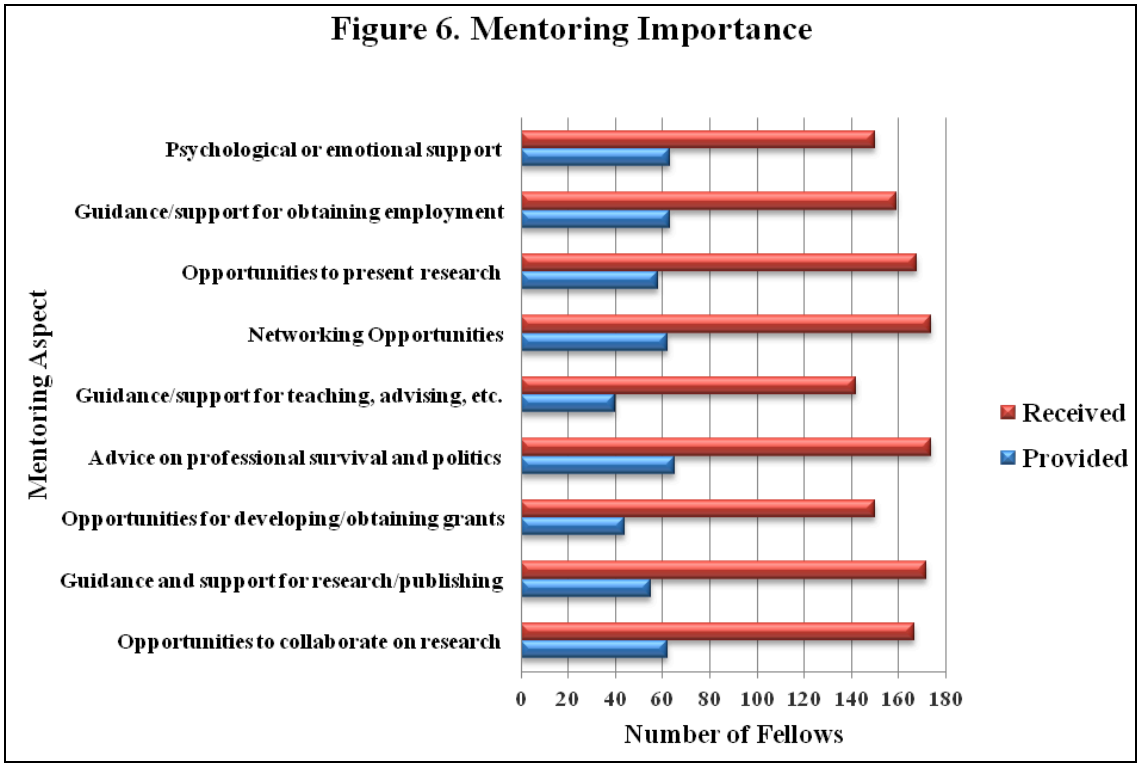


Also, as indicated in Figure 5, the generation of a DOE CSGF community of scholars and the building of collaborative networks — notably, often across generational and disciplinary lines — have been critical outcomes of the Fellowship experience. Many former Fellows have displayed a deep commitment to the DOE CSGF program and mission, continuing to actively contribute to the program through the provision of formal and informal mentoring to other Fellows, screening committee service, networking and collaboration, representation at professional meetings, employment opportunities, and a variety of other activities. Moreover, former Fellows play active roles in outreach, recruiting, engaging, and training the next generation of computational scientists; the Fellows themselves often act as emissaries for the DOE CSGF program, both formally and informally recruiting applicants and serving as information resources and liaisons. As mentioned above, past Fellows increasingly attend the annual conference, serving as speakers, workshop leaders, advisors, and general information resources. Again, not only does the conference serve as an important venue in which they provide insights, guidance, and opportunities for new Fellows, it also is

a networking site through which they establish links among themselves and others working in similar areas. Such CSE community building is critical for creating, advancing, and diffusing knowledge for progress and innovation. Indeed, enduring professional relationships and personal friendships have marked the Fellowship program.



Mentoring too is integral to academic success and, accordingly, the Fellowship program encompasses a number of effective mentoring strategies, not the least of which are resources such as provided by individual advisory meetings and mentor identification. The key importance of mentoring has been indicated by Fellows in their assessment of Conference usefulness and, more, of DOE CSGF usefulness in general. Past Fellows typically serve as mentors and advisors to new DOE CSGF recipients. Also, both formal and informal network development and community building have been central features in support of mentoring relationships through the DOE CSGF program and participation. As is apparent in Figure 6, Fellows recognize the importance of mentoring relationships in general and reported that they value both providing and receiving mentoring.



Furthermore, the required program of study and practicum experiences were designed to expose Fellows to powerful research techniques and approaches and to expand their skill sets to include "areas of heterogeneous high performance computing and software performance optimization."[21] The practicum, in particular, is a 12-week requirement, usually completed during the summer months, which Fellows have undertaken at various sites, as shown in Table 2.

Table 2. Fellow Practicum Sites, 1991-2011

Practicum Sites	Fellows
Argonne National Laboratory	31
Brookhaven National Laboratory	4
Lawrence Berkeley National Laboratory	61
Lawrence Livermore National Laboratory	43
Los Alamos National Laboratory	56
Oak Ridge National Laboratory	30
Pacific Northwest National Laboratory	11

[21] Quotation drawn from a 2011 practicum supervisor comments.

Princeton Plasma Physics Laboratory	3
Sandia National Laboratories – CA	19
Sandia National Laboratories – NM	46
SLAC National Accelerator Laboratory	1
Supercomputer Computations Research Institute	1
Other	13

While the initial practicum must be completed within the first two years of the Fellowship, students often are encouraged to continue or to return for an additional experience — not only for developing their own computational acumen, but also for the important contributions that they make to the laboratory projects and teams. Practicum supervisors consistently use words such as "impressive," "excellent," "amazing," "exemplary," "outstanding," and "remarkable" to describe the Fellows and their progress and contributions.[22] Such descriptions were even more noteworthy given that the practicum projects fall outside of the work the Fellows were following within their own fields. Additionally, the other side of this coin is that the Fellows learned how computational techniques could enhance their other research efforts. Given the "exemplary performance" and "impressive contributions" of the Fellows, it is not unusual for practicum supervisors to suggest that the students extend or pursue additional practica or, even more, to return in postdoctoral positions upon completion of their degrees.

Interestingly, virtually no actual substantively negative statements were offered about the Fellowship experience in any of the survey responses or related comments, even though opportunities to provide them were presented as a matter of course. Although a suggestion was made about holding the conference at other sites (e.g., at the different DOE laboratories), most survey respondents found the Washington, DC, site a benefit and attraction, increasing the likelihood of attendance by former Fellows and other participants. Indeed, as indicated on the DOE CSGF website, meeting in Washington, DC, facilitates conference attendance and participation by DOE leadership and, also, interested Congressional members and staff.

High levels of satisfaction and positive Fellowship experiences were found to be the rule. The Krell Institute has taken an anticipatory

[22] Drawn from practicum supervisor reports.

approach in administering the DOE CSGF, working diligently to determine and address the needs of the Fellows and of the DOE as its first priority. Its strategy has included, among other things, constant inquiry and interaction with the Fellows and with laboratory practicum and project directors; a highly engaged steering committee; self-examination and critique; independent analysis and evaluation; and, importantly, regular attention to and specification of DOE workforce needs and mission.

Education Effects and Attainment

The DOE CSGF has been charged with creating a community of scholars and analysts who can use the latest in HPC resources to blaze new trails in scientific discovery and innovation. To that end, the DOE CSGF program has been dedicated to developing talented individuals with the knowledge and skills to engage the large-scale computer platforms necessary to pursue this mission. It has supported the education and training of students from across the STEM fields — as previously noted and shown here in Table 3 — to stimulate and enable the effective use of advanced computer technologies in inquiry-based CSE to address related challenges and demands in the country's public and private spheres.[23]

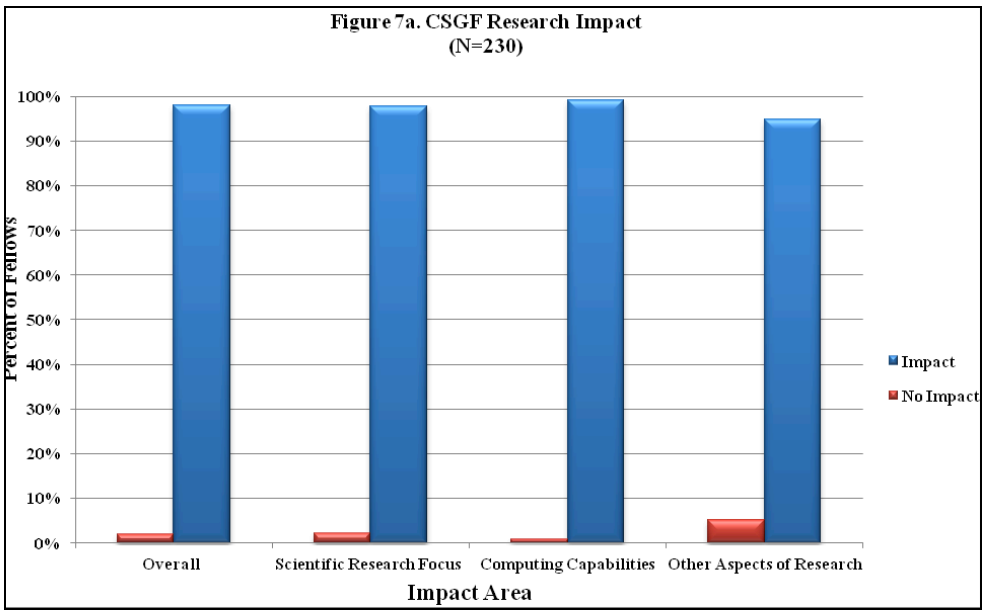
Table 3. Fellow Doctoral Fields, 1991-2011

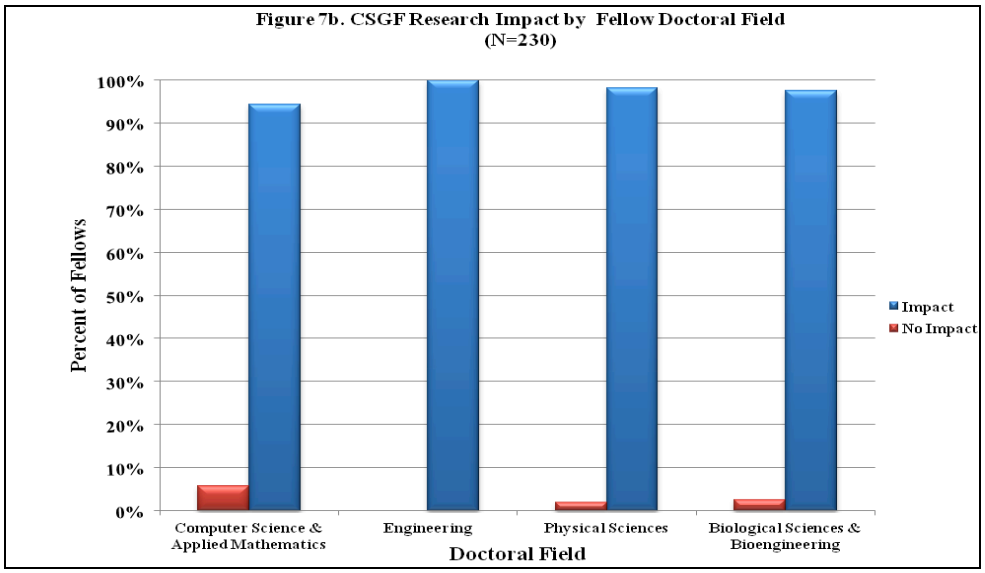
Doctoral Field	%Fellows (N=344)
Physical Sciences	27.03%
Biological Sciences & Bioengineering	13.08%
Computer Science & Applied Mathematics	18.31%
Engineering	41.28%
Social Sciences	0.29%

Moreover, the DOE CSGF has had a definite impact on the research pursued by the students, in substance and approach, stretching them and leading them to explore questions and issues beyond their typical disciplinary areas. Indeed, over 98% of the survey respondents, across disciplinary fields, indicated that the Fellowship directly impacted

[23] Note that, while the earlier DOE CSGF cohorts were dominated by engineering, later groups have reflected greater breadth across STEM fields.

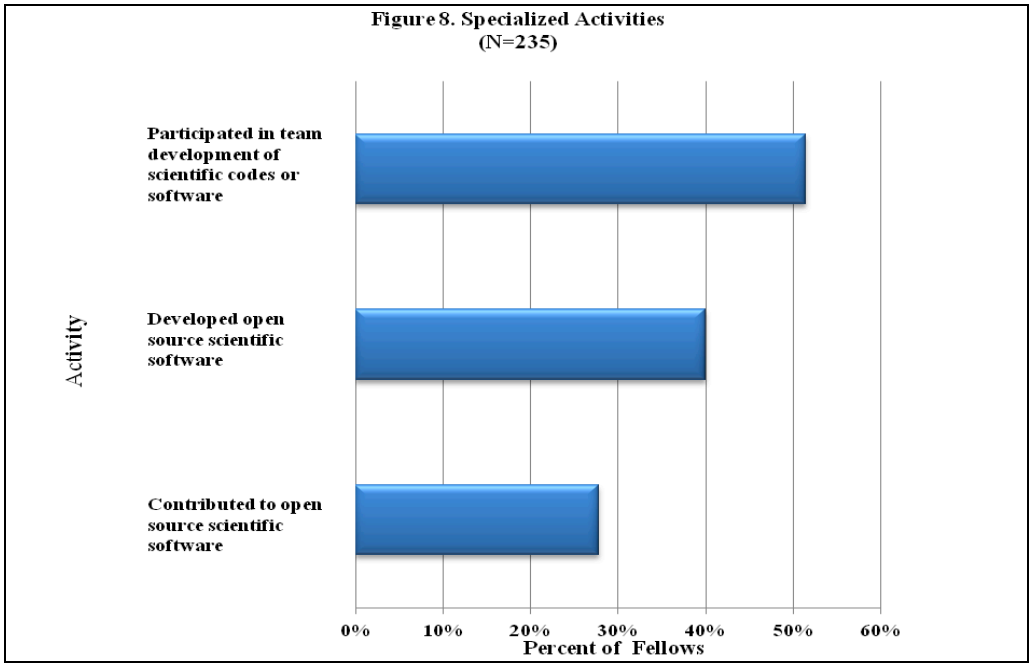
various aspects of their research. This effect referred not only to the methods they used to pursue their research in light of their exposure and training in computational techniques and expanded computing capabilities, but also to their scientific research foci, as shown in Figures 7a and 7b.





Along the same lines, Fellows were able to pursue various specialized activities due specifically to their CSE education and training. As indicated in Figure 8, such activities included, for example, participating in the team development of scientific codes or software and, also,

developing open source scientific software. Also, as might be expected, related activities increased over time within and across fields.



As can be seen below in Figure 9, Fellows in the 1991-2011 cohorts have pursued their doctorates at some of the leading universities in the country, as also represented in the survey respondent pool, of which 227 had completed their degrees, as shown in Figure 10. Comments by survey respondents consistently pointed to the DOE CSGF as critical to their academic success and to their development as scholars and researchers, and for providing them with the tools for their future careers. While referencing the importance of the program of study and practicum requirements, they also repeatedly emphasized the importance of the conference and access to the DOE CSGF network and other researchers in their development as CSE scientists and engineers and to broadening their scientific horizons.

Figure 9. Fellow Doctoral Institutions

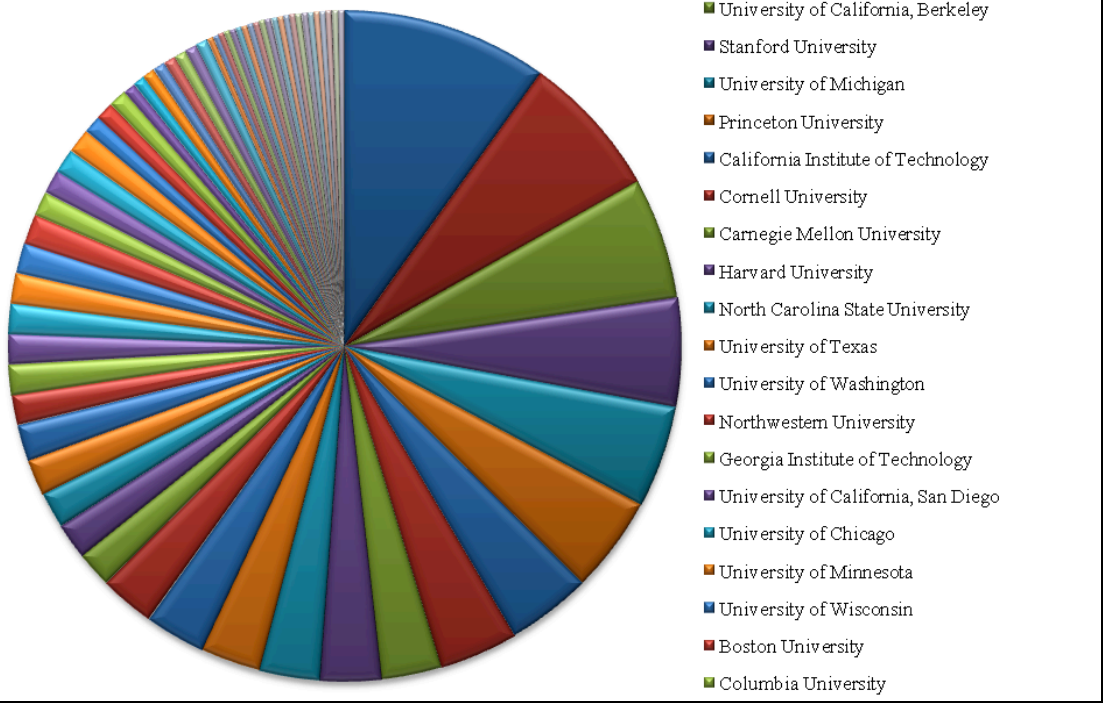
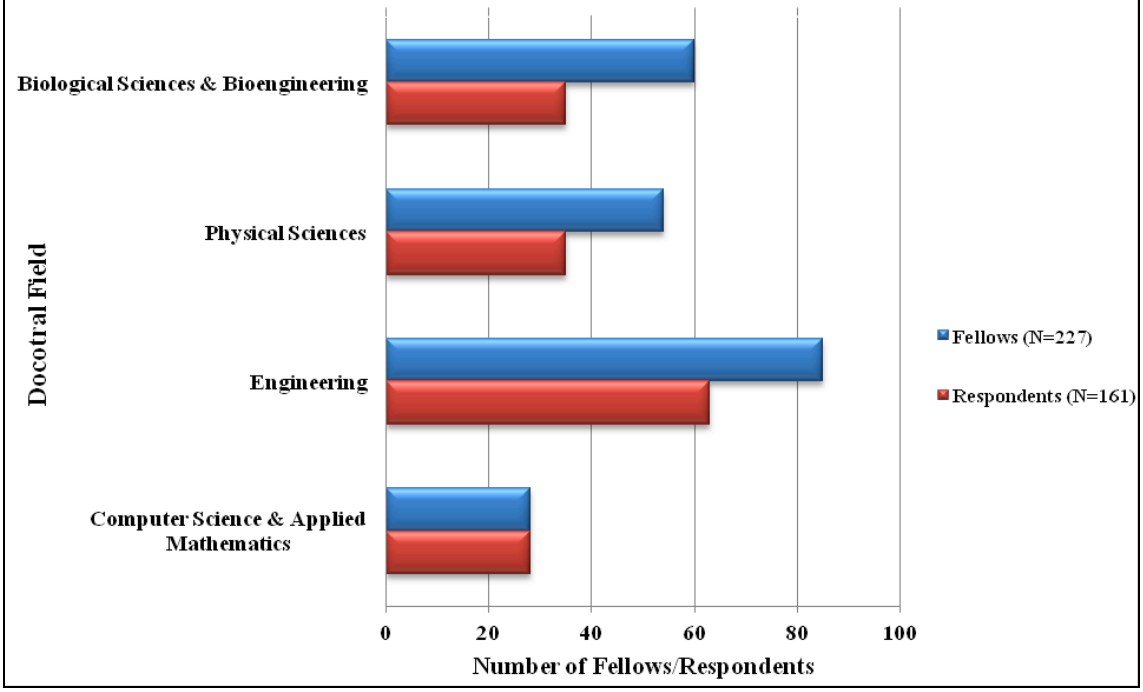


Figure 10. Fellows/Survey Respondents with Completed Doctorates by Field

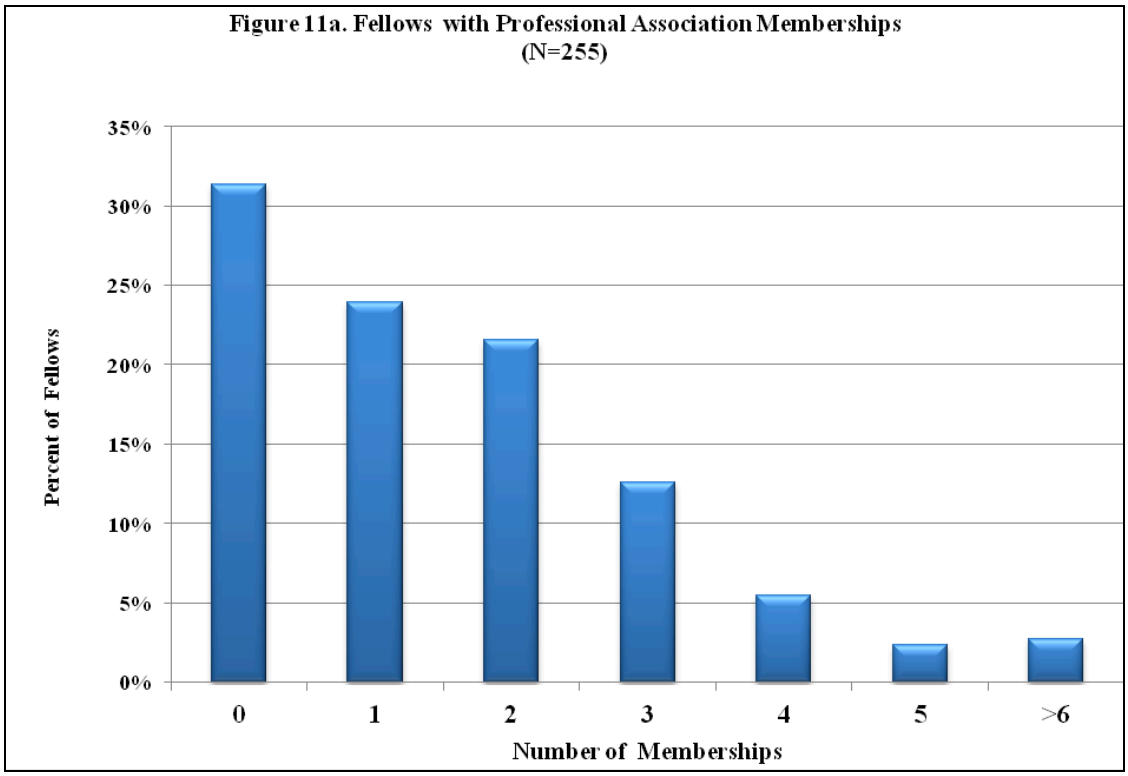


Professional Direction and Employment

All in all, the DOE CSGF provides a practical basis on which to address the looming need for well-qualified computational scientists and engineers, as projected by the DOE in relation to its mission. Development of such a workforce is no small task, and educational attainment and training are only part of the overall picture. As discussed, the CSGF program has taken a multifaceted and comprehensive approach to preparing promising doctoral students to take their place as contributors and leaders in the broader CSE community and workforce. That is, designed to address the research and development activities in DOE and other federal laboratories, academic institutions, and high-technology firms, the DOE CSGF paves the way for various employment opportunities. The program encourages and facilitates access and success for Fellowship recipients in CSE-related careers. Indeed, as previously mentioned, DOE first established the Fellowship as a means for developing a pool of specialized workers with skills particular to its mission and growing needs. Thus, professional development and participation have been critical topics on the DOE CSGF agenda.

A typical indicator of professional community involvement and participation is membership in discipline-based professional associations. However, to date, there is no professional association explicitly identified with CSE as such, which largely reflects its still evolving nature and nascent community.[24] In any case, Fellows have specific STEM disciplinary affiliations to which their doctoral degrees are tied. Therefore, as a first take, the survey simply requested information about Fellow membership in professional associations in general. However, of 255 Fellows for whom information was available, 31% actually indicated no memberships. Still, as shown in Figure 11a, the majority of respondents — 69% — did indicate one or more professional association memberships.

[24] A few professional associations have sections devoted to CSE (e.g., the Society of Industrial and Applied Mathematics), but a separately identified organization has not been established.



An alternative perspective on this issue concerns the multi-disciplinary nature of CSE, which speaks to the DOE CSGF requirement for Fellows to pursue research outside of their major fields. Therefore, moving beyond discussions of professional associations that assume discipline-related membership, the survey requested information on Fellow memberships in associations outside of their individual doctoral fields. As shown in Figure 11b, 30% of Fellows indicated such memberships. Furthermore, active participation involves more than mere membership, especially in regard to leadership considerations. Interestingly, when Fellows indicated involvement in these associations, they also tended to be engaged in special roles and activities. As shown in Figure 11c, of the survey respondents, 54 indicated holding or having held special leadership roles in their professional associations, including organizational officer and board member positions.

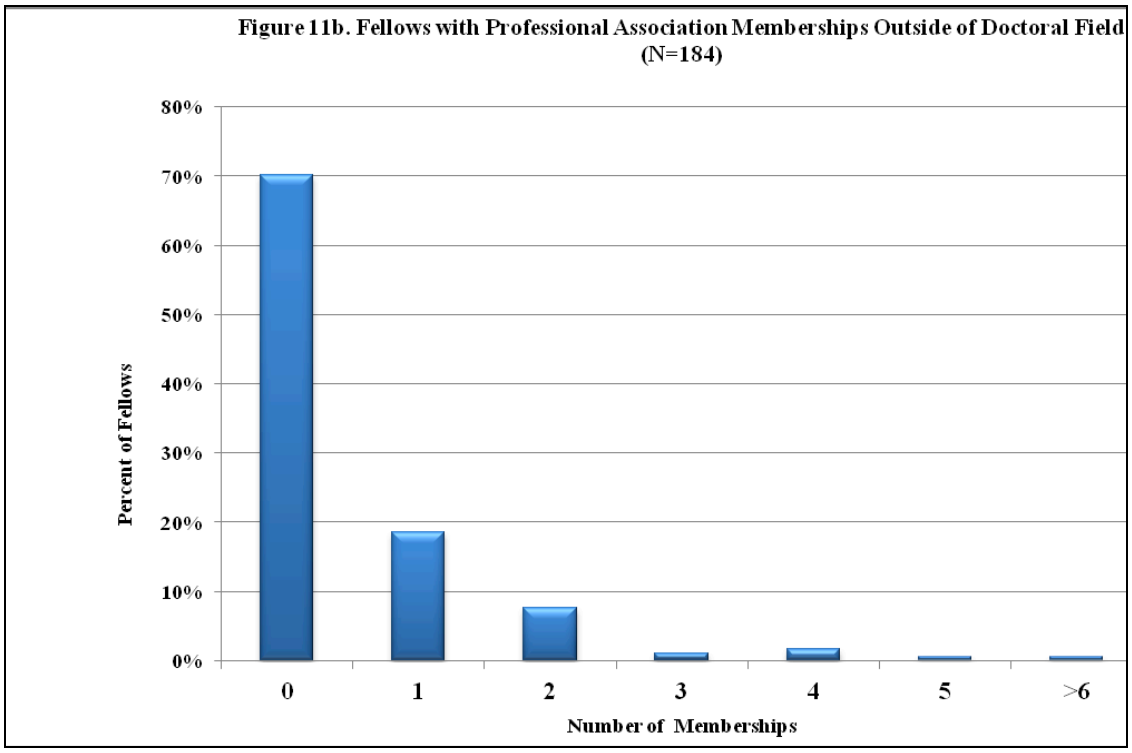


Figure 11b. Fellows with Professional Association Memberships Outside of Doctoral Field
(N=184)
80%
70%
60%
50%
40%
30%
20%
10%
0%
Percent of Fellows
0
1
2
3
4
5
>6
Number of Memberships

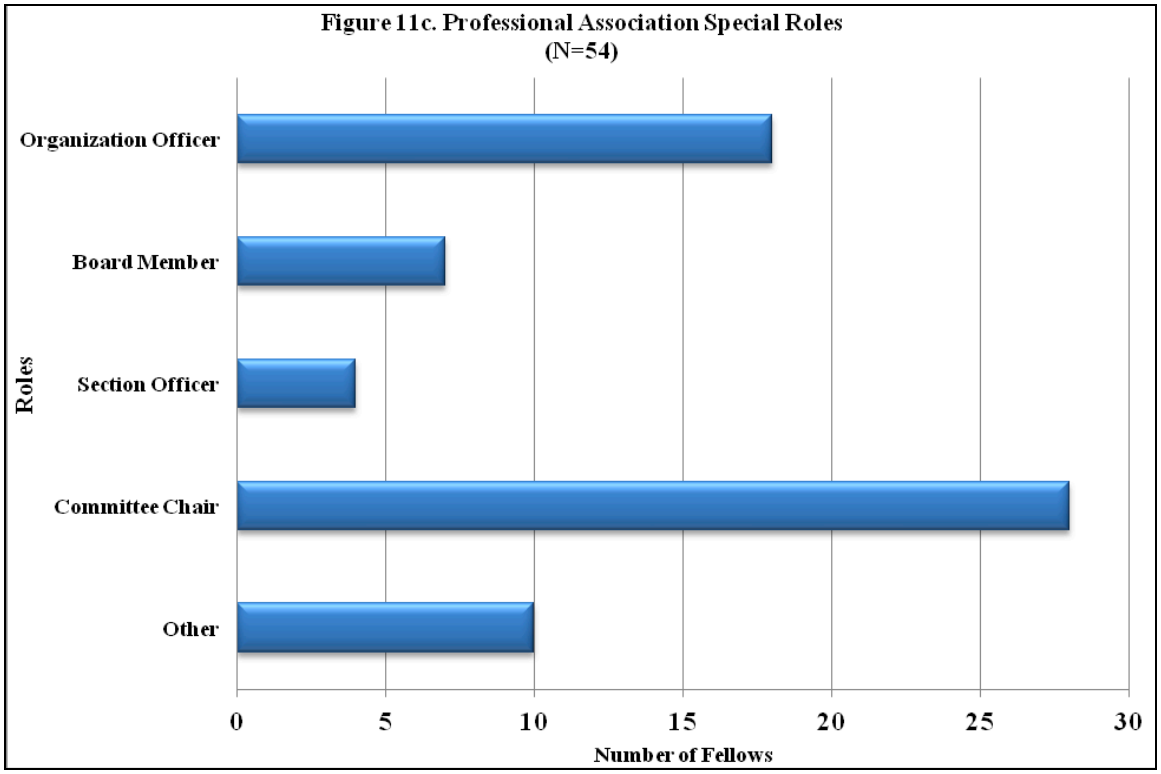


Figure 11c. Professional Association Special Roles
(N=54)
Organization Officer
Board Member
Section Officer
Committee Chair
Other
Roles
0
5
10
15
20
25
30
Number of Fellows

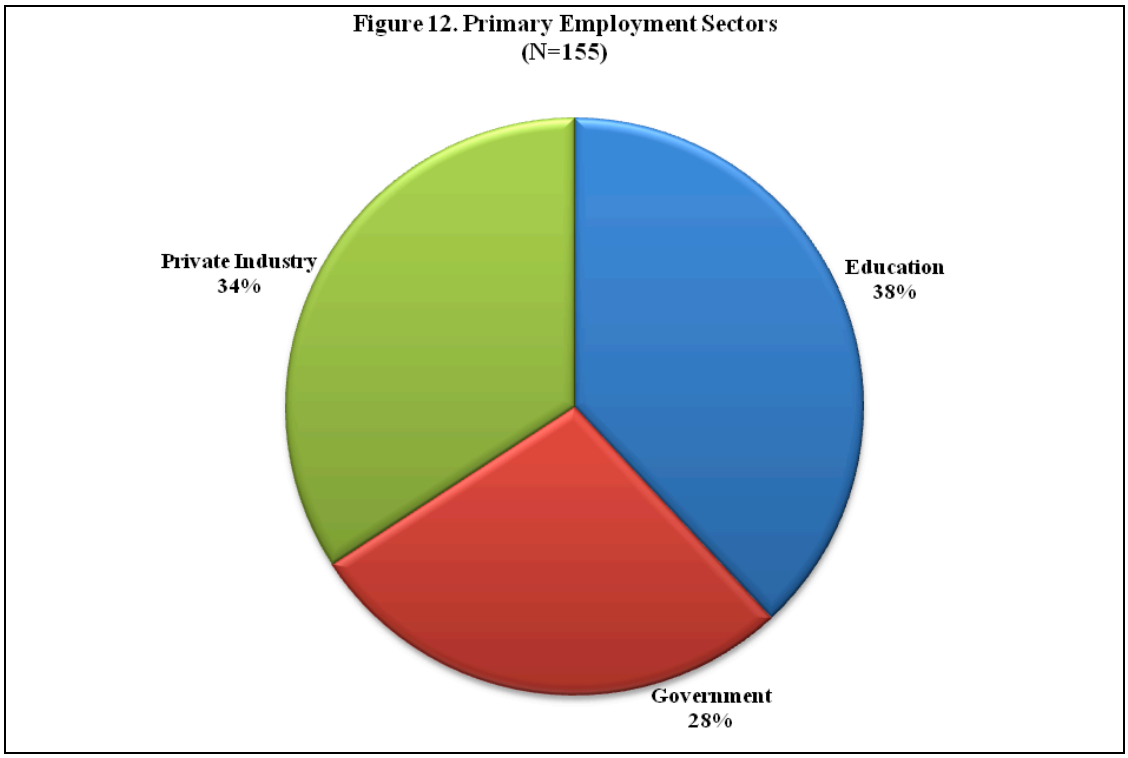
Note that the unevenness of these responses to questions of professional association membership and participation may be an artifact of the data, but, in addition to the fact that there is no CSE-specific organization, it also might point to different kinds of participation taking precedence among computational scientists and engineers and/or to the nature of their particular employment, as will be discussed later.

Regarding Fellow employment, the survey queried a variety of issues, such as employment sector and earnings, and looked particularly at employment in the DOE given the expressed aims of the early Fellowship program to expand the pool of eligible high quality HPC recruits for DOE ends. Related questions focused on employment experiences and also considered position responsibilities and advancement.

According to 2008 figures, 64% of U.S. workers with their highest degree in STEM fields were employed in for-profit firms, 7% in the non-profit sector, 13% in government, and 16% in academia (NSF 2012). However, of employed STEM doctorate holders, 38% were in the for-profit sector, 6% in non-profit, 9% in government, and 47% in academia (NSF 2012).[25] Of survey respondents with completed doctorates, 155 provided employment sector information with, as Figure 12 shows, 28% in government, 38% in education, and 34% in the private (for-profit and non-profit) sector. Furthermore, of 63 current Fellows who had not yet completed their doctorates, 27% indicated plans for employment in government, 44.4% in education, and 11.1% in the private sector (for-profit); the remaining 17.5% were undecided or unknown.[26]

[25] Some indicators for 2010 suggest 35% of STEM doctorate holders in for-profit firms and 41% in academic institutions.

[26] Note that 159 of the survey respondents with doctorates indicated that they were employed, but 4 did not provide sector information.



Of course, a critical issue in relation to the DOE CSGF concerns whether Fellows are employed in CSE-related positions. Note that 82% of U.S. workers with doctorates in STEM fields, but not working explicitly in STEM occupations, still reported jobs that were either closely or somewhat related to their degrees (NSF 2012).[27] Those with backgrounds in CSE appear to have similar occupational outcomes. Of responding DOE CSGF recipients with completed doctorates, as shown in Figure 13, across cohort and field, 138 (89%) reported CSE-related employment. Furthermore, referring to Figure 14, primary employment with DOE was reported by 71 of the Fellows. In fact, an especially telling point is that, of those, 44 (62%) indicated that their employment was in the very same DOE laboratory in which they carried out their DOE CSGF research practicum, showing an arguably direct Fellowship effect. (Of course, this outcome can be attributed to the nature of the work that they carry out in the laboratory. However, that too can be linked directly to their DOE CSGF practicum experience, i.e., that it started the Fellow down a particular research and career path.)

[27] According to 2008 data.

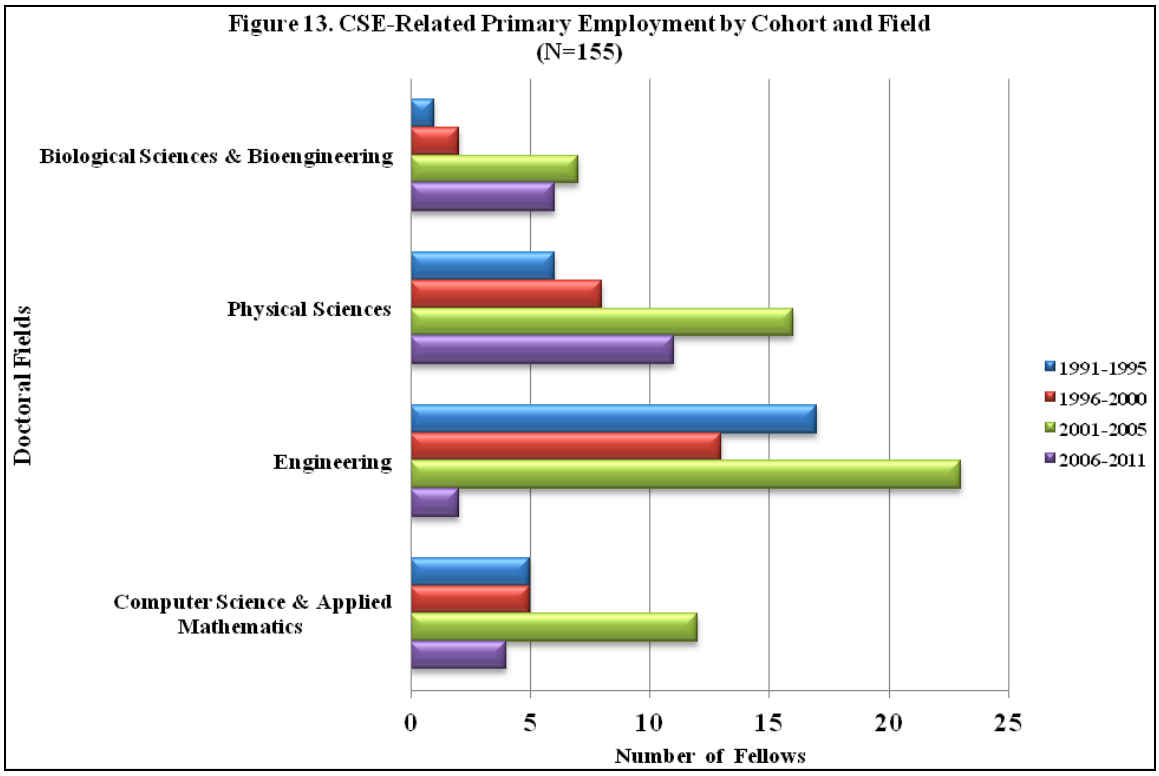


Figure 13. CSE-Related Primary Employment by Cohort and Field
(N=155)
Biological Sciences & Bioengineering
Physical Sciences
Engineering
Computer Science & Applied Mathematics
Doctoral Fields
1991-1995
1996-2000
2001-2005
2006-2011
0
5
10
15
20
25
Number of Fellows

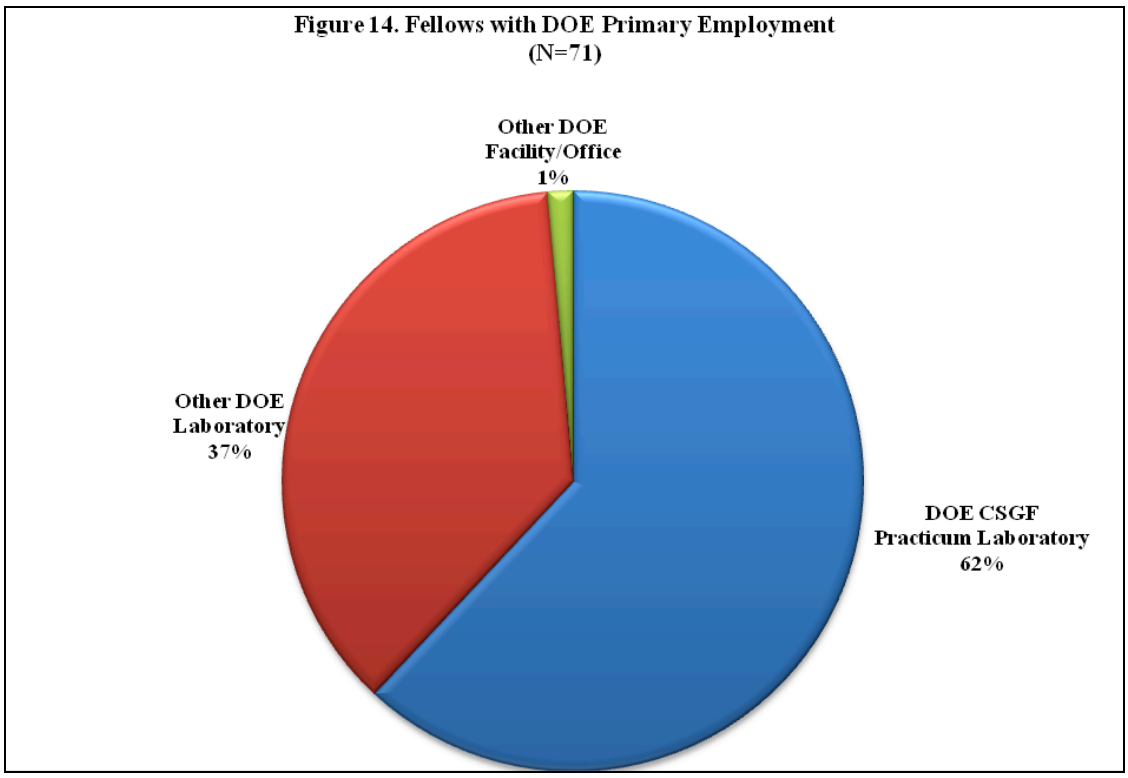
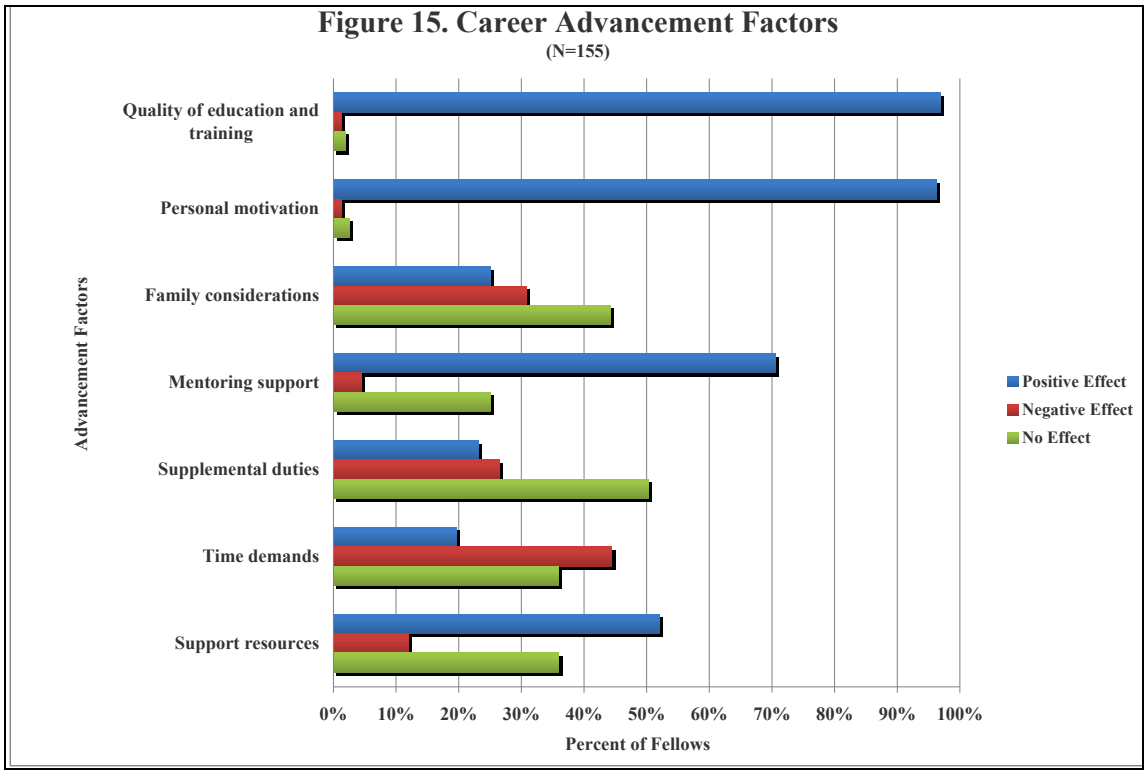


Figure 14. Fellows with DOE Primary Employment
(N=71)
Other DOE Facility/Office 1%
Other DOE Laboratory 37%
DOE CSGF Practicum Laboratory 62%

Beyond the basic issue of employment sector is the more specific concern of career advancement. Typically involving promotions, pay raises, and/or other situationally positive factors, career advancement usually refers to progression from one level to the next and/or other enhanced employment conditions and increased responsibilities. Possibilities for advancement are not only relevant to the individual in a position, but also to the message communicated about the working conditions to others considering similar paths.

In the face of such issues, questions regarding CSE employment are particularly germane to DOE CSGF goals. As already discussed, various aspects of the Fellowship program were devised in support of CSE career development. Therefore, given this understanding, a principal aim of the survey was to capture information on the actual careers and relative outcomes of the Fellowship recipients. The contribution of the DOE CSGF to the CSE field began with an emphasis on educating and training award recipients for related careers.

As can be seen in Figure 15, of employed Fellows with completed doctorates, 97% indicated that, besides their own personal motivation and drive, the quality of their education and training was the most important factor affecting career advancement in their positions. Also, in keeping with earlier discussions, another 71% pointed to mentoring as a critical factor in support of their career advancement. These issues are especially relevant to this study given that they are, in fact, central tenets on which the DOE CSGF program turns.



Also, salary must be mentioned since level of earnings is often a critical factor affecting employment decisions. According to data from the National Science Foundation (2012), workers with STEM degrees, regardless of occupation, typically earn more than workers with comparable-level degrees in other fields, and half of the workers in STEM occupations earned $73,290 or more in 2010 — more than double the median earnings ($33,840) of the total U.S. workforce. For recent STEM doctorate recipients, up to 5 years after receiving the degree, the 2008 median annual salary was $67,000 (NSF 2012).[28] In contrast, the median annual salary of the DOE CSGF survey respondents was $95,673. The mean base salary of the employed Fellows with completed doctorates who responded to related queries was $94,329. Among those Fellows employed in the education sector, the mean base annual salary was $70,351; among Fellows employed in the private sector, the mean base annual salary was $122,100; and among Fellows employed in the government sector, the mean base annual salary was $95,571. Of course, salaries can vary along a variety of dimensions, such as years since completion of the degree. However, while those in the older cohorts and holding the doctorate for 13-18 years tend to be in

[28] These figures were the latest available and were updated in July 2012.

the higher salary ranges, as might be expected, the situation is highly variable across groups.

Overall, Fellows are active contributors across government, private, and education sectors. As mentioned above, the benefit to the DOE also is reflected in the number of Fellows who pursue their careers within or in coordination with DOE laboratories. The development and engagement of a top-notch CSE workforce is critical to the DOE's overall mission and the DOE CSGF encourages and offers Fellows the opportunity to explore related careers, positioning them for employment in DOE laboratories. In addition, many Fellows have taken academic positions, a point that is particularly important given that, as faculty, they serve an important role in furthering CSE as an area of study and in educating and training the next generation of computational scientists and engineers.

A Demographic Note

Again, as noted, DOE CSGF was developed to meet the projected need for trained computational scientists and engineers by DOE and other government agencies and for supporting U.S. leadership in related STEM fields. To reach that goal, the participation of women and minorities in the program also has been raised as an important consideration (ASCAC 2011), especially since women and minorities have been generally underrepresented in degree attainment in STEM fields (NAS 2007, 2011).[29] Put forward in terms of strategic capacity building, these groups have been viewed as a generally untapped and underdeveloped resource.

Since related questions often arise in assessments of the STEM workforce and to further delineate the Fellowship reach and response population, the Krell Institute administers surveys requesting self-identified demographic information. Optional requests for demographic information also are included as part of the application process, with the aim of providing a more detailed picture of the applicant pool and overall Fellow profile, as illustrated in Table 4 using the 2011 outcomes. Also, such information can prove valuable for recruitment and outreach

[29] However, women have reached parity in certain selected STEM fields, most notably in the biological sciences.

planning and for a better-informed understanding of the applicant pool relative to the broader STEM population.

Table 4. DOE CSGF 2011 Applicant and Fellow Demographic Features*

Demographic Feature	% Applicants (N=628)	% Fellows (N=17)
Gender		
Female	21.6	23.5
Male	78.4	76.5
Race/Ethnicity		
African American	3.9	0.0
Asian/ Pacific Islander	12.9	14.3
Caucasian	71.8	71.4
Hispanic	6.5	14.3
Multi-Racial	4.2	0.0
Native American	0.7	0.0
Disability	3.6	0.0

*From Krell Institute surveys.

DOE CSGF is an equal opportunity program open to all qualified persons without regard to race, gender, religion, age, physical disability, or national origin. Accordingly, the Krell Institute has undertaken outreach activities to address this issue and has seen increases in participation and diversity among qualified applicants. For example, in 2011, as seen above, 21.6% of 628 applicants were female. In fact, considering possibilities for graduate school enrollment as required for DOE CSGF recipients, it is important to note that, while "the number and proportion of female undergraduates in computing fields has been declining over recent years, CSE, and especially CSE applied to biological sciences, typically attracts a much higher proportion of females. It is not uncommon for undergraduate applied mathematics programs to have a majority of female students, and it is very common for biology, for example. CSE therefore represents a good opportunity to attract a more diverse student body into computing" (SIAM 2006, p.1). Moreover, recent concerns about scientific workforce capacity have led to demands for greater attention to the potential of all groups to contribute to the larger scientific enterprise in society. DOE CSGF outreach activities are aimed at increasing representation of highly qualified applicants across groups and the Krell Institute has been commended for its efforts in this regard (ASCAC 2011). While their activities speak more generally to questions surrounding the

participation of DOE CSGF recipients and other computational scientists and engineers in related careers and pursuits, they also address efforts to harness the full diversity of intellectual capacity needed to fuel the research enterprise that is critical to scientific advancement and application today.

Integrated Profiles and Community Development

A general goal of this study is to determine ways in which DOE CSGF recipients take part in and contribute to CSE community development. To that end, building upon basic features determined in the previous section, more detailed and individualized information is here engaged to develop Fellow profiles to explore the dynamics, disciplinary and professional cultures, and knowledge production that characterize and mark the related scientific community.

As in any community, membership and participation are defining issues, and the logic of community membership and participation — and, thus, of legitimation — determines the acceptance and diffusion of ideas and information, as well as career opportunities, within and across groups. Accordingly, in this case, scientific communities operate as channels for the generation and dissemination of knowledge, while also serving as sources for mutual recognition and validation. With growing complexity and differentiation characterizing STEM fields and enhanced by technological capabilities and innovation, possibilities for community involvement mark the scientific enterprise and related productivity. The underlying question here is the extent to which the Fellowship itself might be an affective factor determining the dimensions of a related scientific community. These dimensions can vary both independently and interactively according to field and differing structural, disciplinary, and occupational features.

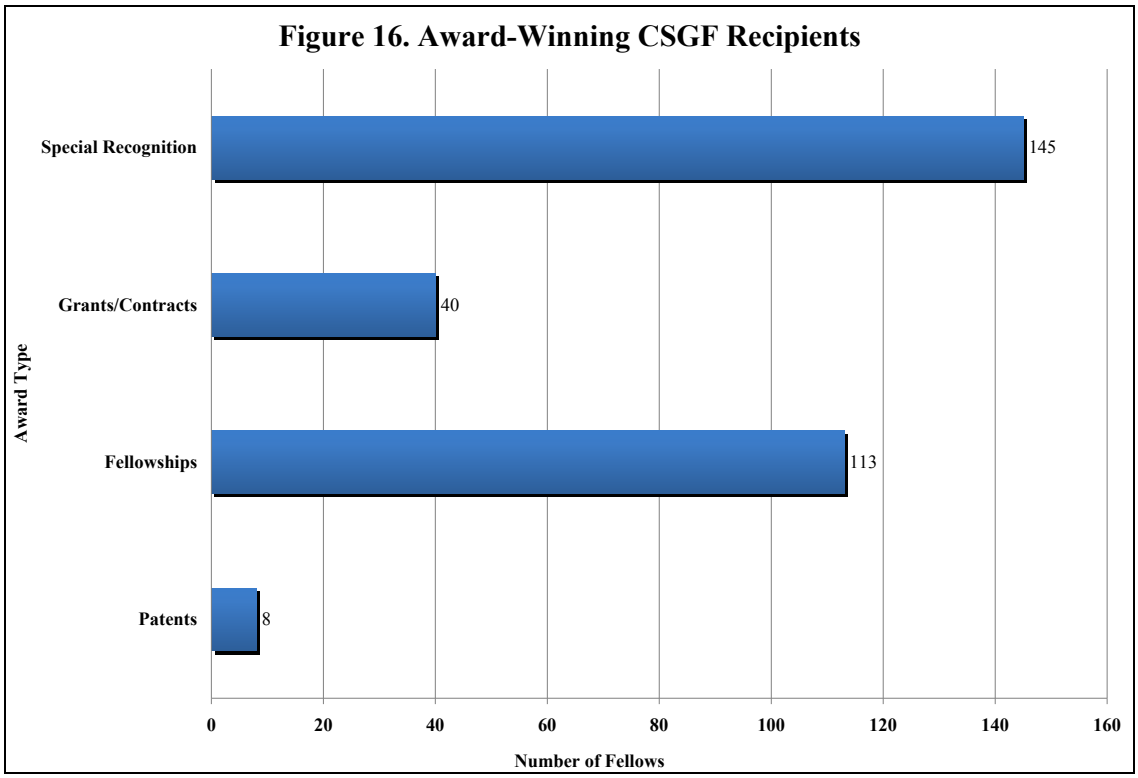
Membership in the scientific community can be marked relative to a variety of participation indicators, such as professional training and socialization — evinced by, for example, attainment of a related advanced degrees, research experience and publications, and professional association memberships — and recognized criteria for excellence, prestige, and reputation, all of which are legitimating factors within designated fields. Therefore, considered especially in terms of scientific field, institutional referents, and professional age and status, and also relying on basic scientometric indicators to gauge participation, the task here is to determine conditions for an emergent community among computational scientists and engineers, in light of their own disciplinary dynamics and directions. The basic aim is to

develop a fuller understanding of the diffusion of STEM talent, which also means employing an analytical stance that directly addresses participation patterns relative to professional relations and outcomes.

Accordingly, criteria identified as community motivations are invoked here relative to DOE CSGF recipients. These include, for example, recognition of expertise, access to resources, visibility, professional advancement, productivity, collegial interaction, intellectual interest, and advancement of knowledge and learning (cf. Beaver 2001; Katz and Martin 1997). Of immediate concern, of course, are the accomplishments of individual Fellows. Specific, individualized data on 170 DOE CSGF recipients were drawn from curricula vitae (CVs), as discussed in Section I, to explore individual productivity and involvement.

Awards and Honors

As a first indicator of accomplishment and community recognition, different types of *awards and honors* bestowed upon DOE CSGF recipients were considered. As can be seen in Figure 16, the vast majority of Fellows — 145 — indicated receiving special awards and honors in recognition of excellence for their work and of outstanding service that they performed. Note too that these awards were not necessarily single occurrences; many individuals received multiple awards, with 387 different ones reported by the 145 individuals. These special recognition awards came from a variety of sources, including private foundations and government agencies. Furthermore, 40 Fellows reported winning 92 relevant grants and contracts, again from a variety of private and public sources (including DOE). Also striking were the 113 Fellows indicating awards of other types of fellowships; counts of fellowships came to 186 across their CVs. In addition, 8 individuals reported patents, both awarded (8) and pending (6).



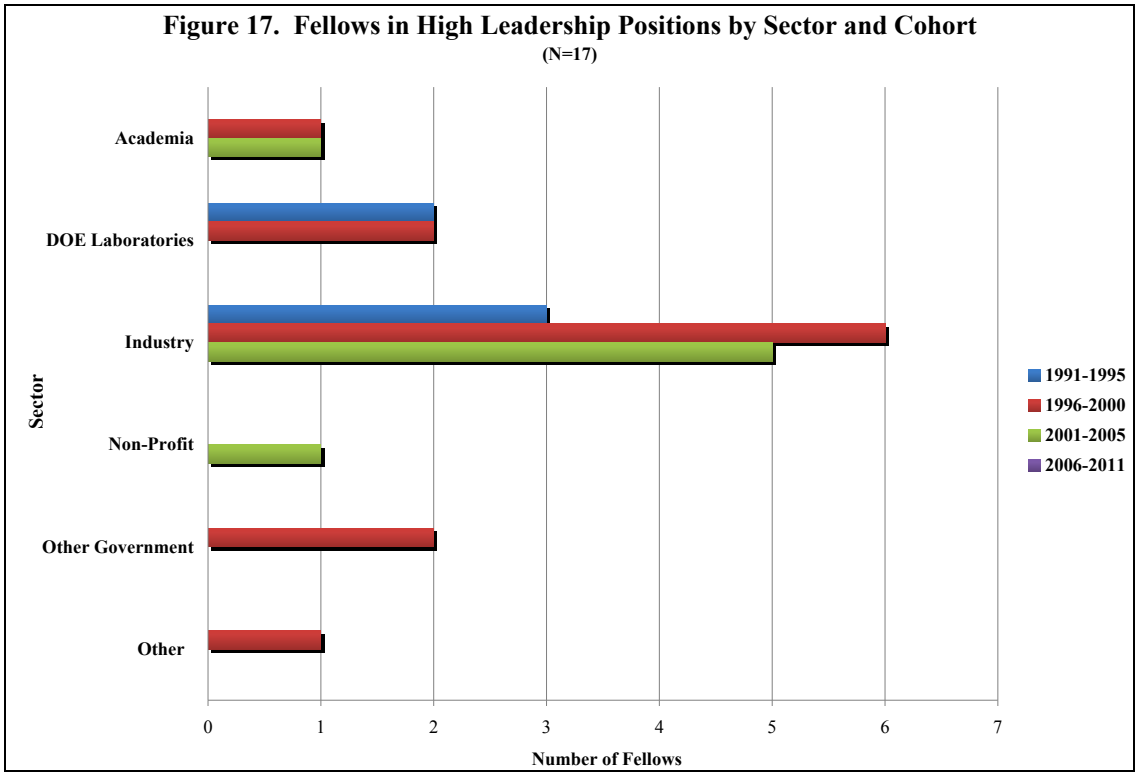
Public Intellectual and Service Activity

Analysis of CVs also made it clear that some Fellows might be viewed as *public intellectuals* or as participating in related *service activities* and roles. While not consistent, some 32 Fellows indicated contributions to the media and public sphere through, among other things, writing reviews, providing special topic interviews, acting as experts and advisors, and developing and contributing to special informational programs and websites. Also, preparation of special reports and service on government committees, review panels, and advisory boards reflect such expertise and recognition. In addition, the CVs reflected a wide range of secondary and optional unpaid service activity roles performed by the Fellows. For example, 31 Fellows indicated serving as instructors and tutors, and 54 specifically listed service as academic and professional mentors. Referee and reviewer service — including work for journals and for funding organizations — also were prominent on 63 CVs, as was assistance to various groups in numerous principal and supportive positions. Furthermore, other factors such as leadership

positions and publications also play a role in framing Fellows in terms of public intellectual and service activities.

Leadership Positions

Some Fellows also were revealed to hold *leadership positions*. Leadership refers in general to processes of organizing and influencing behavior and support among others to accomplish some task or goal (Chemers 1997). While it can encompass informal relations, formal recognition of leadership is here considered relative to its importance not only in professional capacities as scientists and engineers, but additionally in broader community interactions (directly and indirectly). Therefore, the fact that 17 Fellows reported having held such positions across various sectors — with some reflecting multiple positions, as shown in Figure 17 — is somewhat notable. These ranged from team leaders, directors, and managers to organizational presidents and executives, and were, as might be expected, especially apparent among Fellows from the earlier DOE CSGF cohorts — including leadership positions in DOE and other government agencies.



Collaborations

Furthermore, a principal way in which scientific communities have been identified and operationalized in related studies is through *collaborations*, particularly in terms of research and publication. While past studies of scientific productivity tended to focus primarily on the individual researcher, collaboration has been increasingly recognized as critical for related processes, especially given the growing complexity attached to scientific discovery and technological innovation. Indeed, the complex network layers and patterns evinced in collaborative relations are now widely considered indicative of productivity. Collaborations reflect relational structures through which scientists are linked to wider professional communities, calling attention to the nature of networks and interaction.

Among DOE CSGF recipients themselves, with more and more Fellows educated and trained as computational scientists and engineers, greater interconnectedness is obviously possible across cohorts and fields, providing means by which the features of internal CSE epistemic network construction might be determined.[30] Whereas collaborative relationships might begin by chance, intention, or recommendation, or as career expectations (Beaver 2001), keep in mind that DOE CSGF programmatic elements have been instituted to encourage such outcomes. Accordingly, while collaboration networks can be wide-ranging, the issue here is to consider CSGF itself as a path to community development — an especially apt point since, for example, the required practicum experience is grounded in teamwork and the annual conference and several other activities are designed to promote interaction among Fellows. Therefore, the extent to which Fellows might collaborate on research and publications with their practicum laboratory team members or with other Fellows can evidence specific DOE CSGF-influenced networking and community building. Examining the CVs for indications of such co-authorships and research projects after Fellowship completion, 31 Fellows were found to have collaborative relationships with practicum laboratory members and 41 reported collaboration with other Fellows, as shown in Figures 18a and 18b, suggesting a growing community among DOE CSGF participants.

[30] Cf. Wagner and Leydesdorff (2004); Glänzel (2001).

Figure 18a. Fellows with CSGF-Related Collaboration Partners by Field

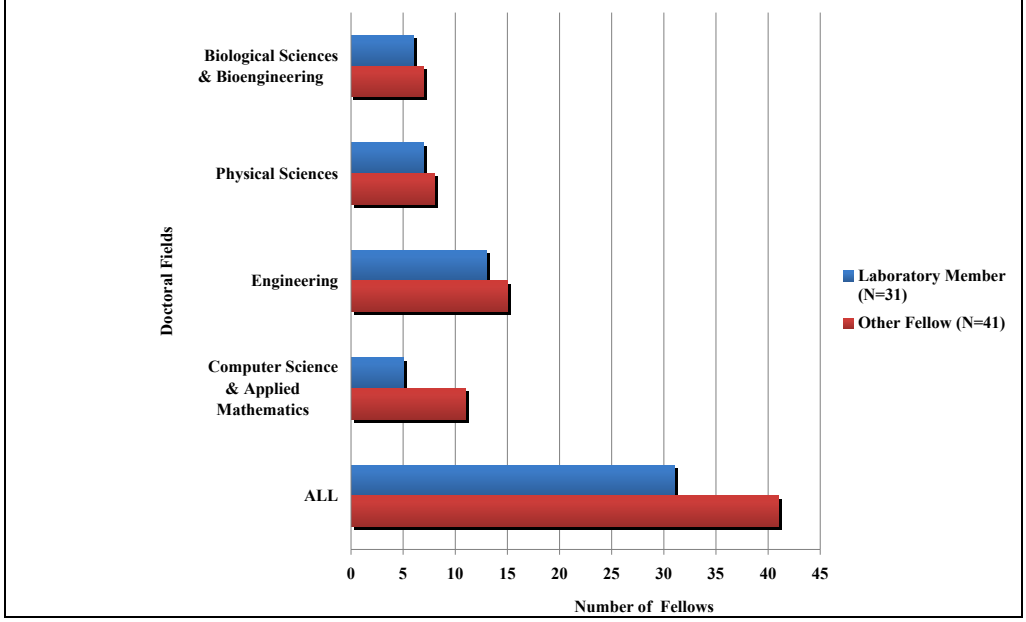
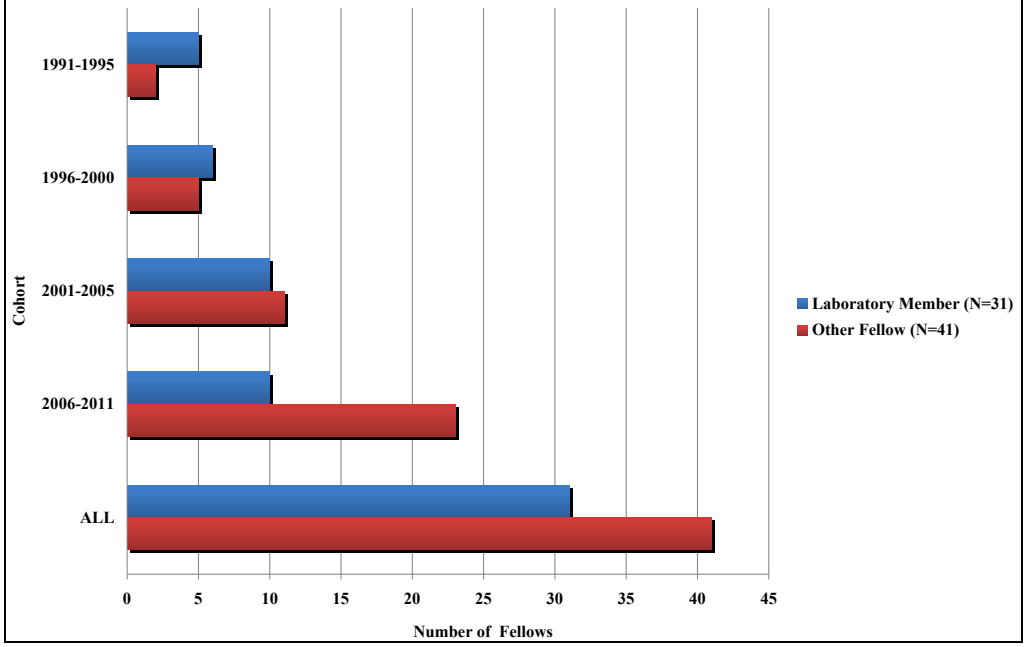
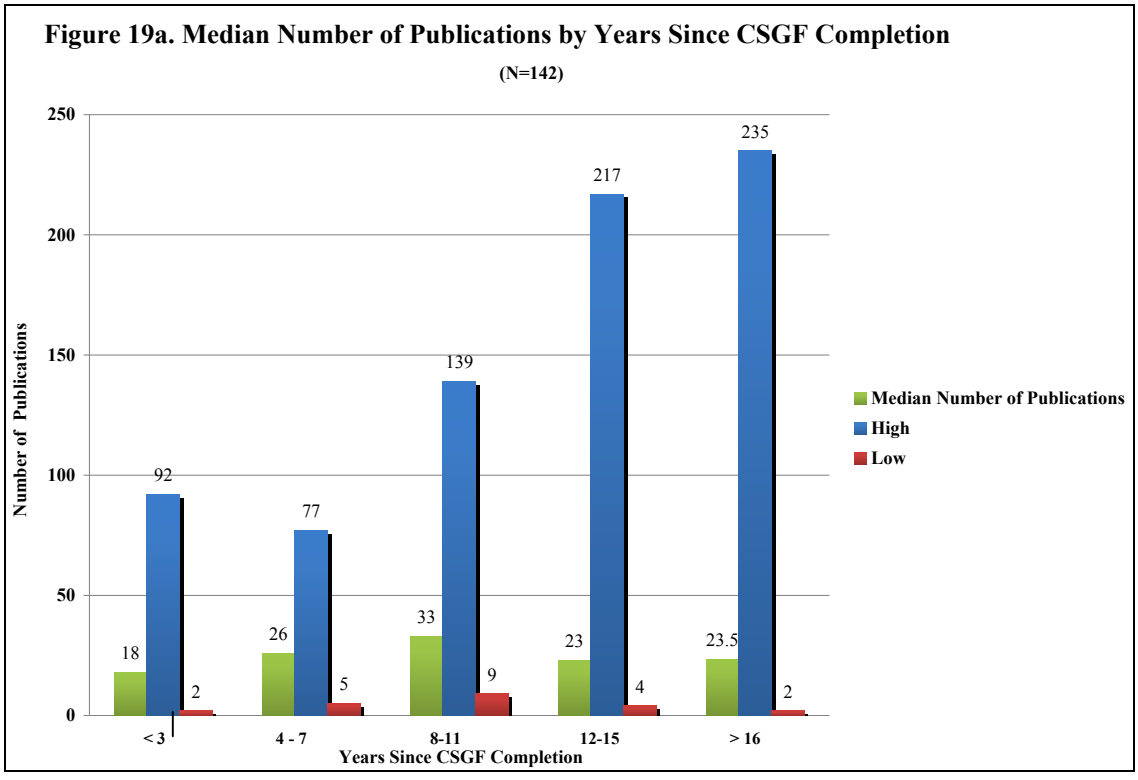


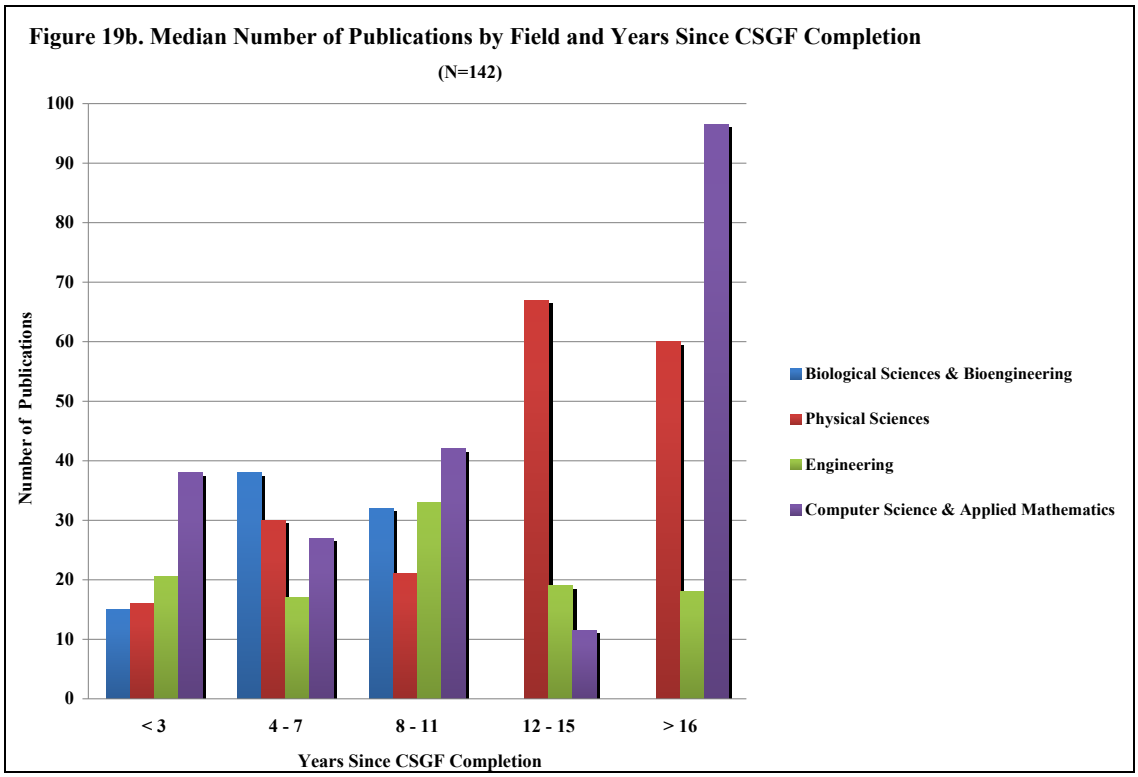
Figure 18b. Fellows with CSGF-Related Collaboration Partners by Cohort



Publications

Extending these issues of productivity and legitimacy, one way in which participation and position in scientific communities has been indicated is through *publications*, especially in peer-reviewed STEM journals. Publication of related articles occurs within a relational structure representing a network of direct and indirect epistemic attachments, and operating as "a mechanism for both gaining and sustaining access to recognition in the professional community" (Beaver and Rosen 1978, p. 69; Beaver 2001). In terms of publications, Fellows tend to be quite professionally active. As shown in Figures 19a and 19b, DOE CSGF alumni for whom CVs were available (142) reflected median numbers of publications of 18 to 33, reflecting contributions to community and knowledge dissemination. Of course, the actual number of publications for individual Fellows in terms of high and low counts can be quite variable and depend on a variety of factors, e.g., discipline and the amount of time necessary to complete research projects on which articles might be based.





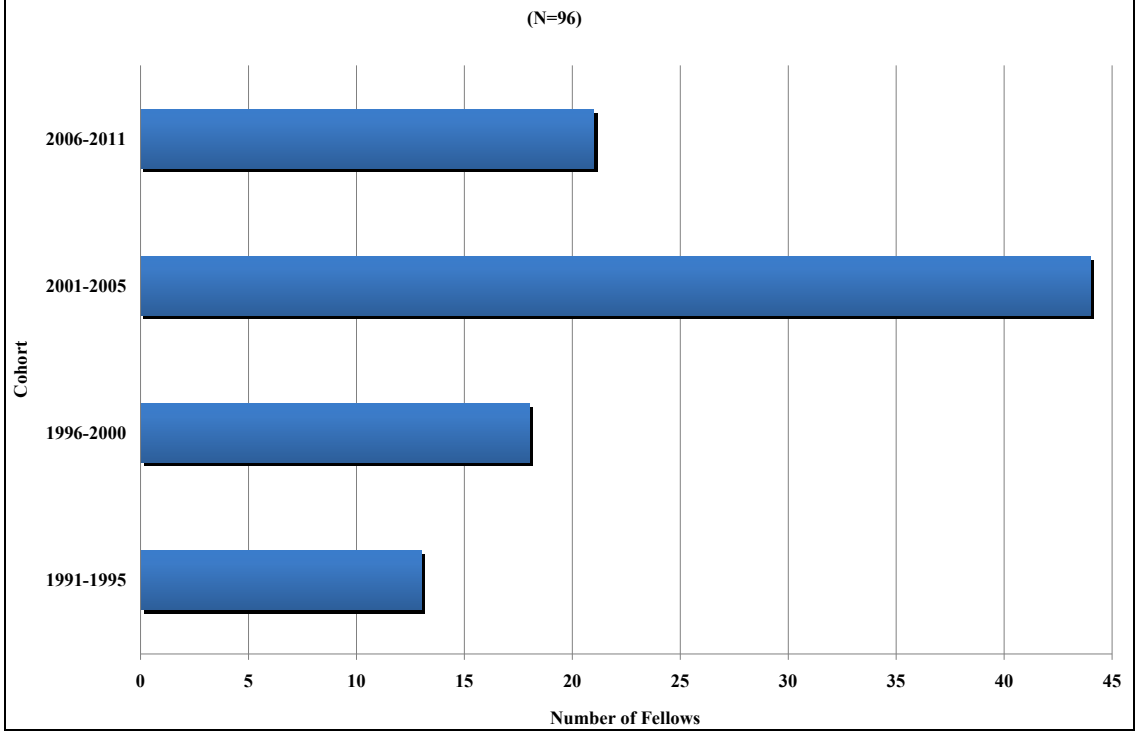
Moreover, *peer-reviewed publications in top-ranked journals* have long been the conventional basis for many of the indicators used to characterize scientific productivity and to evaluate contributions to research and knowledge creation. That is, published articles and assessments of their outlets — the type and status of journals in which they appear — are a paramount consideration in recognizing position and influence within scientific networks. Accordingly, this study proffers an approach for delineating community involvement based on authorship in top-ranked science and engineering journals. Drawing from scientometric perspectives for assessing career relations and productivity, a simplified approach was invoked here to garner insights on the CSE multidisciplinary landscape in terms of participation in scientific communities.[31]

While, as indicated above, DOE CSGF alumni have been somewhat prolific in regard to publishing, the outlets in which they have published is the concern here, especially in light of disciplinary and community

[31] Scientometrics involves scientific measurement and analysis, typically employing bibliometric tools to assess scientific publication impact – although their use is not without controversy. See discussion and references in Stonebraker et al. (2012).

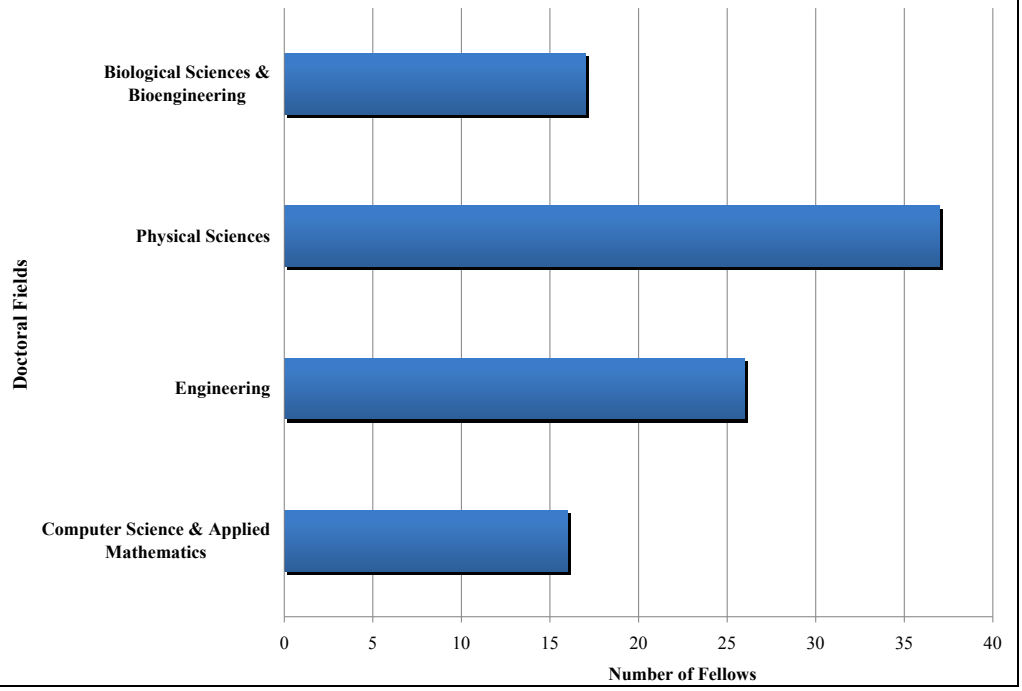
dynamics. Therefore, using a combination of the journal impact factor and Eigenfactor values, convention was followed in identifying top-ranked journals in STEM in general and, more specifically, in Fellow designated fields.[32] The impact factor and Eigenfactor are metrics for ranking the quality of publication outlets and are commonly employed for assessing the scholarly contributions and influence of journals (Fersht 2009; Craig and Ferguson 2009; Garfield 2006; McKerahan and Carmichael 2012; Stonebraker et al. 2012). Looking to determine if CSGF recipients have published in top-ranked STEM journals, a review of information available in their CVs showed that at least 96 Fellows have, in fact, done so, as can be seen in Figures 20a and 20b. Again, the publication outlets for these Fellows have included the overall top-ranked STEM journals — *Science*, *Nature*, and the *Proceedings of the National Academy of Sciences* — and the top-ranked journals affiliated with the various disciplinary areas and subfields in which computational scientists and engineers work.

Figure 20a. Fellows with Publications in Top-Ranked STEM Journals by Cohort



[32] From ISI Web of Knowledge/Thomson-Reuters *2010 Journal Citation Reports*, Science Edition; http://www.eigenfactor.org/methods.php

Figure 20b. Fellows with Publications in Top-Ranked STEM Journals by Doctoral Field
(N=96)



Interviews and Fellow Perspectives

The DOE CSGF was established to help develop a qualified workforce with the knowledge and skills to advance the DOE national agenda and meet the environmental, economic, and security challenges of today and the future. To that end, the DOE has instituted programs aimed at developing computational talent and increasing excellence in pursuit of its mission and as a contribution to national wellbeing. Central to its efforts championing the related STEM enterprise has been the DOE CSGF, developed to maximize the education and training of its recipients, especially as regards HPC. While the Fellowship objectives refer to a generally encompassing rationale and motivation, they at the same time provide a platform on which the DOE CSGF outcomes can be explored in both broad and specific terms. Beginning with the goal of enhancing the STEM workforce, computational scientists and engineers are treated as fundamentally critical to societal advancement.

However, although the DOE CSGF was established with the goal of producing eminently qualified and talented candidates who can employ HPC and other robust technologies in support of the STEM research infrastructure, the value of the DOE CSGF is not simply assumed here. Rather, it is a matter for investigation, and exploring the accomplishments and contributions of DOE CSGF recipients is a vital task for documenting and determining Fellowship impacts in both direct and indirect terms. Accordingly, particular attention must be given to, for example, scholarship, leadership, recognition, collaboration, and service. Such interrelated areas are linked intimately to how science is conducted and used in society, thereby providing a basis on which to identify and assess Fellowship impact. By considering DOE CSGF effects and influence on individual Fellows, a more detailed picture of recipient outcomes and programmatic impacts can be determined relative to disciplinary and professional dimensions.

Thus, interviews were employed here as a research strategy to supplement and extend the findings in the previous sections. Using interviews to explore the paths followed by the Fellows, framed by their choices, decisions and perspectives, can illuminate differences that might be more obscure in surveys or variable on CVs. In this sense, the

interview strategy complements the CV and survey-based findings for a more detailed and finer grained picture of the outcomes in question. While, by themselves, interviews can be viewed as offering only individual or idiosyncratic opinions and perspectives, when incorporated as part of the larger research strategy, they can address and provide insight into Fellow perspectives and the broader issues in question. Indeed, they can help to demonstrate linkages between programmatic elements and computational research and applications.

The organizational logic for the interviews was based on the set of considerations delineated in conducting the survey and CV analyses, offering a framework for analyzing, interpreting, and integrating findings. To that end, basic guiding questions were developed as initial considerations:

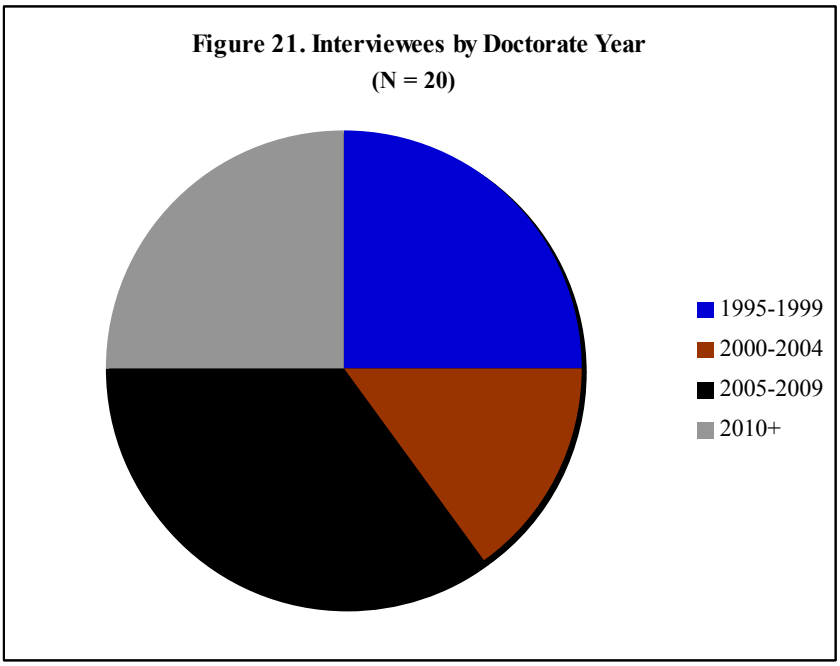
- How would you describe your DOE CSGF experience?
- Has the DOE CSGF and CSE been relevant to your career and professional development?
- Have you participated in relevant organizational activities (in general and, more specifically, in CSE-related areas)?
- What have been/are the contributions and significance (if any) of your work and other professional activities both in and beyond your field?

These questions were expanded and supplemented to capture a broad range of information on the program and its effects from the Fellows' perspectives. The overall concern was to learn as much as possible about participant perceptions of the nature and impact of the DOE CSGF program.

Approach

As mentioned, this section is based on in-depth semi-structured interviews with 20 DOE CSGF alumni Fellows. Interviewees were randomly selected within groups determined by Fellowship cohort and doctoral field to ensure general representation over the program's history. Of the selected individuals, 15 were male and 5 were female, with an age range spanning late 20s to mid-late 40s. Also, as shown in Figure 21, their doctorates were completed between 1995 and 2010,

with a third receiving them in engineering; the rest were in the physical sciences, biological sciences, and computer science and applied mathematics. All interviewees were employed, holding positions in government-funded laboratories, universities, and industry.



Interviews were transcribed and analyzed as text through both deductive and inductive approaches,[33] informed particularly by content and discursive analytic methods. Used for analyzing texts and large corpora of related documents, discourse analysis allows for the identification of textual patterns and makes replicable valid inferences from the data to their context (Baker 2006; Schiffrin et al. 2001; Krippendorff 1980). Adapted for use in this study, a hermeneutic approach to discourse analysis was employed, with interview content interpretation based on the systematic identification of specific characteristics of the related texts in terms of *lexicon*, *syntax*, and *morphology*. From this common set of features, various indexing and classification schemes were derived to provide links to specified items both within and across texts, thus allowing for *thematic inferences* that tie the contents of specific interviews to their DOE CSGF-related and

[33] Cf. Liu (2007).

community contexts. Such classifications or categories help to make sense of the common connections among individual interviewees, whether through job choice, practicum experience, or some personal identification. For example, one important category by which the interviews were classified from a Fellowship perspective was based on practicum location. Interestingly, although the interviewees were randomly selected, for the most part they were equally distributed among practicum sites, as can be seen in Table 5.

Table 5. Interviewee Practicum Sites

Practicum Site	Interviewees
Argonne National Laboratory	3
Lawrence Berkeley National Laboratory	3
Lawrence Livermore National Laboratory	3
Los Alamos National Laboratory	3
Oak Ridge National Laboratory	2
Pacific Northwest National Laboratory	3
Sandia National Laboratories – NM	3

Also, a basic lexicon of relevant *lemma* terms was established for analytical purposes; a lemma is the foundational linguistic term from which other terms are derived. Similarly, keywords — i.e., terms indicating the semantic typology of the different interviews — were determined for analytical purposes. Thus, for example, thematic keywords such as *fellowship, mentoring, collaborate, laboratory, computational science, service*, and so on, were designated and then used to perform various occurrence, association, and concordance analyses. The basic analysis included determination of word frequencies drawn from occurrence values relative to a list of 1000 lexical units or words, including various elements of speech (e.g., nouns, verbs, adjectives, adverbs, etc.). Word associations show keywords and their significant one-to-one relationships with other words within the textual corpus, and concordances involve the examination of actual occurrence contexts and specificity referencing explicit word usage. Together, these approaches constitute the primary interpretive components for analyzing the interviews.[34]

[34] Cf. Baker (2006).

While each Fellow had their own individual story to tell about the paths they had followed in their personal and professional lives, they all shared a common bond through their DOE CSGF experience. Indeed, in considering both commonalities and differences, evidence was clear of the power that the DOE CSGF program held not only to find talented individuals, but also to cultivate them to become leaders and innovators who are changing the future of their respective fields. Employing content analysis of the interviews, references to items associated with the Fellowship, including the annual conference and related network, were examined. In addition, the practicum experience, career choice, mentoring, and service related activities were explored.

To that end, a basic task was determining associations among words and terms and their variations in the related discourse of individuals in their roles as Fellowship recipients and as leaders in their fields. First considered were specific keywords — *fellowship, computational science, laboratory, career, collaboration, network, conference, mentoring, and service* — selected based on conceptual relevance and preliminary textual mapping, which were then used to identify other lexical units occurring in the same contexts. Also, in light of the overall focus of the study, concordance analyses were run for the same nine keywords as means for further considering the contexts of specific word usage. Word frequencies and associations within the interviews were analyzed to gain insight into the impact of the Fellowship on recipients.[35]

As mentioned, the textual corpus was comprised of the 20 transcribed interviews that were conducted with alumni DOE CSGF recipients. As a point of reference, note that, together, the interviews contained 4,626 lemmas.[36] To ensure statistical reliability, the threshold for inclusion was a minimum of 6 occurrences for the corpus.[37] For purposes of this study, the relatively common occurrence of words related to the Fellowship itself is especially telling. As shown in Table 6, the "fellowship" lemma (fellowship and related words and phrases, e.g., fellow, fellows, fellowship experience, Krell, DOE CSGF fellow, etc.) was itself the third most used lemma, occurring 589 times. The

[35] T-Lab Pro 6.0 textual analysis software was used to perform the analysis (http.//www.tlab.it).
[36] Also, the interviews contained 6,086 words and 6,792 contexts.
[37] T-Lab determines the threshold value choice using an algorithm based on low frequency range detection relative to the corpus size.

"computational science" and "research" lemmas occurred 493 and 202 times, respectively. Further, the lemmas for "mentoring," "collaboration," and "network" occurred 196, 176, and 74 times, respectively. Research in discourse analysis and linguistic studies, and also in ethnographic and interview methodologies, suggest that such occurrences indicate the critical role of such utterances as markers of relevance and impact (Fairclough 2003; Schiffrin et al. 2001). The point here is that the common reference to terms such as "fellowship" and even "science" potentially reflects internal perspectives or opinions that were voiced by the interviewees.

Table 6. Interview Lemma Occurrences

Rank	Lemma	Occurrences
1	think	808
2	work	629
3	fellowship	589
4	Computational Science	493
8	laboratory	346
13	research	202
17	mentoring	196
18	collaboration	176
28	software	138
36	teach	117
42	engineer	109
44	science	107
46	conference	105
53	service	100
71	network	74

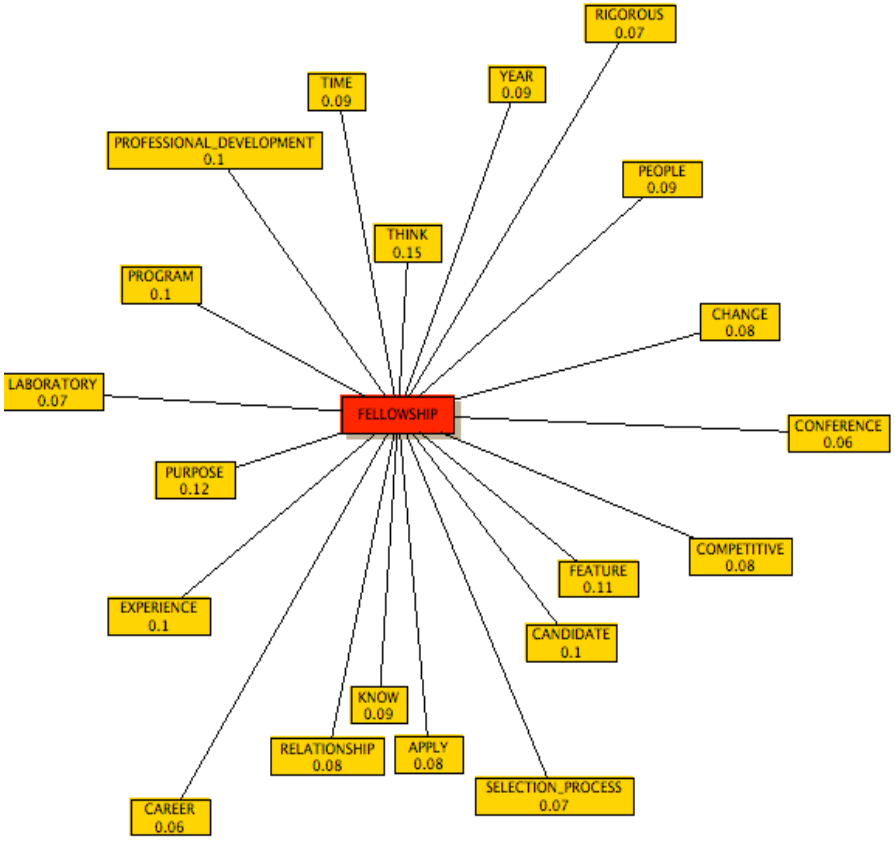
Word Associations

The strength of association was measured for particular lemmas in order to examine the lexical units with which they were associated or co-occurred within the interviews. This type of examination aids in determining contextual meanings of the selected words. Again, of special interest are the word associations with the aforementioned selected keywords — *fellowship, computational science, laboratory, career, collaboration, network, conference, mentoring, and service* — whose frequencies lend support to notions positing their potential

substantiation of related issues. Word association radial diagrams for the selected keywords (Figures 22-30) are presented to depict the strength of association between each central lemma and the lemmas most significantly associated with it on a one-to-one basis, i.e., indicating words with high degrees of associations with the keywords.[38] The distance from the central lemma represents strength of association, with numerical values corresponding to the indicated similarity coefficients or association indices. These coefficients, reflecting a value range of 0 to 1, are utilized to analyze the co-occurrence of terms within the context by employing binary data that captures the relative presence or absence of the two terms.

As shown in Figure 22 below, high level word associations with *fellowship* follow conventional lines showing strong associations with *purpose, change, rigorous, competitive, attractive candidate, and professional development*.

Figure 22. Associations with Fellowship



[38] The radial diagrams are presented in graphML format in order to show the structural properties of the graph.

Similarly, Figure 23 shows high level word associations for terms related to *computational science*. For example, as expected, computational science has the strongest relationships with *engineer*. Additionally, other *computational science* references followed traditional assumptions indicating the field and included words such as *science, mathematics, chemistry, and biology*. Of course, this finding is as expected since Fellows tend to discuss issues related to computational science in respect to various disciplines and within the larger STEM context.

Figure 23. Associations with Computational Science

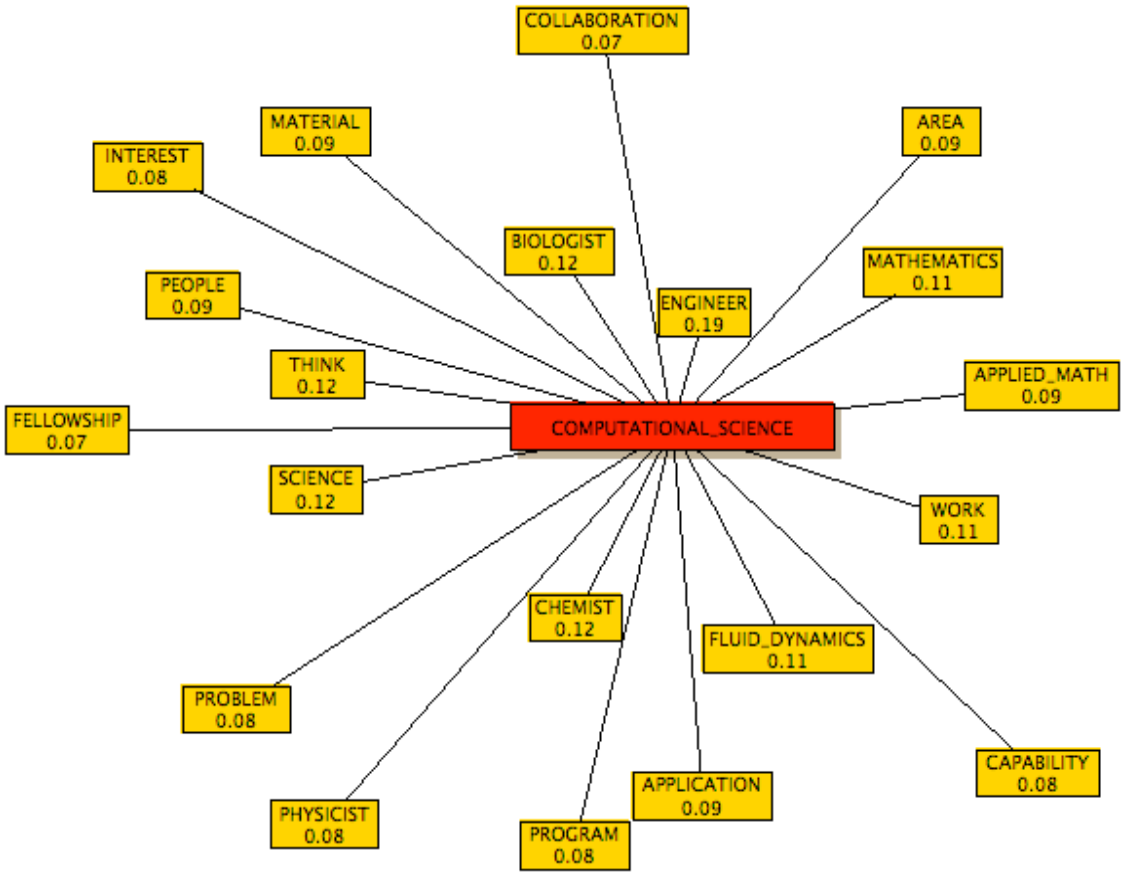
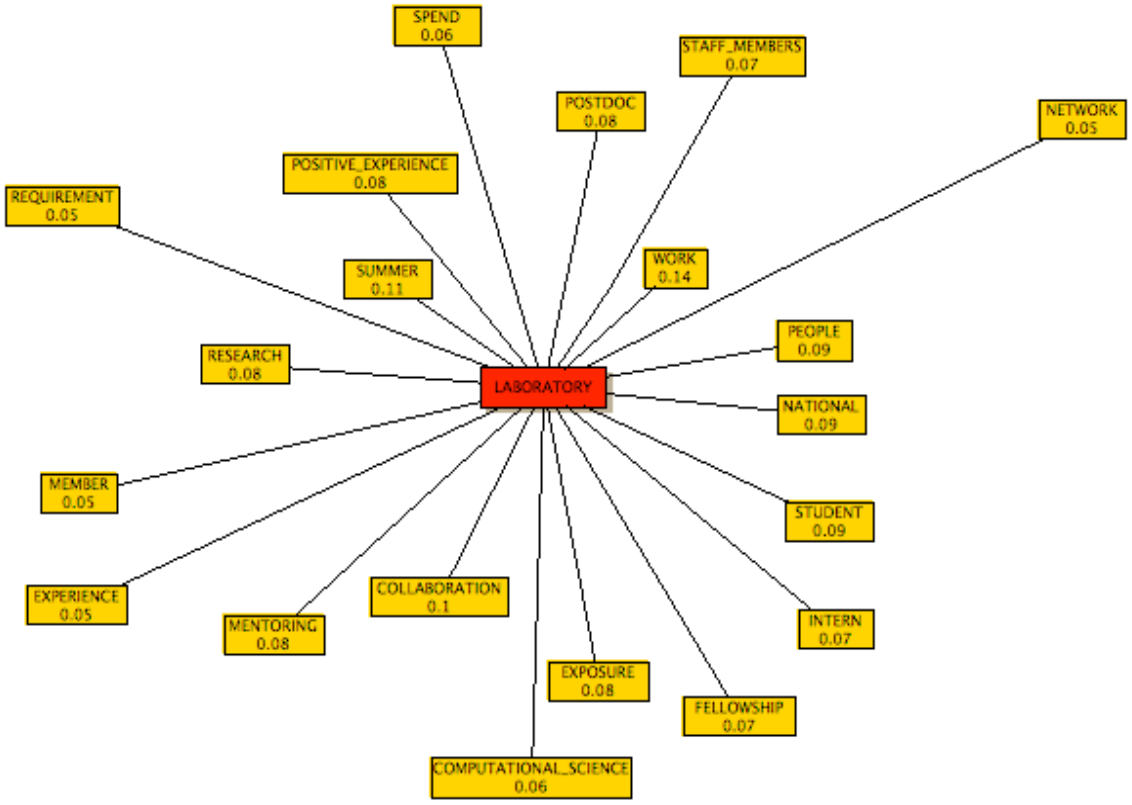


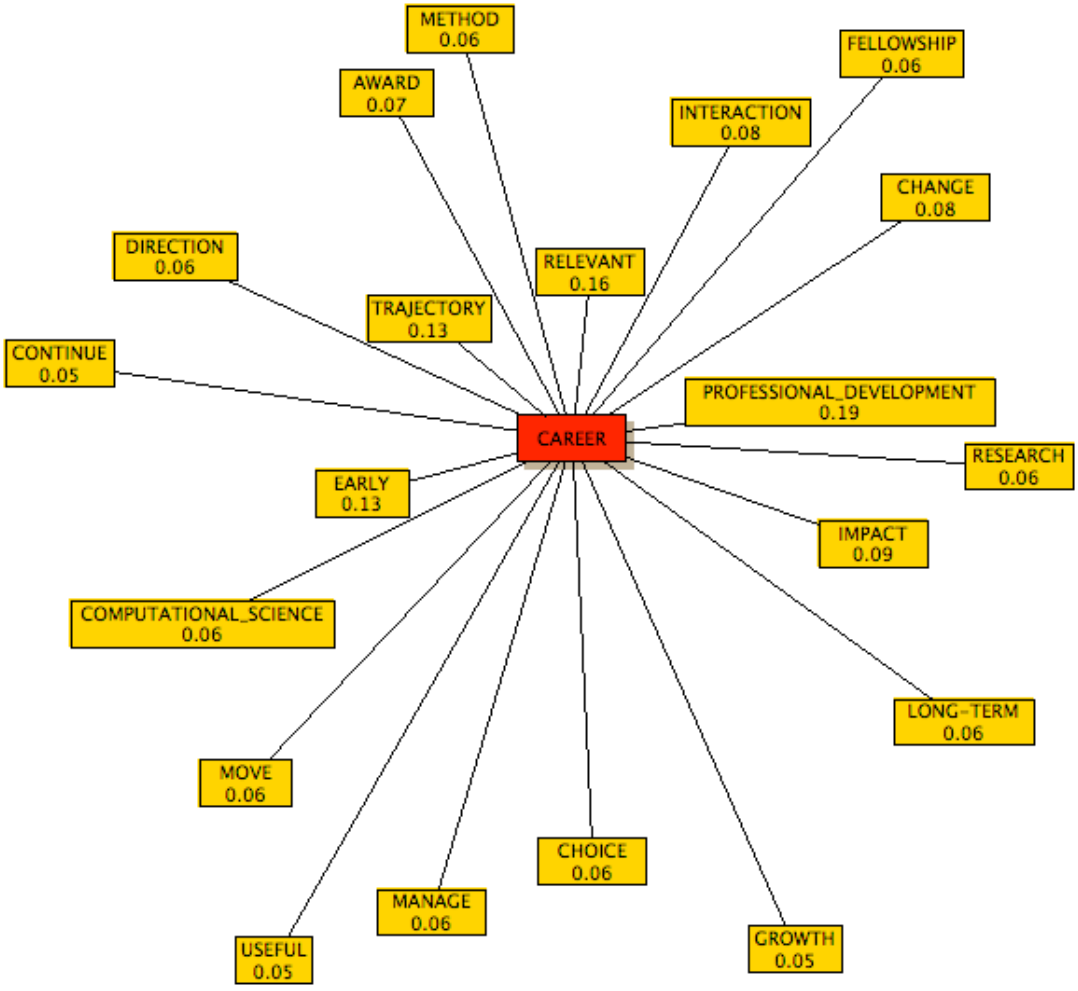
Figure 24 shows associations with *laboratory*. Again, these relationships follow expected patterns since the majority of practicum experiences take place in one of the national laboratories. Their influence is evident in the strong associations with the terms *summer, exposure, intern, fellowship*, and *positive experience*. Moreover, a quarter of the Fellows interviewed went on to careers in national laboratories, reflected in *work*, and the associations with *collaboration* and *mentoring* extend to both practicum experiences and career decisions.

Figure 24. Associations with Laboratory



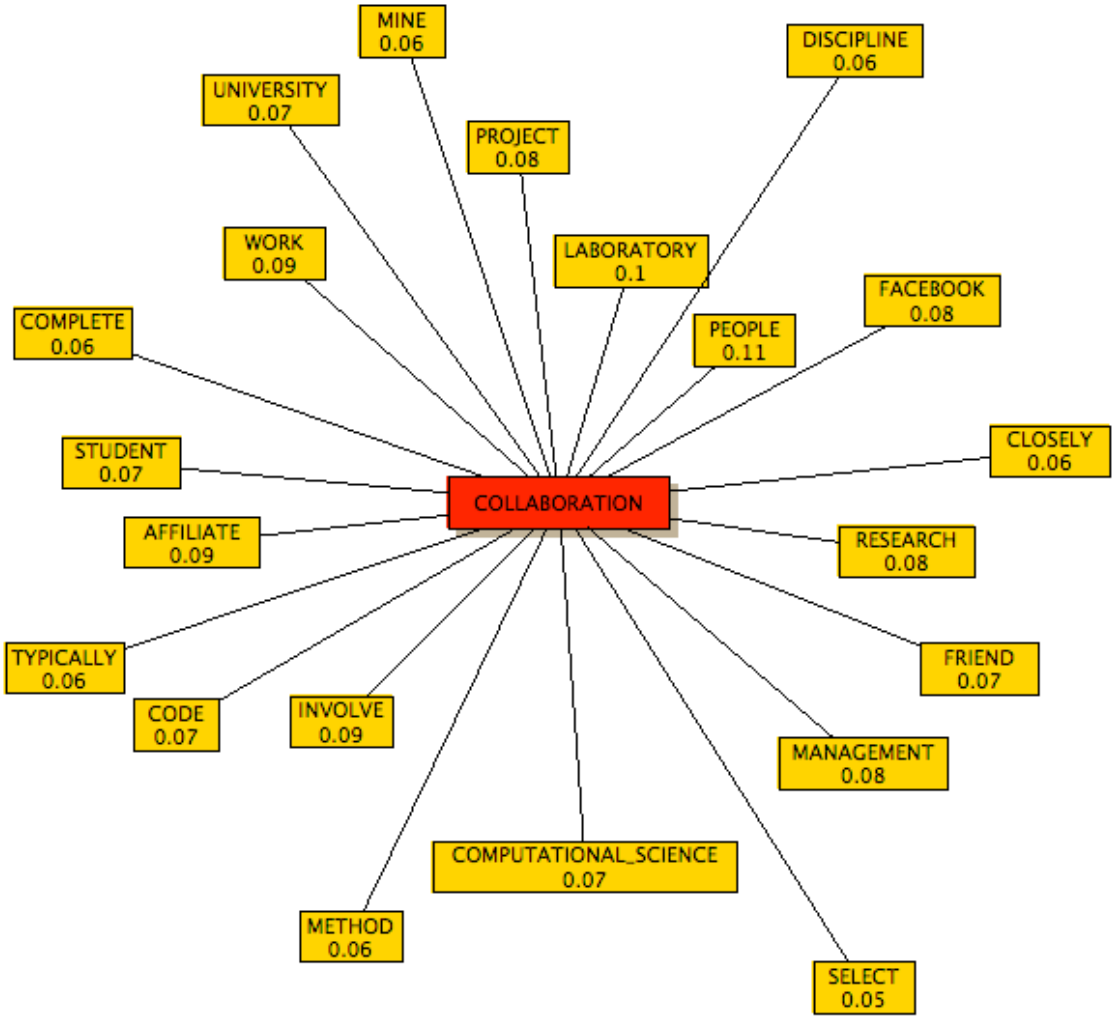
In regard to *career*, the strong associations with *relevant, fellowship*, and *computational science*, as shown in Figure 25, are especially worth noting given their pertinence to the current study. Moreover, strong relationships between *career* and *change* and between *career* and *impact* suggest their importance to Fellows in their chosen careers.

Figure 25. Associations with Career



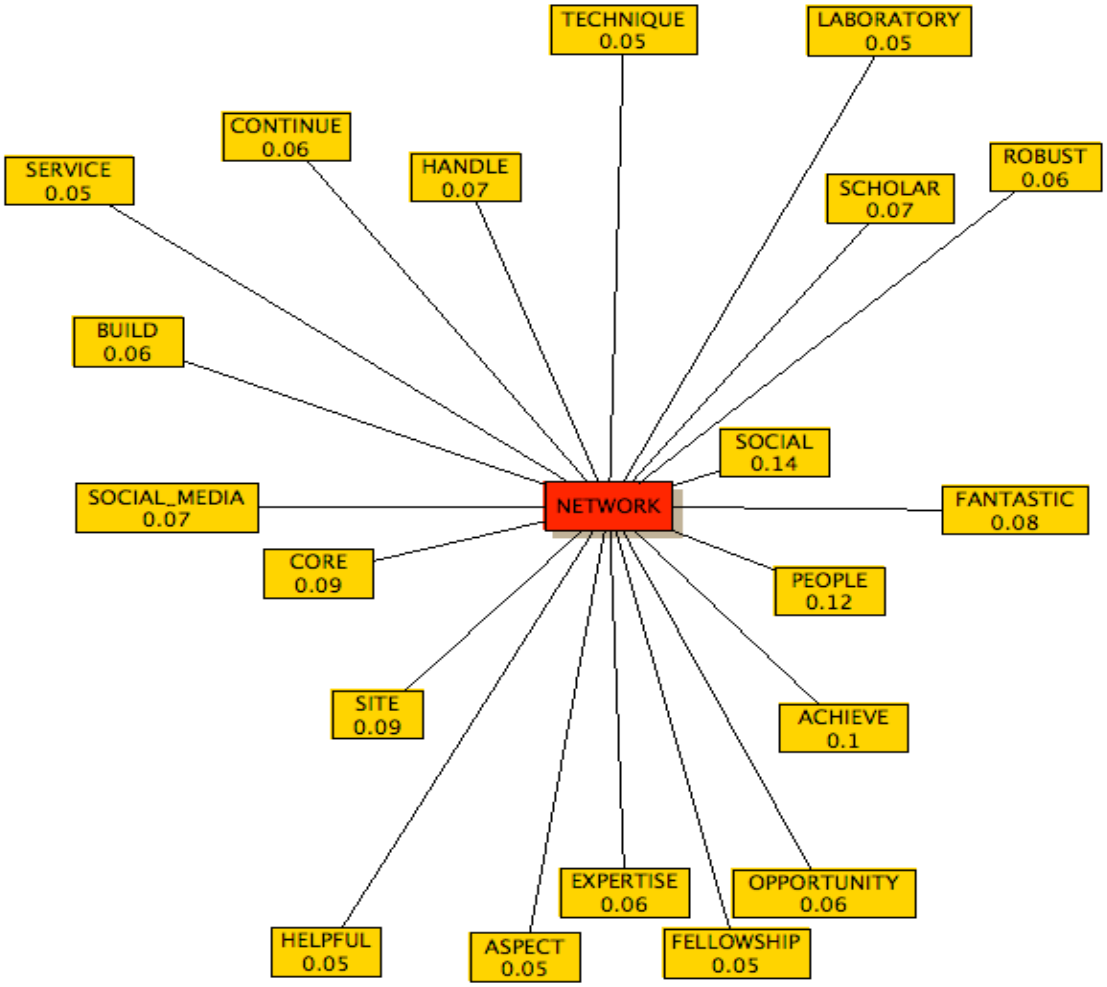
As can be seen in Figure 26, *collaboration* too shows a strong association with *computational science*. Interestingly, *Facebook* also is strongly associated with *collaboration*, highlighting the role of social media. The association between *laboratory* and *collaboration* is especially notable in that a number of interviewees spoke about the opportunities their practicum laboratory experiences afforded for collaboration.

Figure 26. Associations with Collaboration



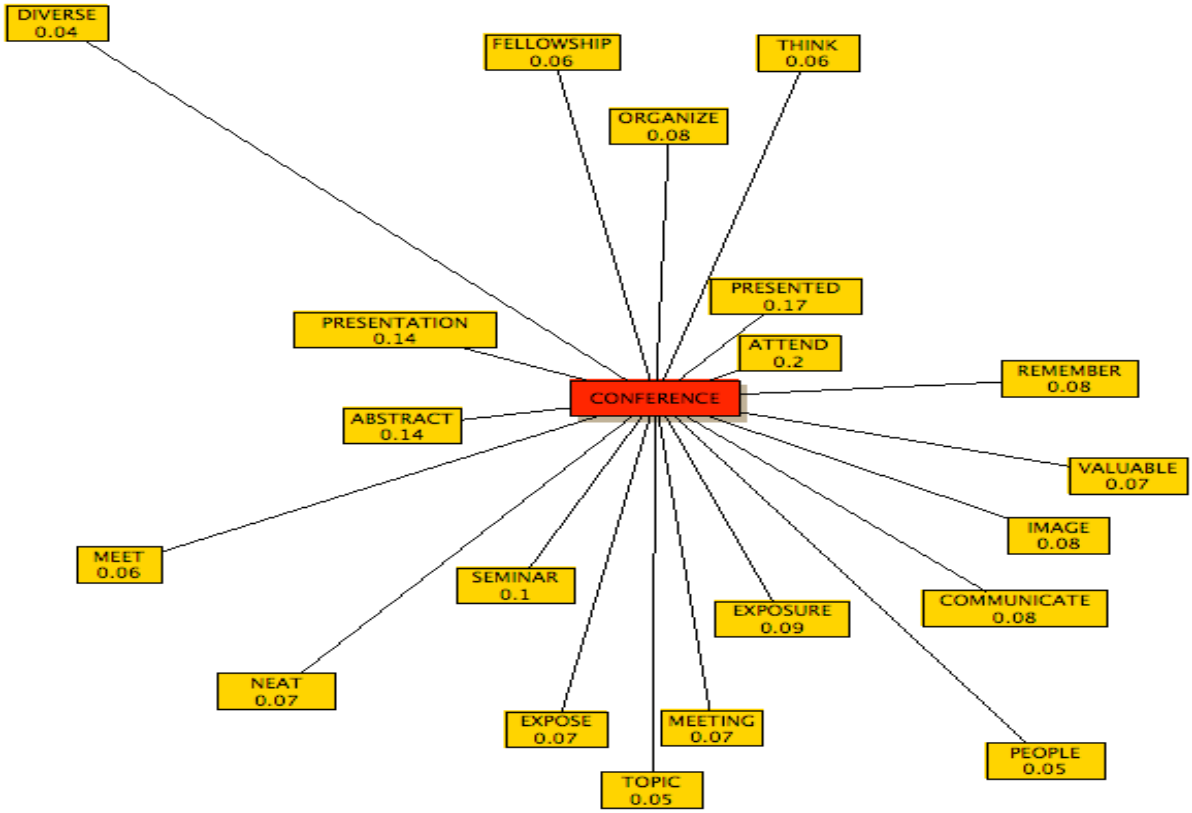
The keyword *network*, represented in Figure 27, also provides a good comparison point with *collaboration*, given its different associations within the corpus. The network of scholars and Fellows were represented through the terms *big, robust, fantastic, helpful*, and *fellowship*. Other references were represented through the terms *social* and *social media*; in fact, the strongest relationship with *network* was with the *social.* Note that all expressions related to *network* were positive.

Figure 27. Associations with Network



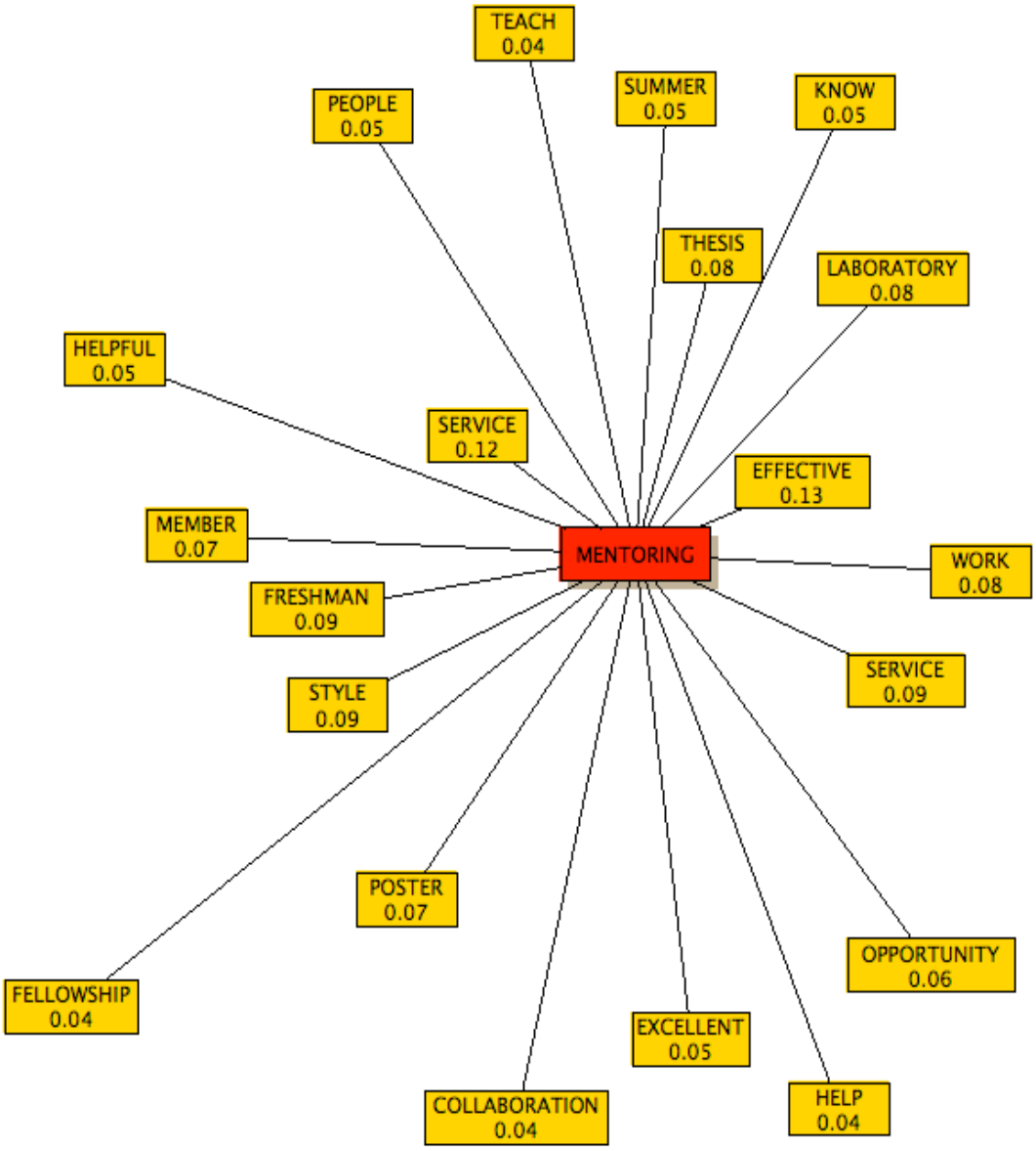
Associations with *conference*, shown in Figure 28, followed traditional lines and emphasized the various aspects of the annual CSGF conference. *Abstract, presentation, attend, seminar, organize*, and *meeting* describe involvement at or with the *conference*, while strong associations with *valuable* describe thoughts and assessments on the *conference.* Of course, it also has a strong association with *fellowship*.

Figure 28. Associations with Conference



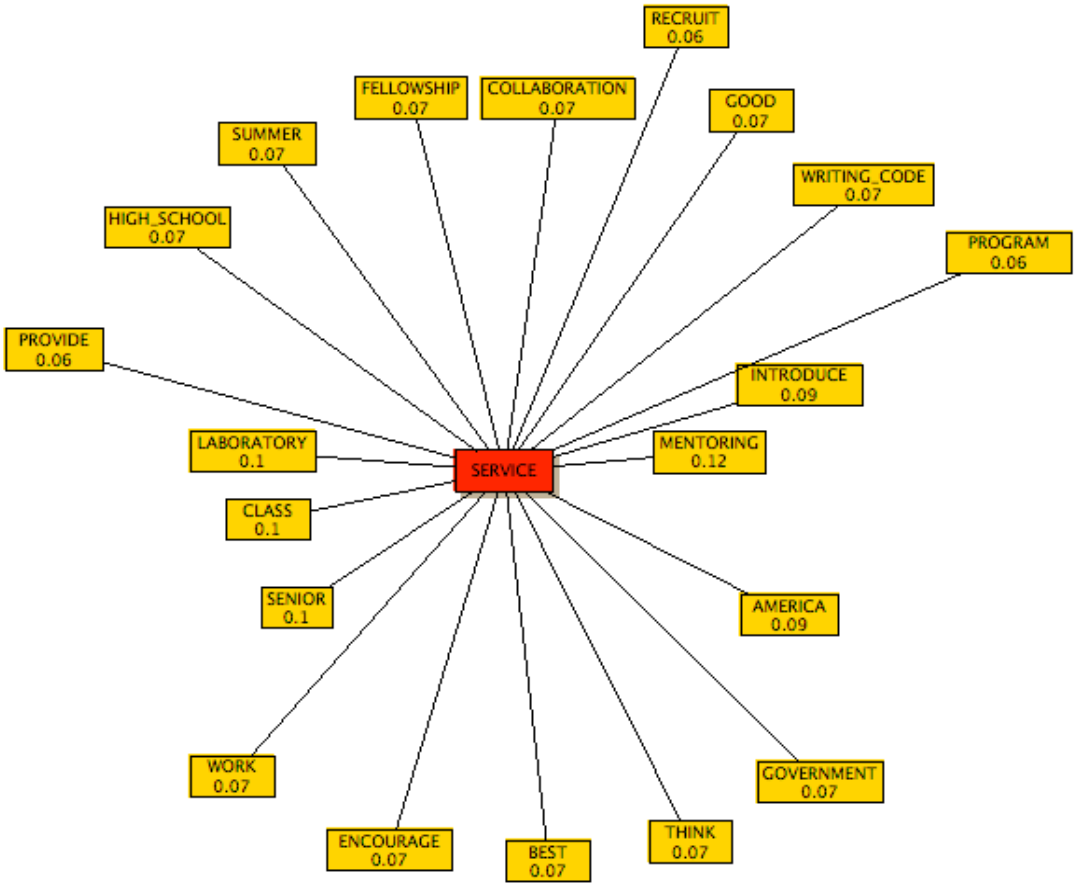
High level associations for the word *mentoring* span the range of the mentor/mentee relationship, as reflected in Figure 29. Thus, *service, teach, effective*, and *work* as well as *helpful, summer*, and *thesis* are all attached to *mentoring*. The strongest association was between *mentoring* and *effective*.

Figure 29. Associations with Mentoring



Interestingly, as seen in Figure 30, the strongest association reflected with *service* was *mentoring*. Both *mentoring* and *writing code* express forms of service, while *high school, summer, class, fellowship, and laboratory* all express periods or places where individuals might performed service.

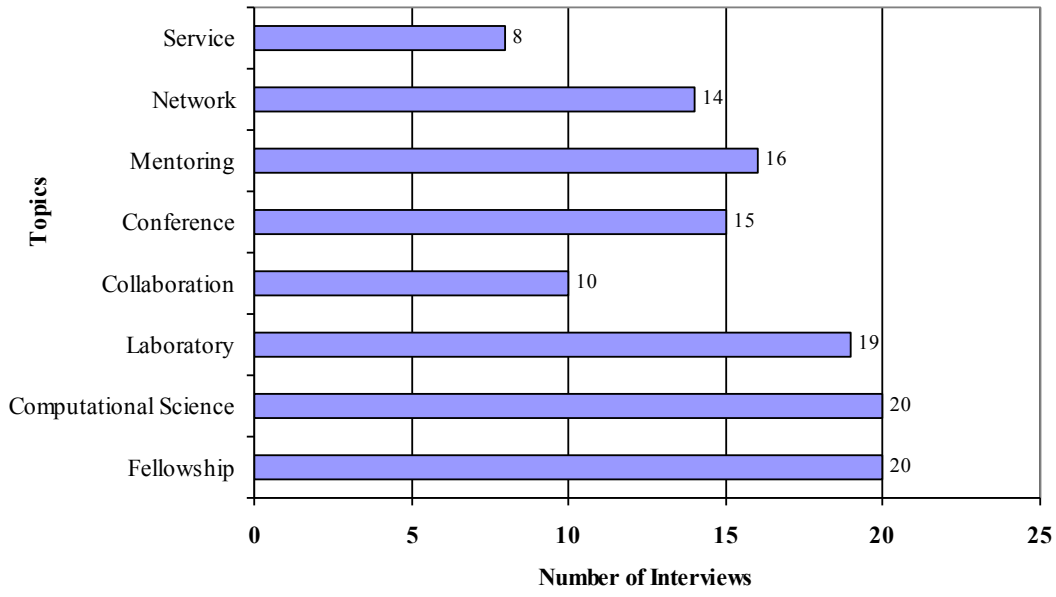
Figure 30. Associations with Service



Concordances

To further facilitate interpretation of terminological significance within the context of interview statements, a concordance analysis — consisting of in-context searches — was performed on the keywords as delineated above. As can be seen in Figure 31, *fellowship* and related words were present in all 20 interviews, as was *computational science*. *Laboratory* was found in 19, *collaboration* in 10, *conference* in 15, *mentoring* in 16, *network* in 14, and *service* in 8. More than simply understanding the number of interviews in which these terms were present, which indicates their centrality and importance relative to DOE CSGF impact, this analysis also considers how they were used in the interviews and provides representative examples of Fellow statements.

Figure 31. Interview Topic Concordances



Fellowship

The Fellowship was discussed by the interviewees also in terms of their experiences and views of its effects. For instance, as expressed by one Fellow,

> *If you're stuck in your pigeonhole, which is what science is, to some extent, more and more becoming, you're not exposed to these ideas.*

And the DOE CSGF kind of breaks you out of that because of the course requirements, because of the practicum, because of the conferences, because of everything.

Regarding perceptions about the purpose of the fellowship, the following statement also captured a broad sentiment of several of the interviewees.

If the purpose of the fellowship was to encourage people to get involved in computational methods and perhaps support DOE work, from my perspective it was just about perfect, because that's exactly what it did for me. I've never worked anywhere other than DOE labs.

Taking it a step farther,

Yes, that's kind of different because, to some extent, I think the DOE CSGF was trying to create people who don't naturally exist in the academic environment, and I think that was one of the more exciting aspects of it.

In terms of overall feelings on the fellowship, nearly all were positive, indicating that it was a career changing experience.

The Fellowship really had a direct impact on the direction I took in my career…. Had I not had the fellowship, I might have selected a different advisor, worked on something else, and so it definitely started my career off in a certain way, and I'm glad it also forced me to take classes in computer science and, I guess, applied math. Since I'd already done a master's in math, that wasn't really an issue, but it did also, I suppose, help me get started on interdisciplinary work, which I continue, obviously, to this day.

The Fellows commonly spoke about the DOE CSGF in comparison to other fellowship programs and providers, such as from the National Science Foundation and the Department of Defense. Although the most common comparisons made related to the amount of funding provided, other issues such as requirements, conferences, and networking were

also described. For most, the DOE CSGF provided an experience that could not be replicated.

> DOE *CSGF is very unique, and if DOE CSGF does not exist, there is no replacement in terms of the absolute topnotch computational science graduate program. It is not a valid substitute to say NSF or DOD or any of these other programs because none of them have the deeply invested pedagogical intervention that it offers.*

The importance of funding also was stressed in terms of recruiting students to pursue CSE.

> *What it illustrates, though, is students do have to think about funding, and so when the government provides, in this case through the Department of Energy, a fellowship, they are really giving serious encouragement to those students to go into a certain area. So, if the government wants to develop a certain area, like computational science, then this really does help. It certainly put me on that path, and I might not have gone on that path otherwise.*

In speaking of the future of the program, many of the interviewees were willing to participate and support it or were already involved. The following statement is an example of just how strongly some Fellows felt about their experience.

> *Well, I just really hope that the DOE CSGF program continues. If there's anything I can do to help make it continue, then I'll do that, because there isn't a fellowship program that's as good, as well managed, as well defined. I think the goals and objectives of the DOE CSGF are so clear, and I think the way that they're carried out are more clear than any other fellowship there is, and I think other fellowships should learn from the DOE CSGF. For that reason, I'll do anything to make sure the DOE CSGF continues.*

Computational Science

On the relationship between DOE CSGF and computational science, most participants were highly supportive of the program for recruiting students to the field:

If I ever run across somebody who is interested in computational science, I always think of the DOE CSGF first, because it was a really wonderful experience and I enjoyed almost every minute of it.

Furthermore, how the alumni Fellows saw themselves within CSE and whether or not they considered themselves computational scientists was a topic of interest, with many stressing the relationship to various disciplinary fields.

That's a really interesting question, and a difficult one, actually. I think of myself as a computational biologist, and I think of computational biology as a computational science.

From all indications in the interviews, DOE CSGF alumni are leaders and innovators in their respective fields and in the area of computational science in general. Many are involved in projects across sectors from academia to national laboratory work, and to industry as well in areas such as finance and social networking. Moreover, they think of themselves in transformative terms, as pushing the boundaries of their fields of study.

I really want to be part of the group of people that tries to resolve these questions and lays the groundwork for the next epoch of computational science in chemistry and material science.

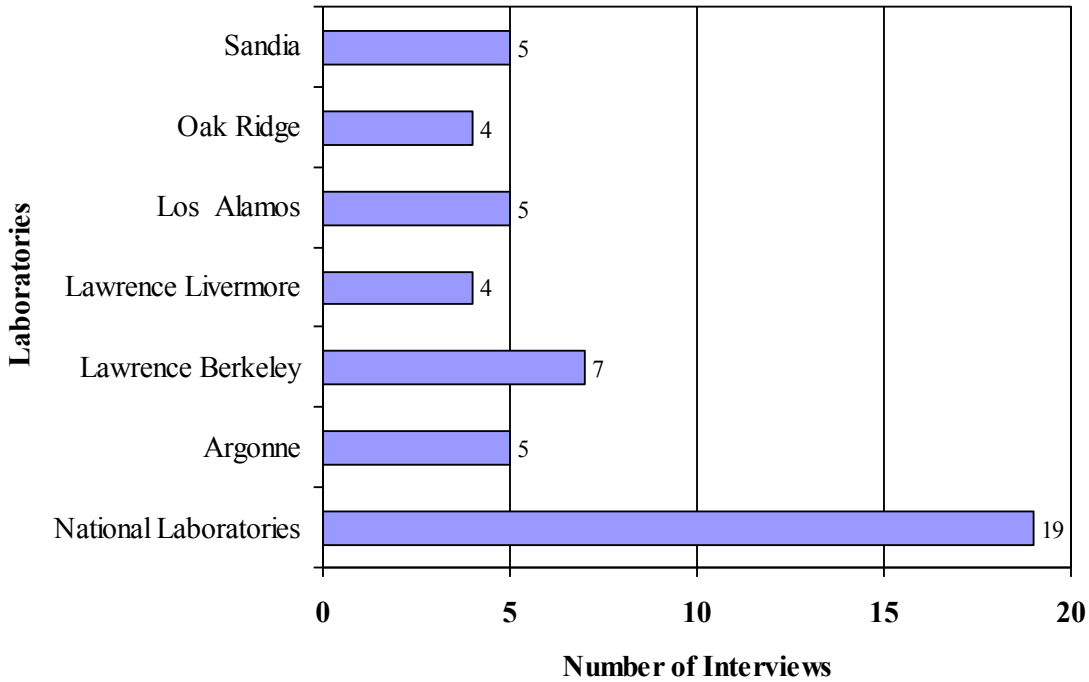
They also are considering change in a variety of ways, including thinking about what they do as affecting their fields in other terms, as expressed here:

Transformational is a really strong term. I don't know if anything I'm doing is transformational. I do think that there need to be more women in computational science, so I think about it in that sense — about running a lab that's all women, that's all computation, and having the women be the system administrators — because when you stereotypically think of a system administrator, you don't think of a woman.

Laboratory

Laboratory-related references, including the names of the various national laboratories, came up repeatedly in the interviews, in part because at least a third of the interviewees currently work at one of the laboratories and because they were the sites where most Fellows fulfilled their practicum requirement. While national laboratories were referenced in general in 19 interviews, as shown in Figure 32, individual laboratories were specified in 4 to 5 interviews, and Lawrence Berkeley was talked about most often, with references in 7 interviews.

Figure 32. Interviews Specifying National Laboratories



The general feeling about the practicum was expressed in the following comment:

> *To me, my practicum experience especially represents the right way people should do computational science, period – and, therefore, is something that should be templated.*

It is clear that the practicum had a significant impact on many of the Fellows, due in large part to the mentoring that often went hand in hand with the practicum. In some cases, such as the one mentioned below, the Fellows even went on to replicate their experience based on the value they saw in it.

> *I tell them that, as a recruiting tool, to say look at the breadth of expertise… and this is true at all the national labs, but of course I'm a little bit biased towards Argonne. This environment is unique compared to academia, and it was something that I learned at PNNL, and I try and make sure that it exists here.*
>
> *The model of academia is a mentoring of one to N, meaning one faculty member teaches N students…. First of all, the student will never be able to get enough time with the faculty member if they're competing with N other students and, second, you're entirely limited to whatever that faculty member knows. Whereas in the national lab, with there being hundreds of staff members and only dozens of interns, for each intern there can be one to five staff members who might be helping them on a regular basis and teaching them in the way that I was taught.*
>
> *So I'm a huge advocate of the practicum experience model for interns, and that's why I try and make sure that, whether or not they're DOE CSGFs, that all of my interns basically get that experience.*

Since an important part of the DOE CSGF mission was to develop a pool of computational scientists and engineers for the national laboratories, it is of little surprise that the practicum also was used to not only cultivate these individuals, but also to acclimate them to such environments.

> *I had such a great experience on the practicum and thought, this is someplace where I know I fit in. I've got friends here, I have the support infrastructure, and I can see myself being successful.*

Career

According to many of the Fellows, the DOE CSGF was an important influence on their career paths. Statements like the following showed up repeatedly:

> *Just basically the entire trajectory of my career so far wouldn't have happened without DOE CSGF.*

Similarly,

> *I am very grateful for the DOE CSGF support that I enjoyed at a very early stage in my career. It gave me the independence to work on high-risk and high-reward research as a graduate student and helped me get started on a career in computational science and collaboration with DOE.*

Even those who did not draw a direct link between the Fellowship and their careers still saw it as helpful in the grand scheme of things.

> *I don't think my advisor liked the fellowship so much after I was in it because it did require so many classes to be taken. In hindsight, as a student, I like that because it did kind of push me into other areas and, you know, I had to take a ton of computer science, and I wouldn't have probably taken that otherwise, and it's ultimately been good for my career.*

Collaboration

Discussions of collaboration went beyond mere reference to collaborating on a research paper or project to address the collaborative role of a computational scientist or engineer as part of a team. For example,

> *If we add a new development, then it's usually done in collaboration with the support engineers because they'll be the ones talking with the customers and understanding what exactly their need is. Then they will work with us, the software developer engineers; we will*

together put together a plan of how we can satisfy the customer's needs.

Some Fellows also expressed different viewpoints on being a computational scientist. This point is made below while a Fellow notes how universities use collaborations between departments to fill gaps.

Different places are handling it differently. Some places hire people; some universities hire people. Some universities set up collaborations between CS and biology, and all these things are being tried, and people are definitely making progress. But part of the problem is the senior people have to start appreciating the computer science and the computational biologist people as colleagues, not as service providers.

Conference

The conference was another prominent aspect of the program about which three-quarters of the interviewed Fellows spoke.

I think the best part about it for me was attending the conferences and just getting to see all the different kinds of problems that computational science can address.

Although attendance at the conference is required for new students, many alumni Fellows continue to participate in it because of the opportunities to network, to see friends, and to hear and discuss information on relevant scientific topics.

I have attended DOE CSGF every single year that I have been invited to go, and I intend on attending it every year as long as I am able.

Also mentioned in Section II of this report, one individual offered a suggestion for changing the conference from the Washington, DC, area, as indicated below.

That was one thing I would suggest changing…. Going around to visit the various labs I think would be tremendously helpful, or perhaps on a semiannual basis. But the content of the conferences

is always good. The contacts you get through the Fellowship are always very good. It's very generous compensation, so I wouldn't change that or the practicum.

Mentoring

Two-thirds of the interviewees mentioned mentoring relationships, either having a strong mentor or acting as one. Several DOE CSGF alumni served as mentors in part because of the mentoring they received and thought it was their duty to give back. Also, of those who were acting as mentors to university students, most had encouraged their mentees to apply for the DOE CSGF.

My point is that, going all through this, there's been lots of mentoring that people have taken the time to do for me, and part of that then is there's a certain expectation to pay it forward. I can't pay those people back for taking the time out of their schedules to do it, but I can certainly pay it forward.

As often as the topic of mentors came up in relation to academia, it occurred even more in relation to the practicum. This is because of the nature of the experience and the fact that it is the ideal environment for providing a host of potential mentors for a student.

It was such an amazing experience to be in a work environment where, as opposed to academia, they actually have people whose job it is to help others do stuff they don't know how to do. The computer people there…taught me basically everything I know about compilers, parallel computing, debugging, and programming language.

It is worth noting that some practicum team leaders were mentioned in several interviews, accompanied by praise and gratitude for the impact they had on future work and directions.

This is one thing that I'm very happy that I have been able to leverage having a very large number of people whom I consider my mentors.

My practicum advisor is at the absolute top of my list.

Network

The vast majority of interviewees talked about networking in some way, including networking opportunities at conferences, how networking with other Fellows aided in job placement, and the role networking played in collaboration efforts.

> *Even without the perks of the funding or whatever, it was just a great network, and it is a great network to have.*

Social networking too was an important topic that arose in several interviews. One Fellow in particular talked about their career and how they used computational science in the creation of social networking sites.

> *Right now, basically, I'm using somewhat similar techniques to model how people, users, behave in social networks and social media. The abstraction there is that instead of having a group of neurons that talk to each other via chemical synapse, you have real people, and they talk to each other through social media or Facebook or whatever.*

Service

Service — and volunteering in particular — also are related to the notion of giving back to society, and the interviewees tended to embrace this idea, especially in regard to sharing what they had learned. Mentoring, again, was especially discussed in terms of service and was the issue raised most frequently in this regard.

> *I've been fortunate enough to have excellent mentors in my own experience, so a lot of it has been sort of through osmosis, seeing how they have mentored students in the past, and realizing that you need to focus on what is good for the student and good for the mentored more than what is good for you as the mentor. So I try to say what do I need to provide to let you get your work done and then, beyond that, try and get out of their way so that I'm not a hindrance to them. But if they want help or advice or guidance in anything, I try to provide that as best I can.*

General Comments

Based on interviews with 20 random DOE CSGF recipients, the analysis and comments offered in this section are not meant to be exhaustive. Rather, they are linked to and provide "texture" for the overall study, helping to illustrate the underlying structures and dynamics that determine the bigger picture. The interviews were semi-structured, on the one hand, to provide more detailed information on the issues pursued in the survey and CV analyses on the DOE CSGF recipient outcomes and programmatic impacts. On the other hand, open-ended questions and flexibility were built into the interviews to allow for clarification, participant expression, and sensitivity to varying experiences, interests, and opinions.

All of the interviewed Fellows spoke highly of their Fellowship experience, and almost all made similar mention of their practicum. Usually, they mentioned the practicum site by name and described the nature of their work and their advisor. Almost all — 19 of the 20 — also described what they considered other valuable features of the program, most commonly the course requirements and the funding. Moreover, these points also were used to draw points of comparison and to distinguish DOE CSGF — in very positive terms — from other fellowships.

Most interviewees suggested that they are leaders in their respective fields and chosen professions and are working on projects that they described as innovative with the potential to impact the future in positive ways. Explicitly pointing to their scholarship as such, references to, for example, recognition and awards for groundbreaking research, patents, and the establishment of cross-disciplinary projects and programs were made by the Fellows. Interestingly, especially given concerns about recipient roles and Fellowship impacts, discussions of scholarship were framed largely in terms of practical applicability. Knowledge creation in particular was tied explicitly to broader impact and societal benefit. The Fellows appeared, as a whole, to be very driven and high achieving, with clear future goals for themselves and their work. Also, while not typically discussed directly as such, community building too was evidenced in references to recruitment, mentoring, collaboration, and networking activities with other Fellows.

Conclusion

STEM workforce capacity has been a prominent topic on policy agendas in the U.S. and elsewhere, and calls for computational expertise and HPC resources in particular have been growing in prominence in both public and private spheres. Indeed, already back in 1991 in response to related projections for its own workforce needs, the DOE established the DOE CSGF program to ensure an adequate pool of individuals trained in computational science and engineering. Over time, DOE CSGF has played a critical role in educating and training scientists for DOE laboratories and for other government agencies, academia, and industry. Indeed, the DOE CSGF represents a major investment in STEM in service to the country. Reaching across disciplinary boundaries, it is a fundamental force in knowledge creation, development, and application. It has played "a key role in training the next generation of researchers who are skilled in harnessing the potential of high performance computing to advance science and engineering."[39] Aimed at developing and maintaining the computational and computing infrastructure, including HPC resources and tools, the DOE CSGF provides resources to ensure that DOE's and other national laboratories are engaged as sites of research and mentoring for computational scientists and engineers.

Managed by the Krell Institute, the DOE CSGF program has consistently garnered high praise by recipients. The superior benefits and opportunities that the DOE CSGF offers have made it one of the most sought-after and effective fellowships available in terms of support, education, and training in related fields and otherwise. They also have operated to maximize contributions to knowledge and community building and to the broader DOE mission. The rigorous approach employed by the DOE CSGF is unmatched and the curricular and laboratory practicum requirements facilitate translating knowledge into discovery and practice. At the conferences, in addition to presenting their own work, Fellows learn about other kinds of research undertaken by their colleagues and have opportunities to interact with each other, DOE laboratory managers and personnel, and other CSE experts,

[39] From a 7 March 2011 charge letter for a review of DOE CSGF to the ASCAC Chairman from the Director of the DOE Office of Science.
[http://science.energy.gov/~/media/ascr/ascac/pdf/meetings/mar11/Csgf_ascac_charge.pdf]

including those who serve on DOE CSGF selection and steering committees. Not only does the Fellowship offer a comprehensive education and training opportunity, it does so across fields. It requires that students expand their limits; they must reach beyond their specific disciplines to develop an understanding of the broad application and importance — indeed, the necessity — of computational approaches in solving the problems of today's increasingly complex and expanding world.

Furthermore, scientific productivity today is a highly networked, dynamic, and interactive process. Indeed, scientific and technological innovation in today's complex world is, almost by definition, the result of collaboration and teamwork (Rykroft and Kash 1999). The digital domain in particular offers innovative ways to collaborate and communicate findings, extending networks and productivity. Social media and online networking have been recognized as important means for community building and, more, for enhancing productivity. Online social networks — whether mainstream or targeted specifically to scientists — offer mechanisms for researchers to meet and exchange ideas. In contrast to traditional scientific communities, especially those based primarily on face-to-face contact, such mechanisms facilitate interaction, communication, and the diffusion of knowledge across time and space (Ginsparg 2011). Moreover, in addition to digital networks, tools like blogs and wikis are increasingly popular means for disseminating research findings. Characterized particularly by collective intelligence and shared knowledge, this environment has been referred to as Science 2.0 (Tapscott and Williams, 2008). Although, in keeping with convention, the issue of publications as career indicators was broached in Section III, diverse media today serve as avenues for dissemination to reach broad audiences and the Science 2.0 environment also renders notions of scientific productivity much more complex than traditional notions based on stock indicators like publication counts.

In the face of new dynamic and interactive ways to conduct and disseminate research, the Krell Institute has supported several digital networking sites for Fellows, including web meetings, Facebook and LinkedIn groups, and private wikis for past and current Fellows and "friends of the program." The Krell Institute also has undertaken

various tracking efforts as part of its efforts to maintain contact and encourage the involvement and participation of former Fellows. Additionally, DOE CSGF print and online publications — featuring articles on practicum experiences, projects at the DOE laboratories, Fellow profiles, research collaborations, events, etc. — offer further means for continuing communication.[40] Together with face-to-face networking at the annual conference and other sponsored events, such activities are critical to community-building efforts and to instituting CSE as a field.

The purpose of this study was to document the effects of the DOE CSGF on the individuals who were awarded the Fellowship between 1991 and 2011, as well as to understand the accomplishments and contributions of the Fellows to the scientific community and to society more generally. Taking all of the components of the study together, it is clear that DOE CSGF recipients can be characterized as playing important roles as computational scientists and engineers and as community builders and leaders. DOE CSGF recipients are arguably high achievers by nature and their successful outcomes and engagement of the Fellowship were to be expected, especially given the rigorous and competitive selection process and the continual evaluation and commitment required by the program. By linking individual elements with institutional and external realities and needs, the DOE CSGF program itself has operated to identify and involve individuals who might serve not only the field and their own professional goals, but also the national agenda and society more generally, both directly and indirectly. Accordingly, Fellows act as partners in providing support and assistance for fulfilling needs delineated in the DOE CSGF objectives. This point was supported across the research platforms and strategies, and reflected in both the overall and individual Fellow profiles.

Fellows use the program of study and the practicum to expand their research capabilities. Moreover, working with some of the top scientists in the world, the practicum also provides focused mentoring and recognition by and entrée into the growing CSE community. The generation of a "community of scholars" and the building of collaborative networks — notably, often across generational and

[40] E.g., *Deixis* magazine, *Deixis* online, community newsletters, etc.

disciplinary lines — has been a critical outcome of the Fellowship experience. Indeed, in addition to personal friendships, enduring collaborative relationships have been typical among the Fellows themselves. The salience of this point is grounded in recognition of collaboration as a principal factor determining scholarly productivity and efficacy.

The transformative service role of mentor was expressed consistently by Fellowship recipients. Mentoring was identified as a primary activity for Fellows — mentoring to students within their institutions and, significantly, also to students at other institutions who have established contacts through disciplinary and Fellow networks. In fact, formal and informal network development has been a central feature in support of mentoring relationships through the fellowship programs and the value of mentoring relationships has been indicated consistently by Fellows.

Fellows also reported high levels of service and leadership. While particularly true, as might be expected, in their professional associations among those who belong to them, Fellows also engaged in volunteer and other service activities outside of these venues (including, for example, community organizations, government agencies, local schools, etc.). As tutors, project leaders and participants, leaders and members on advisory boards and committees, and so on, the Fellows actively contribute to the overall societal wellbeing.

Through an exploration of career directions and outcomes that influence broader community development, the study presented here can help to illuminate affective factors for the development and implementation of Fellowship features for "growing" CSE talent. Furthermore, the productivity and impact analyses can serve to better contextualize the Fellow and program contributions. The multi- and inter-disciplinary nature of CSE offers avenues for integrating research to address related issues in a broader context, and more discipline-specific and discipline-spanning understandings of research, career interaction, and knowledge creation can generate relevant data for use by analysts and policy makers.

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Appendix A: Methodological Notes

As indicated, data for this study were drawn primarily from three sources: 1) a general survey, 2) Fellow curricula vitae, and 3) semi-structured interviews.[42] Whether referencing the survey, curricula vitae, or interviews, major limitations to keep in mind are problems of recall and perception and the point that not all issues were addressed equally by or for all Fellows in the samples. However, taken together as a comprehensive approach, they provide a roadmap and analytic direction for understanding the broader dynamics that shape the relationships and outcomes of interest.

- **Survey**

The 2012 DOE CSGF Survey was aimed at developing a comprehensive overview of individuals awarded the Fellowship during the 1991-2011 period. Meant to gather information on their Fellowship experiences and on their educational and career outcomes in particular, the survey instrument was designed as a broadly inclusive query on the Fellows across cohorts and doctoral fields. In an effort to provide at least a rudimentary sense of data continuity and to capture similar types of information, crucial survey components and questions were determined through an in-depth examination of the DOE CSGF program features and of related surveys previously conducted by the Krell Institute and of information already present in their DOE CSGF database. Also, the survey instrument design was informed by a review of literature on effective strategies for educational attainment and professional development and a consideration of assessment strategies for other prominent fellowship programs.[43] In general, a desire for future data comparability, tracking, and contextual placement dictated modeling the Survey instrument as much as possible in keeping with other database formats and categories.

The self-administered questionnaire was distributed electronically using individualized confidential links to 335 Fellows through an online

[42] Information was gathered separately via these means, but, ideally, future efforts will look to structure and combine them to increase the number of cases and general coverage.
[43] E.g., National Science Foundation, Ford Foundation, Gates Foundation, etc.

survey service.[44] The number of Fellows was determined by the availability of validated contact information and a number of tracking and contact efforts were undertaken to obtain as many responses as possible. Two information notices announcing the upcoming survey were first sent via e-mail in December 2011 to all Fellowship recipients with validated contact information, and the survey instrument was tested (and revised accordingly) during the first week of January 2012. The survey was launched via e-mail on 12 January 2012, with follow-up reminders on 19 January, 25 January, and 1 February. Telephone calls were also made to Fellows during this period to encourage participation, and a final reminder was sent on 7 February 2012, the last day of the survey. The total number of respondents was 236, for an overall 70% response rate to the survey.[45]

In general, the data collected through the Survey imparted information on the distribution of and relationship among the various instrument items regarding the characteristics of fellowship recipients along a variety of dimensions, as discussed in the main text. This information provided a basis for general assessments of Fellowship impact and Fellow accomplishments and the data was used to build a set of measures to characterize DOE CSGF participation and to determine the extent to which they relate to program participation and career trajectories. Straightforward contingency tables and cross-tabulations presenting frequency distributions and central tendencies, variation, and other pertinent information showing the relative associations and distributions of such items were developed as basic descriptive and analytical contributions allowing for a generally contextualized depiction of Fellowship recipient outcomes.

- **Curricula Vitae**

Curricula vitae (CVs) were coded to capture more focused individualized data.[46] They represent self-reports by Fellows on their careers and roles as computational scientists and engineers and as broader community members. The CVs were collected through various means. Their submission was requested on all of the Survey

[44] Survey Monkey [http://www.surveymonkey.com]
[45] See Appendix C for the survey instrument.
[46] See Appendix D for the CV coding protocol.

announcements and reminders, as delineated above; initial and follow-up telephone calls were made to Fellows requesting them; and intensive online searches were conducted to locate as many CVs as possible. As indicated in the main text, these efforts resulted in the collection of CVs for 170 Fellows.

Regarding the use of both the impact factor and Eigenfactor values for determining the top-ranked journals, both factors were used to provide a broader perspective and representation of journal status across Fellow disciplinary fields. (Also, as a technical consideration, the factors can be adapted for use within distinct disciplinary contexts.)

- **Interviews**

The interviews were conducted by telephone, generally lasting 1 to 1.5 hours. However, due to their open-ended and flexible structure, any given interview could last between 0.75 and 2 hours. Note that the interviewees were selected without intervention by or consultation with the Krell Institute staff; nor were they previously known by the researcher. The interviewee list was determined according to three basic criteria — cohort (fellowship year), degree field (discipline), and employer category — and individuals were randomly selected within delineated groups to achieve overall DOE CSGF representation. (Degree institution also was considered, but did not change the overall representation or sampling pattern.)[47]

[47] See Appendix E for Interview Guide.

Appendix B: Survey Instrument

The 2012 DOE-CSGF Survey

Survey Instructions

We are seeking information, at the request of the Department of Energy (DOE), from past and current recipients of the DOE Computational Science Graduate Fellowship (CSGF) for a study of Fellowship outcomes. Your participation is vitally important to this effort. Responses to this survey will provide insights on the education, careers, and Fellowship experiences of the Fellows. *All information that you provide will be treated as confidential* and will not be reported in any way that will allow individual identification without your express permission.

Survey Instructions

- The survey requires about 20 minutes to complete; please allow enough time to finish the survey in one sitting.
- Please respond as completely as possible. If you cannot answer a given question or part of a question, simply proceed to the next one and continue from there.
- Directions are provided throughout the survey. Note that not all questions will apply to all respondents and you may be asked to skip certain questions.
- You will have the opportunity to make additional comments throughout the survey. Please feel free to do so.

You may direct any questions to DOE CSGF Survey Information at Email Me or at 515-598-2723.

Thank you for taking the time to complete this survey.

The 2012 DOE-CSGF Survey

DOE CSGF Experience and Community Building

Your DOE CSGF status is

- ○ Current Fellow
- ○ Past Fellow

A1. Please rate how useful you found the DOE CSGF for the following items:

	Very Useful	Somewhat Useful	Neutral	Not Very Useful	Not At All Useful	N/A
Collaborative opportunities	○	○	○	○	○	○
Interaction with researchers in your field	○	○	○	○	○	○
Interaction with researchers in other fields	○	○	○	○	○	○
Opportunities to develop mentoring relationships	○	○	○	○	○	○
Intellectual stimulation and exchange	○	○	○	○	○	○
Knowledge attainment in other fields	○	○	○	○	○	○
Practical experience in other fields	○	○	○	○	○	○
Job attainment	○	○	○	○	○	○
Publishing opportunities	○	○	○	○	○	○
Professional growth and direction	○	○	○	○	○	○
Financial support	○	○	○	○	○	○
Appreciation of and identification with Computational Science and Engineering as a field	○	○	○	○	○	○
Other *(Please specify in the Comments box below)*	○	○	○	○	○	○
Please rate the overall usefulness of the DOE CSGF Fellowship	○	○	○	○	○	○

Comments

A2. Overall, how *satisfied* were/are you with your DOE CSGF experience?

	Very Satisfied	Somewhat Satisfied	Neutral	Not Very Satisfied	Not At All Satisfied	Do Not Know
Satisfaction with DOE CSGF experience	○	○	○	○	○	○

Comments

A3a. Have you ever attended a DOE CSGF Conference?

- ○ Yes
- ○ No *Please skip to question A4a*

The 2012 DOE-CSGF Survey

A3b. If you have completed your Fellowship, how many DOE CSGF Conferences have you attended since completion?

	None	1	2-3	4-6	7 or more	Uncertain
Number of DOE CSGF Conferences	○	○	○	○	○	○

A3c. Please rate the usefulness of the DOE CSGF Conference for the following items:

	Very Useful	Somewhat Useful	Neutral	Not Very Useful	Not At All Useful	N/A
Collaboration opportunities	○	○	○	○	○	○
Interaction with researchers in your field	○	○	○	○	○	○
Interaction with researchers in other fields	○	○	○	○	○	○
Opportunities to develop mentoring relationships	○	○	○	○	○	○
Intellectual stimulation and exchange	○	○	○	○	○	○
Opportunities to present your research	○	○	○	○	○	○
Opportunities for feedback on your research	○	○	○	○	○	○
Contacts for obtaining employment	○	○	○	○	○	○
Postdoctoral opportunities	○	○	○	○	○	○
Networking opportunities	○	○	○	○	○	○
Other *(Please specify in the Comments box below)*	○	○	○	○	○	○
Please rate the overall usefulness of the DOE CSGF Conference	○	○	○	○	○	○

Comments

A4a. Have you ever encouraged students and/or colleagues to pursue Computational Science and Engineering as a field of study?

○ Yes

○ No

Comments

The 2012 DOE-CSGF Survey

A4b. Have you/would you recommend the DOE CSGF to students?

- Yes
- No

If No, please indicate your reason(s).

A4c. If you have recommended the DOE CSGF to students, have any of those students applied?

- Yes
- No
- Do not know
- Not Applicable

Comments

A5. Collaboration with DOE CSGF Fellows

	Yes	No
A5a. Have you ever *contacted* another (current or past) DOE CSGF Fellow for information or advice?		
A5b. Have you ever *collaborated on research* with another (current or past) DOE CSGF Fellow?		
A5c. Have you ever *published research* with another (current or past) DOE CSGF Fellow?		

Comments

If you are a current DOE CSGF Fellow, please skip question A6 and continue to question A7.

A6. Collaboration after completing your fellowship

	Yes	No
A6a. After completing the Fellowship, have you ever contacted your DOE laboratory practicum supervisor or team members for information or advice?		
A6b. After completing the Fellowship, have you ever collaborated on research with your DOE laboratory practicum supervisor or another member of your DOE laboratory practicum team?		

Comments

The 2012 DOE-CSGF Survey

A7. Published Research

	Yes	No
A7a. Have you ever published with your DOE laboratory practicum supervisor?	○	○
A7b. Have you ever published with another member of your DOE laboratory practicum team?	○	○

Comments

A8. Mentoring

	Yes	No
A8ba. Have you ever been mentored by another (current or past) Fellow?	○	○
A8b. Have you ever served as a mentor to another (current or past) Fellow and/or others? *(If No, please skip to A8d)*	○	○

Optional Comments

A8c. How frequently have you engaged in the following aspects of providing mentoring to Fellows and/or others ?

	Often	Sometimes	Never	N/A
Opportunities to collaborate on research	○	○	○	○
Guidance/support for publishing	○	○	○	○
Opportunities for developing and obtaining research grants	○	○	○	○
Co-authored publications	○	○	○	○
Advice regarding professional survival and politics	○	○	○	○
Guidance/support for teaching, student advising, etc.	○	○	○	○
Opportunities to network with other scholars, publishers, editors, etc.	○	○	○	○
Opportunities to present research	○	○	○	○
Guidance/support for obtaining employment	○	○	○	○
Guidance/support for obtaining grants, contracts, fellowships, and other resources	○	○	○	○
Psychological or emotional support	○	○	○	○

Optional Comments

The 2012 DOE-CSGF Survey

A8d. To what extent do you value the following aspects of mentoring <u>that you have received?</u>

	Highly Value	Value	Somewhat Value	Do Not Value	N/A
Opportunities to collaborate on research	○	○	○	○	○
Guidance/support for my research	○	○	○	○	○
Guidance/support for publishing	○	○	○	○	○
Advice regarding professional survival and politics	○	○	○	○	○
Guidance/support for teaching, student advising, etc.	○	○	○	○	○
Opportunities to network with other scholars	○	○	○	○	○
Opportunities to present research	○	○	○	○	○
Guidance/support for obtaining employment	○	○	○	○	○
Guidance/support for obtaining grants, contracts, fellowships, and other resources	○	○	○	○	○
Psychological and emotional support	○	○	○	○	○

Comments

A9. Please rate the impact that your Fellowship has had on the following:

	High Impact	Some Impact	A Little Impact	No Impact	N/A
Your scientific research focus	○	○	○	○	○
Your computing capabilities	○	○	○	○	○
Other aspects of your research *(Please specify in the Comments box)*	○	○	○	○	○

Optional comments

A10a. Have you participated in any team development of scientific codes or scientific software suites?

○ Yes *(If Yes, please specify codes and software suites in the Comments box)*

○ No

Please specify codes and software suites

The 2012 DOE-CSGF Survey

A10b. Have you any developed open source scientific software?

- Yes *(If Yes, please indicate software names, as well as comment on who has used your software, in the Comments box)*
- No

Please indicate software names and who has used your software.

A10c. Have you ever contributed to any open source scientific software projects?

- Yes *(If Yes, please specify software projects in the Comments box)*
- No

Please specify software projects.

Please continue to Section B, EDUCATION.

The 2012 DOE-CSGF Survey

B. Education

B1. Please list all colleges (including 2-year) and graduate institutions you have attended as well as each degree earned (if any), including your doctoral institution(s) and degree(s).

B1a. Institution

Institution Name	
Branch or city of institution	
State	
Country (if not USA)	
Years attended (from and to)	
Major Field of Study	
Type of Degree Granted (B.S., M.S., etc.)	
Year of Degree	

B1b. Institution

Institution Name	
Branch or city of institution	
State	
Country (if not USA)	
Years attended (from and to)	
Major Field of Study	
Type of Degree Granted (B.S., M.S., etc.)	
Year of Degree	

B1c. Institution

Institution Name	
Branch or city of institution	
State	
Country (if not USA)	
Years attended (from and to)	
Major Field of Study	
Type of Degree Granted (B.S., M.S., etc.)	
Year of Degree	

The 2012 DOE-CSGF Survey

B1d. Institution

Institution Name	
Branch or city of institution	
State	
Country (if not USA)	
Years attended (from and to)	
Major Field of Study	
Type of Degree Granted (B.S., M.S., etc.)	
Year of Degree	

B1e. Institution

Institution Name	
Branch or city of institution	
State	
Country (if not USA)	
Years attended (from and to)	
Major Field of Study	
Type of Degree Granted (B.S., M.S., etc.)	
Year of Degree	

B1f. Institution

Institution Name	
Branch or city of institution	
State	
Country (if not USA)	
Years attended (from and to)	
Major Field of Study	
Type of Degree Granted (B.S., M.S., etc.)	
Year of Degree	

The 2012 DOE-CSGF Survey

B1g. Institution

Institution Name

Branch or city of institution

State

Country (if not USA)

Years attended (from and to)

Major Field of Study

Type of Degree Granted (B.S., M.S., etc.)

Year of Degree

B1h. Institution

Institution Name

Branch or city of institution

State

Country (if not USA)

Years attended (from and to)

Major Field of Study

Type of Degree Granted (B.S., M.S., etc.)

Year of Degree

B2. Please indicate your high school/secondary school graduation (or equivalent) year.

Example: 1965

B3.What is the state (U.S.) or country of the high school/secondary school you last attended?

B4. What was your academic standing at the time of your initial (successful) DOE CSGF application?

- Undergraduate student/Graduate school applicant
- First-year graduate student
- Second-year graduate student

B5a. Have you completed your doctoral degree?

- Yes *If yes, skip to Question B6*
- No

The 2012 DOE-CSGF Survey

B5b. If you plan to complete your doctoral degree, please provide the projected month and year of your doctoral completion. *Example: Month 06/Year 2013*

Month

Year

B5c. If you do not plan to complete your doctoral degree, please indicate the primary reason for not completing it.

B6. In your estimation, how many years of full-time study *(or the equivalent)* **were/will be required <u>after the bachelor's degree</u> to complete your doctorate?**

	3	4	5	6	7	8	9	more than 9
Equivalent years of full-time study	○	○	○	○	○	○	○	○

Optional Comments

Please continue to Section C, EMPLOYMENT/CAREER. If you have <u>not</u> received your doctoral degree, please continue to C1. If you have received your doctoral degree, please skip to C2a.

The 2012 DOE-CSGF Survey

C. Employment/Career

Please answer Question C1 if you have not yet received your doctorate . Otherwise, please skip to Question C2a.

C1. Please indicate in what sector you expect to find your main source of employment after receiving your doctoral degree.

- ○ Education
- ○ U.S. Government
- ○ Industry/Business
- ○ Private Foundation
- ○ Nonprofit, other than private foundation
- ○ Unknown
- ○ Other *(please specify in Comments box)*

Comments

C2a. Do you currently belong to any professional societies or associations?

- ○ Yes
- ○ No

Approximate number of professional associations to which you currently belong:

C2b. Do any of the professional societies or associations to which you belong represent fields/disciplines other than your primary field/discipline?

- ○ Yes *(please note in Comment box how many)*
- ○ No

Optional Comments

The 2012 DOE-CSGF Survey

C2c. Have you ever held any special positions/roles or performed special tasks on behalf of a professional organization in which you were a member? *Mark all that apply.*

- ☐ No
- ☐ Yes: organizational officer (e.g., president, vice-president, secretary, treasurer, etc.)
- ☐ Yes: board member
- ☐ Yes: section officer
- ☐ Yes: committee service
- ☐ Yes: Other *(please specify in Comments box)*

Comments

C3. In what other kinds of service and leadership activities have you participated?

If you have not completed your doctorate, please continue to D1.

C4a. Are you currently working for pay (or profit)? *This includes postdoctoral appointment, self-employment, or temporary absence from a job (e.g., due to illness, sabbatical, vacation, or parental leave).*

- ○ Yes *(If Yes, please skip to question C5a)*
- ○ No

The 2012 DOE-CSGF Survey

C4b. If you are not working for pay, what are your reasons for not doing so? *Mark all that apply.*

- ☐ Retired
- ☐ Suitable job not available
- ☐ Laid off from a job
- ☐ Student
- ☐ Family responsibilities
- ☐ Chronic illness or permanent disability
- ☐ Do not need or want work
- ☐ Recently completed degree and looking for employment
- ☐ Other *(Please specify in Comments box)*

Comments

C4c. If you are not working for pay, when did you last work for pay (or profit)? *Example: Month 02/Year 2009*

Month

Year

C4d. Have you EVER worked for pay or profit after receiving your doctoral degree?

- ○ Yes
- ○ No

Comments

C5a. After receiving your doctoral degree, has your primary employment ever been in a Computational Science and Engineering related field?

- ○ Yes
- ○ No

Comments

The 2012 DOE-CSGF Survey

C5b. After receiving your doctoral degree, have you ever had primary employment within the DOE? *Please mark all that apply.*

- ☐ Yes, in the DOE laboratory where I undertook my DOE-CSGF practicum
- ☐ Yes, in a different DOE laboratory from where I undertook my practicum
- ☐ Yes, in another DOE facility or office
- ☐ No

If your primary employment after receiving your doctoral degree was within the DOE, please specify the DOE laboratories, facilities, or offices in which you accepted primary employment.

C6a. Current/last Employment Sector: For what type of employer did you work during your current or last employment? *If you had more than one employer, please refer to your principal or primary job.* **Please mark one only.**

- ○ **Education:** U.S. 4-year college or university, other than medical school
- ○ **Education:** U.S. medical school (including university-affiliated hospital or medical center)
- ○ **Education:** U.S. university-affiliated or academe-related research institute
- ○ **Education:** U.S. 2-year college, junior or community college, or technical institute
- ○ **Education:** U.S. preschool, elementary, middle, or secondary school
- ○ **Education:** Foreign educational institution
- ○ **Education:** Other *(Please specify in Comments box)*
- ○ **Government:** Foreign government
- ○ **Government:** U.S. military service
- ○ **Government:** U.S. federal government (civilian employee)
- ○ **Government:** U.S. state government
- ○ **Government:** U.S. local government (city, county, etc.)
- ○ **Government:** Other *(Please specify in Comments box)*
- ○ **Private Sector:** Non-profit organization
- ○ **Private Sector:** For-profit company or organization
- ○ **Private Sector:** Self-employed or business owner
- ○ **Private Sector:** Other *(Please specify in Comments box)*

Comments

The 2012 DOE-CSGF Survey

C6b. What was your occupation (job title or position) on your primary current/last job?
Please be as specific as possible, including any area of specialization. (Example: College Professor - Computer Science)

C6c. Was your current/last job a postdoctoral appointment? *Postdoctoral appointment refers to temporary positions in academia, industry, or government, primarily providing additional education, training, or research opportunities.*

- Yes
- No

C7a. Is/was your current/last principal employer an educational institution?

- Yes
- No *(If No, please skip to question C8)*

C7b. If your current/last employer is/was an educational institution, please indicate your primary and secondary work activities.

	Primary	Secondary	Does Not Apply
Teaching			
Research and development			
Administration			
Professional services			
Other *(Please specify in the Comments box)*			

Comments

C8. If your current/last principal employer is not an educational institution, is it an academic-related organization or agency? (e.g., think tank, research center, etc.?)

- Yes *(Please specify in the Comments box)*
- No

Comments

The 2012 DOE-CSGF Survey

C9a. Please indicate your basic annual salary (before deductions) in your current/last principal employment position. ***(Do not include bonuses, overtime, or supplemental compensation. If not salaried, please estimate your earned income, excluding business expenses)***

- ○ Under $35,000
- ○ $35,000 - 49,999
- ○ $50,000 - 64,999
- ○ $65,000 - 74,999
- ○ $75,000 - 84,999
- ○ $85,000 - 94,999
- ○ $95,000 - 109,999
- ○ $110,000 - 124,999
- ○ $125,000 - 149,999
- ○ $150,000 - 174,999
- ○ $175,000 - 199,999
- ○ $200,000 - 299,999
- ○ $300,000 - 399,999
- ○ $400,000 - 499,999
- ○ $500,000 or more

C9b. Was this salary or earned income based on working full time?

- ○ Yes
- ○ No

Comments

C9c. If your current/last position is an academic position, please indicate the applicable salary period.

- ○ 9-10 months of salary
- ○ 12 months of salary
- ○ Other *(Please specify in the Comments box)*

Comments

The 2012 DOE-CSGF Survey

C10a. What effect have the following factors had on the rate of your career advancement or development?

	Positive Effect	Negative Effect	No Effect
Quality of education and training	○	○	○
Personal motivation	○	○	○
Family considerations	○	○	○
Mentoring support	○	○	○
Supplemental duties	○	○	○
Time demands	○	○	○
Support resources	○	○	○
Other *(Please specify in Comments box)*	○	○	○

Comments

C10b. Importance of the DOE CSGF experience for your career

	Very Important	Somewhat Important	Slightly Important	Not Important
How important has your DOE CSGF experience been for your career advancement possibilities?	○	○	○	○

Comments

C11a. While working at your current/last primary job, did you also have a secondary job? *(This can include part-time, evening, or weekend work)*

○ Yes

○ No *(If No, please skip to Question D1)*

Optional Comments

C11b. If you have/had a secondary job at your current/last primary job, what was your occupation (job title or position) on your secondary job? *Please be as specific as possible, including any specialization. (Example: Adjunct College Professor - Applied Mathematics)*

Please continue to Section D, PERSONAL BACKGROUND

The 2012 DOE-CSGF Survey

D. Personal Background

D1. What is your date of birth?

Date MM / DD / YYYY

D2. What is your sex?

- Female
- Male

D3a. What is your Race/Ethnic Self-Identification? *Please mark the race or ethnic group(s) with which you are principally identified.*

- Asian/Asian American *(Please specify in the Comments box)*
- Alaska Native
- Black/African American
- Native American Indian
- Native Pacific Islander
- White
- Mexican American
- Puerto Rican
- Other Hispanic *(Please specify the Comments box)*
- Other *(Please specify in the Comments box)*

Comments

D3b. Are you a citizen of the United States?

- Yes
- No *(If No, please specify citizenship in the Comments box)*

Comments

D4. What is (or what do you consider to be) your hometown and state (U.S.) or home country?

The 2012 DOE-CSGF Survey

D5. Parents' Education

	Mother	Father
Education drop down menu		

D6. What is/was your marital status?

	Marital Status
At the start of your Fellowship	
Currently	

D7. How many children did/do you have ?

	Number of Children
Children at the start of your Fellowship	
Children Currently	

Please continue to Section E, CONTACT AND FOLLOW-UP INFORMATION

The 2012 DOE-CSGF Survey

E. Contact and Follow-Up information

E1. What is your name?

E2a. Institutional Affiliation/ Work Address

Company:
Address:
Address 2:
City/Town:
State:
ZIP:
Country:
Email Address:
Phone Number:

E2b. Is this Institutional Affiliation/Work Address your preferred contact address?

- Yes
- No

E3a. Home Address

Address:
Address 2:
City/Town:
State:
ZIP:
Country:
Email Address:
Phone Number:

E3b. Is this Home Address your preferred contact address?

- Yes
- No

The 2012 DOE-CSGF Survey

E4. Other Connections

Email (if not already indicated)

Website 1

Website 2

Blog

Other

E5. Are you willing to participate in a formal interview concerning your education, DOE CSGF experience, career, and related accomplishments?

- Yes
- No
- Maybe

E5. Please use this space to provide additional relevant comments on your education, career, the DOE CSGF program, or other related issues, if desired.

THANK YOU!!!

Appendix C: Curriculum Vitae Coding Protocol

Category	Information	Definition/Values
Individual		
	ID	DB provided username
	Coding date	Date coding started
	Coder	Staff member coding the CV
	CV full or partial	Values: full, partial, unsure, bio statement
	First name	DB provided
	Middle name	DB provided
	Last name (current)	DB/CV provided
	Last name (previous)	Any previous names held, such as maiden name
	Race/Ethnicity (from CSGF records)	Drop down using census data choices from http://www.census.gov/population/www/socdemo/race/racefactcb.html
	Gender	Male/Female (if unsure, leave blank)
	Marital status (current)	From Census: http://www.census.gov/prod/2003pubs/c2kbr-30.pdf (SEE NOTE BELOW)
	Marital status at start of fellowship	From Census: http://www.census.gov/prod/2003pubs/c2kbr-30.pdf (SEE NOTE BELOW)
	Children (current)	Enter number listed
	Children (start of fellowship)	Enter number listed
	National origin	Country of birth/citizenship
	Citizenship	DB provided
	US citizenship	US citizenship?
	PRA	Permanent resident alien?
Education: code of each degree		
	Degree Type	B.S., B.A., M.S., M.A., Ph.D., Sc.D., etc.
	Degree year	Year degree conferred
	Degree institution	Institution attended (use NSF institution codes)
	Degree field	Field of study (use NSF field codes)

Employment: code for each job based on title, type/position, and/or place/institution		
	Year job started	Year job started
	Year job ended	Year job ended
	Employer	Employer name
	Job type	Job type by position, title and field
	Sector	Job categories by sector: academia, industry, DOE lab, DOE appointment, other government
	Job title if no job type	Job or position title
	Disciplinary Field	Field of study or teaching
	Notes	
Publications: include breakdown counts for books, articles, chapters, and other (e.g., reports, but only if included in the total count; eØÅÌude fellowships, patents, and grants); code for each publication year		
	Publication Type	Type of publication (Use codes for books, book chapters, journal articles, reports, conference proceedings, etc.)
	Publication Year	
	Publication Count	Number of publications by category for the year, journal articles will include number of HI journal articles.
	High Impact Journal	List of high impact journals. Select if publication was in one of these journals.
	Journal code	Specific codes for selected journals
	High impact journal year	Year published if high impact journal
	High impact journal count	Number of articles in high impact journals for that year
	Notes	
Special Recognition awards (excluding fellowships, patents, and grants): code each award		
	Award name	Official name of the award
	Year	Year awarded
	Source/organization	Source or organization presenting or sponsoring the award
	Award field/discipline	The field or discipline in which the award is made (if applicable)
	Notes	

Fellowships: code for each fellowship including DOE CSGF		
	Fellowship name	Official name of fellowship awarded
	Start/Declined year	Year fellowship started or, if declined, year declined
	Fellowship declined	Default is "N"; choose yes if fellowship declined
	End year	Year fellowship ended
	Type	Type of fellowship (e.g., graduate student, dissertation, postdoctorate, etc.)
	Source/organization	Source or organization (fellowship sponsor)
	Field/discipline	Field or discipline required by fellowship
	Notes	
Grants/Contracts: code for each grant or contract		
	Official ID	Official ID if available (e.g., NSF, NIH, etc. Grant number)
	Start year	Year grant or contract awarded
	End year	Year grant or contract expires
	Source/Organization	Source of grant or contract
	Amount	Dollar amount of the total award
	Role	Role of fellow in grant/contract execution (e.g., PI, Co-PI, GRA, Consultant, etc.)
	Notes	
Patents: code for each patent		
	Patent number	Patent number
	Patent year	Year patent issued
	Patent status	Pending or granted
	Patent US	Indicates if patent is a US patent
	Patent Int'l	Indicates if patent is an international patent
	Patent licensed	Indicates if patent was licensed
	Patent sold	Indicates if patent was sold
Professional Association Memberships		
	Number of current professional association memberships	Number of current professional association memberships
Professional Association positions/participation: code for each position		
	Organization name	Official name of the organization
	Major position(s)	Any major position held in the organization, see related codes (e.g., president, vice president,

		secretary, treasurer, board member)
	Major position years	Number of years major position held
	Other positions held	Other positions held (e.g., committee chair, committee membership, etc.)
Miscellaneous/Other		
	Additional Information	Include any other relevant information (e.g., community activities or positions, volunteering, etc.)
Notes		
	Notes	Additional Observations Include notes about any problems in coding CV information Indicate updated areas if after completion of initial input
	Coder: check here if you have encountered any problems or issues with this CV	Box to check if the coder has any questions or problems with coding the CV
	Date last update	Last date/time a change was made to the record
	Update coder	Name or user name of person who last coded or updated information

Race: Use Census 2000 categories (following Office of Management and Budget (OMB) standards for Federal data on race and ethnicity). Minimum categories for race: American Indian or Alaska Native; Asian; Black or African American; Native Hawaiian or Other Pacific Islander; White; Some Other Race. Minimum categories for ethnicity: Hispanic or Latino, Not Hispanic or Latino.

Marital Status: Use Census 2000 categories: Now married; Widowed; Divorced; Separated; Never Married

Appendix D: Interview Thematic Coding Categories

- **Fellowship Experience**
  - Valuable feature(s)
  - Laboratory team
  - Networking
  - Compared to other fellowships
  - Skill Development/Learning
  - Conference participation/assessment
    - Past
    - Present
    - Future
  - Negative aspects
  - Relevance
  - Suggestions
- **Collaboration**
  - Outside Academia
  - Outside University
  - Within University
  - Outside Field
  - Within Field
  - Within Sector
  - Across Sectors
  - National/International
  - Fellowship factors
    - Fellows
    - Laboratory team
    - Others
- **Establish New Activities/Programs**
  - Center/Facility/Institute
  - Courses
  - Department/Area of Study
  - Workshops
  - Programs
- **Community Building**
  - Committees
    - Faculty
    - Student
  - Programs
  - Recruit
    - Faculty
    - Student
      - Academia
      - Field
      - University
    - Workers/Colleagues
    - Trainees
  - Scholarship Effects
    - Future
    - Present
  - CSE field identification
  - Broadening participation
- **Contracts/Grants/Fellowships**
  - Types
  - Sources
- **Service**
  - International
  - National
  - Local
  - State
  - Local
  - Professional Association
  - University
  - Non-Profit
  - Other
- **Leadership**
  - Academic
  - Community
    - International
    - National
    - State
    - Local
  - Government
    - Federal
    - State
    - Local
  - Industry
  - Professional Associations
  - Non-Profit
  - Other
- **Mentoring**
  - Given/Received
    - Faculty
    - Student
    - Trainee
    - Supervisee
    - Postdoctoral
  - Fellows
  - Laboratory team
  - Other
- **Public Intellectual**
  - Courts
    - Federal
    - Local
    - State
  - Government
    - Federal
    - Local
    - State
  - Non-Governmental Media
  - Other
- **Scholarship**
  - Awards
    - Articles
    - Books
    - Other
  - Cross Field Effects
  - Models
  - Innovations, other firsts
  - Patents
  - Intellectual impact
  - Broader impact
  - Other
- **Special Recognition/Awards**
  - Types
  - Sources
- **Other Accomplishments/Contributions**
- **CSE relevance**
- **DOE relevance**
- **Future Plans**