Building a diverse and inclusive HPC community for mission-driven team science

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Abstract—The U.S. Department of Energy (DOE) has been a long-standing leader in driving advances in science and technology through advanced computing. However, DOE laboratories are currently facing urgent workforce challenges, particularly in terms of underrepresentation from key communities, including people of color, women, persons with disabilities, and first-generation scholars. This paper introduces the work carried out as part of the ECP Broadening Participation Initiative, which aims to address workforce challenges through a lens that considers the distinct needs and culture of high-performance computing (HPC). The work focuses on three main efforts: hosting Intro to HPC Bootcamps, expanding the Sustainable Research Pathways (SRP) internship and workforce development program, and establishing an HPC Workforce Development and Retention Action Group. The paper also highlights various workforce efforts throughout the computational science community and explores opportunities for future work aimed at broadening participation in HPC.

Building the workforce to tackle big problems through HPC team science

The U.S. Department of Energy (DOE) is a long-standing leader in scientific discovery enabled through high-performance computing (HPC). Associated with 118 Nobel Prize winners, the 17 DOE national laboratories conduct a wide array of basic and applied science research, with emphasis on solving big problems through mission-driven team science. DOE's investments have pushed the growth of computational and data-enabled science and engineering as a foundation of scientific and technological progress in conjunction with theory and experimentation [1]. Computational science—at the intersection of mathematics and statistics, computer science, and core disciplines of science and engineering—is revolutionizing not only the traditional physical sciences, but also life sciences, social sciences, humanities, business, finance, and even government policy [2].

As we tackle next-generation challenges and problems otherwise intractable—bridging scales and domains through new multiscale and multiphysics algorithms that exploit advanced computing architectures, incorporating complex workflows that couple modeling/simulation and experimental/observational data, leveraging AI/ML tools for enhanced insight, and working toward greater scientific reproducibility—we face a new era of complexity.

Past success has relied on developing a highly inter- and multi-disciplinary workforce and culture that fosters cross-disciplinary communication and not only exploits but also celebrates the unique expertise of each field. The combined expertise of diverse teams is increasingly essential, including applied mathematicians, computer scientists, domain scientists, and research software engineers,[1] along with project coordinators, social scientists, and more [3]. Moreover, various studies have shown that diverse organizations and groups are more creative, innovative, and productive [4], [5].

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[1] https://us-rse.org, https://society-rse.org,

HPC Workforce Challenges

DOE national laboratories, like many other scientific research organizations, face growing needs and challenges in recruiting and retaining a skilled workforce in the computing sciences [6], [7], [8], [3]. HPC has additional constraints stemming from its reliance on a workforce versed not only in advanced computing but also in multi- and interdisciplinary science and engineering domains, which also face challenges in recruiting and retaining underrepresented populations.[2] Government and academic sectors face fierce competition for talent attracted to lucrative industrial workplace benefits. Moreover, the changing U.S. demographics and higher attrition rates among people from underrepresented groups present additional challenges.

Cultivating the HPC workforce appears to be an over-constrained problem: growing needs, higher competition, changing workforce demographic profiles, and higher attrition rates in demographic groups currently underrepresented in HPC, but growing in the general workforce population. Moreover, while HPC has successfully cultivated a technically diverse workforce and many successful recruitment models exist, widespread reliance on existing social and professional networks has largely resulted in a homogeneous workforce.[3] [4] [5] The challenge is not only to develop new approaches to broaden the reach but also to change longstanding recruitment, onboarding, and retention practices to create and sustain an inclusive and diverse HPC workforce.

HPC Workforce Progress

Addressing these workforce challenges requires broad community collaboration to change the culture and demographic profile of computational science. Impactful DOE-wide programs such as SULI,[6] GEM,[7] VFP,[8] CCI,[9] and activities in the wider computing community [9], [10], [11] are making headway. Likewise, events such as *Advanced Computing for Social Change* [12], *The Pipeline Workshop* [13], and *Scaling HPC Education* [14] are pioneering innovative formats to engage underrepresented students in HPC. In addition, various communities are exploring strategies to improve HPC education and training; for example, a working group [15] made recommendations for overcoming key challenges in undergraduate-level education in computing and HPC, including building an HPC educator community and developing and providing inexpensive HPC hardware as teaching tools. Meanwhile, laboratory-specific initiatives are addressing challenges in workforce and training, capitalizing on each lab's unique perspectives, culture, and regional connections to underrepresented populations.

ECP Broadening Participation Initiative

The DOE Exascale Computing Project (ECP)[10] [16] is a research, development, and deployment project spanning multiple national labs as well as academic and private institutions. Beginning in 2016, ECP has engaged 1,000 researchers over seven years on the development of an integrated scientific computing software stack for use on exascale supercomputers (capable of executing 10^{18} operations per second) and the demonstration of new and faster capabilities in a wide variety of applications in chemistry, materials, energy, Earth and space science, data analytics, optimization, AI, and national security [17]. Advanced software technologies—including programming models and runtimes, mathematical libraries, data and visualization packages, and development tools that constitute the Extreme-scale Scientific Software Stack (E4S)[11]—form a community software ecosystem that underpins ECP applications and is unlocking the potential of advanced computing across all scales [18].

The technical breadth and sustained multi-lab collaboration of ECP have provided a unique and com-

[2] As discussed in a 2023 NSF report, https://ncses.nsf.gov/pubs/nsf23315/, women and racial and ethnic minorities are underrepresented in U.S. science and engineering programs.

[3] https://nationallabs.org/staff/diversity

[4] According to a 2021 study of nine HPC and HPC-related conferences, women represent only 10% of all HPC authors, doi:10.1145/3458817.3476164 .

[5] A 2018 *Wired* article discusses reasons for underrepresentation of women and minorities in technology fields, https://www.wired.com/story/computer-science-graduates-diversity.

[6] DOE Science Undergraduate Laboratory Internships (SULI, https://science.osti.gov/wdts/suli) encourage undergraduate students to pursue STEM careers by providing research experiences at DOE laboratories.

[7] The GEM Fellowship Program (https://gemfellowship.org) seeks to recruit high-quality underrepresented students looking to pursue degrees in applied science and engineering.

[8] The DOE Visiting Faculty Program, (VFP, https://science.osti.gov/wdts/vfp) seeks to increase the research competitiveness of faculty members and their students at institutions historically underrepresented in the research community.

[9] The DOE Community College Internships Program (CCI, https://science.osti.gov/wdts/cci) seeks to encourage community college students to enter technical careers relevant to the DOE mission.

[10] https://exascaleproject.org

[11] https://e4s-project.github.io

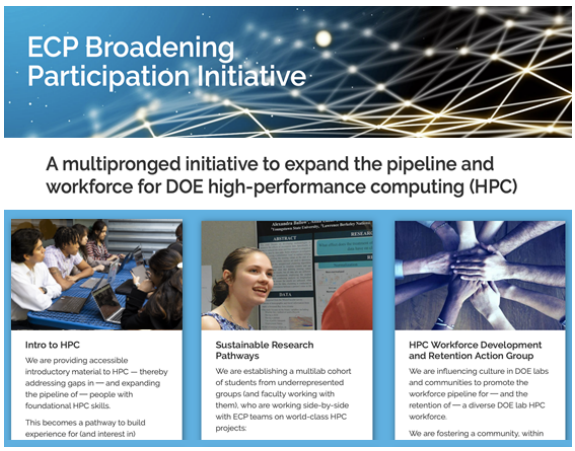

FIGURE 1. The ECP Broadening Participation Initiative features three complementary thrusts.

pelling opportunity for the DOE HPC community to address workforce challenges through a lens that focuses on the distinct needs and culture of DOE high-performance computing, with its emphasis on mission-driven team science [7]. Consequently, in August 2021 the *ECP Broadening Participation Task Force* was established, with members representing eight DOE national laboratories—Argonne (ANL), Brookhaven (BNL), Lawrence Berkeley (LBNL), Lawrence Livermore (LLNL), Los Alamos (LANL), Oak Ridge (ORNL), Pacific Northwest (PNNL), and Sandia (SNL)—as well as the DOE Office of Science computing facilities: Argonne Leadership Computing Facility (ALCF), National Energy Research Scientific Computing Center (NERSC), and Oak Ridge Leadership Computing Facility (OLCF). After clarifying the most urgent workforce challenges in the DOE computing sciences and surveying relevant ongoing work, the task force leveraged ECP's unique position as a broad effort spanning the DOE computational research ecosystem to launch the *ECP Broadening Participation Initiative*.[12] The initiative embodies a collaboration among ECP investigators, facilities staff, and education and workforce professionals. On a path toward a post-ECP role, it has expanded to invite participation from all lab staff in the DOE computing sciences.

As shown in Figure 1 and discussed in the following sections, the ECP Broadening Participation Initiative features three complementary thrusts: (1) launching the *Intro to HPC Bootcamp*, an immersive program designed to engage students in energy justice using project-based pedagogy and real-life science stories to teach foundational skills in HPC, scalable AI, and analytics, while exposing students to the excitement of DOE mission-driven team science; (2) expanding the *Sustainable Research Pathways* (SRP) internship and workforce development program as a multilab cohort of students from underrepresented groups (and faculty working with them), who collaborate with DOE lab staff on world-class R&D projects; and (3) establishing an *HPC Workforce Development and Retention Action Group* to foster a supportive and inclusive culture in DOE labs and communities.

These three thrusts provide paths for student engagement and retention at multiple points of the HPC workforce timeline, increasing access to and enhancing the DOE HPC community. If you imagine the HPC academic and career pathway as a superhighway, as depicted in Figure 2, we envision the three thrusts as on-ramps at different points, each meeting students (and lab staff) where they are, providing support and preparation, and offering access at appropriate points in an individual's journey. Through these three thrusts, the ECP Broadening Participation Initiative supports the full life cycle of the academic and career pipeline.

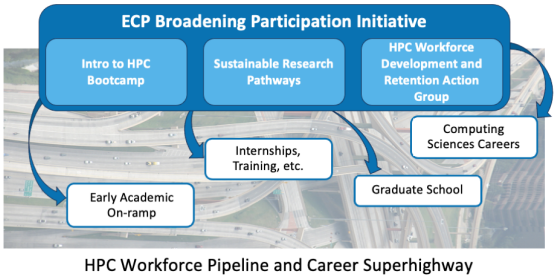

FIGURE 2. The ECP Broadening Participation Initiative supports the full HPC workforce pipeline, from on-ramps to career retention.

Introduction to HPC Bootcamp

The Introduction to HPC Bootcamp serves as the first entry point onto the HPC career superhighway for students early in their academic careers. The bootcamp is designed to engage students who may not know how or why HPC could help them accomplish their academic and scientific goals, while also preparing them for internships and inspiring them to continue their studies in graduate school.

[12] https://www.exascaleproject.org/hpc-workforce

To this end, the first Intro to HPC Bootcamp[13] was developed and organized by the advanced computing facilities at ANL, LBNL, and ORNL in collaboration with Sustainable Horizons Institute, taking place in August 2023 at LBNL [19]. The bootcamp brought together 60 students[14] to work in project groups supported by 14 trainers made up of national lab staff and academic partners[15] and 10 peer mentors.[16] Each group of students explored one of seven energy justice projects developed from DOE science that examined issues related to sustainable energy usage and alternatives, social impact of climate risk and resilience, and energy equity in the United States.[17] The bootcamp focused on raising awareness of the power and benefits of HPC, engaging more students from historically underrepresented groups in HPC by fostering a sense of belonging and exposing students to opportunities in HPC, especially at DOE labs.

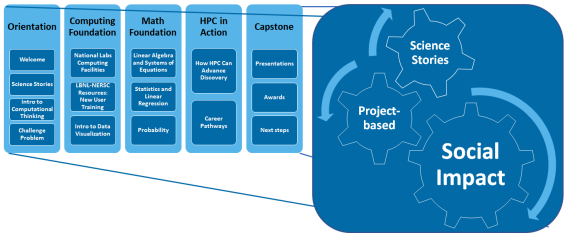

FIGURE 3. The framework of the Intro to HPC Bootcamp focuses on solving problems with mission-driven social impact to engage new communities in HPC.

The bootcamp utilized culturally relevant pedagogy and project-based learning to engage students in addressing social impact questions related to energy justice. As shown in Figure 3, the five-day bootcamp began by building community and a friendly learning environment, motivating participants through socially relevant scientific problems, while exposing students to foundational concepts in computing, HPC, mathematics, and analysis. Learners worked throughout the week on their projects, culminating in a presentation on the final day. Throughout the bootcamp, students had opportunities to hear from lab staff about their paths to the national labs and HPC careers.

To ensure an engaging and inclusive bootcamp, we included a diverse set of organizers, trainers, and mentors to develop and facilitate the program. The team had expertise in computational science, advanced computing, energy justice, diversity, education, workforce development, and program evaluation. Collaborators came from multiple DOE labs, Sustainable Horizons Institute, the DOE Office of Economic Impact and Diversity, and academia. Alongside the bootcamp trainers, peer mentors provided guidance on technical concepts, collaboration, workshop expectations, and presentations.

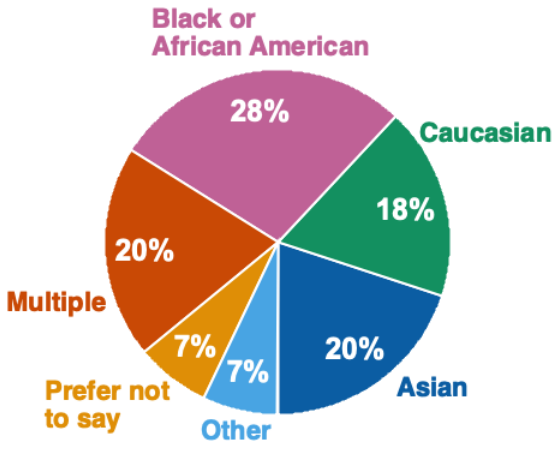

FIGURE 4. Breakdown of demographics of participants of the Intro to HPC Bootcamp in August 2023

A pivotal step in developing the bootcamp was a *Train the Trainers* workshop, essential for building effective team collaboration and introducing the bootcamp concept to the DOE lab staff who would serve as materials developers and trainers. During the workshop, the team considered strategies for modifying existing HPC training materials through the lens of engaging new communities and project-based learning.

The bootcamp application was designed to lower the barriers for students historically underrepresented in HPC, asking why students wanted to attend the bootcamp without requiring a letter of recommendation or CV. Of the over 300 students who applied, 60 were chosen to attend; all had some experience with computing but little or no background in HPC. Nearly eighty percent were undergraduates, along with a mix of master's, Ph.D., and community college students. As shown in Figure 4, the 60 students were diverse racially, with African Americans/Black representing the largest group at 28%, followed by Asian and multiple race (20%) and Caucasian (18%). Nearly all partici-

[13] https://shinstitute.org/intro-to-hpc-bootcamp
[14] https://shinstitute.org/intro-to-hpc-participants
[15] https://shinstitute.org/intro-to-hpc-project-leaders-and-trainers
[16] https://shinstitute.org/intro-to-hpc-peer-mentors
[17] https://shinstitute.org/intro-to-hpc-energy-justice-projects

pants (98%) identified as a member of at least one underrepresented group, including 48% first-generation scholars and 57% female participants. For these 60 students, travel, lodging, and food were covered, and a $500 stipend was provided at the end of the bootcamp to ensure all students, regardless of financial context, would be able to attend.

Preliminary feedback about the bootcamp has been positive. Of the 54 students who responded to a post-bootcamp survey, 85% said they are interested or very interested in a career in HPC, and 90% said they are interested or very interested in a career at a DOE national lab. In responses to the post-bootcamp survey, many students expressed changes in potential future plans because of their experience at the bootcamp:

> *[The Intro to HPC Bootcamp] exposed me to work and life at a national lab and motivated me to consider such work ... If not at a national lab, it has definitely motivated me to look into non-industry jobs that more greatly benefit the public good. I think I would find that incredibly meaningful and fulfilling, and that is very important to me in a career and something I've been searching for ...*

Building on bootcamp successes, we plan to increase access to introductory HPC materials by building in adaptability and customization. Potential paths to increase sustainability and access to the program are through faculty partnerships, asynchronous bootcamp components, providing local offerings, and creating curriculum components to progressively build HPC skills for more advanced learners. By reaching more participants, we are working to build a sustainable pipeline of talent for DOE national labs, preparing students for internship opportunities and providing them with tools to succeed in the next steps of HPC careers.

Sustainable Research Pathways

Sustainable Research Pathways (SRP)[18] is a comprehensive workforce development program designed to increase the participation of underrepresented groups and institutions in research and development at DOE national labs and to address pressing needs in the advanced scientific computing workforce. SRP serves as an on-ramp for undergraduate and graduate students with some experience and interest in computing or computational science and engineering. Started as a partnership between Sustainable Horizons Institute and LBNL in 2015 [20], SRP expanded beyond LBNL in 2022 as part of the ECP Broadening Participation Initiative. The 2022 SRP cohort was comprised of a highly diverse group of faculty, students of faculty, and independent students who collaborated with DOE lab staff, as shown in Figure 5. In 2023, the program further expanded through a partnership with ECP and seven labs (ANL, BNL, LBNL, LLNL, LANL, ORNL, SNL) from the Computational Research Leadership Council. During summer 2023, SRP facilitated nearly 200 faculty and student collaborations at 10 DOE national labs, and work is underway to prepare for the summer 2024 cohort.

FIGURE 5. Students and faculty in the first ECP Broadening Participation SRP Cohort in 2022 collaborated with staff at 10 DOE laboratories on topics involving advanced software technologies, scientific applications, and hardware/integration.

Figure 6 illustrates the program components and timeline. SRP begins with extensive recruitment of faculty, students, and DOE staff members for participation in an interactive virtual *SRP Matching Workshop*, where participants engage in successively more focused interactions, providing them with the opportunity to explore common interests and potential collaborative summer projects. At the conclusion of the workshop,

[18] https://shinstitute.org/sustainable-research-pathways-2024-workshop

participants indicate their matching preferences, which are used to create two-way matches (requiring that both parties have expressed interest in working together). Following the matching process, the resulting teams develop brief project plans/proposals for the summer experience, and then funded teams are onboarded at their assigned DOE lab. In addition to pursuing their summer research projects, participants attend local seminars and social events at their host laboratory, as well as virtual cohort-wide SRP activities that help build a multilab SRP community. Volunteer committees provide participants with professional development and leadership opportunities; recent activities have included game nights, wellness events, and seminars on work/life balance. After the summer internship, the *Catalyzing Ubiquitous Learning Through InoVaTive and Engaging (CULTIVATE) Conversations* program serves to maintain contact with the cohort with the aim of helping develop inclusive workforce ecosystems through facilitated conversations. Participants often showcase their SRP accomplishments at scientific conferences.

SRP faculty alumni accomplishments include DOE Early Career, ASCR-RENEW, and ASCR FAIR awards and nomination for the Presidential Awards for Excellence in Science, Mathematics and Engineering Mentoring. Student participants have been hired full-time at LBNL, LLNL, and PNNL; decided to pursue graduate degrees; won best poster awards; been awarded the DOE Computational Science and Stockpile Stewardship Graduate Fellowships and Fulbright scholarships; presented their research at prestigious venues such as the Supercomputing and SIAM CSE conferences; and participated in programs such as the Argonne Training Program on Extreme-Scale Computing[19] and the ORNL Artificial Intelligence Workshop.

SRP forms meaningful and lasting connections between faculty, students, and DOE lab staff, while helping to build inclusive HPC research and development ecosystems. Community building activities start at the virtual SRP Matching Workshop and continue during the summer experience and beyond through CULTIVATE Conversations.

HPC Workforce Development and Retention Action Group

While the *Intro to HPC Bootcamp* and *Sustainable Research Pathways* prepare students to enter the HPC career superhighway, we recognize the vital importance of cultivating an inclusive ecosystem, not only to welcome and retain them, but also to foster an environment where they can thrive, meet their potential, and express their full selves. As shown in Figure 2, we complement work to engage students in the HPC workforce pipeline with activities aimed at creating a culture of inclusion. The *HPC Workforce Development and Retention (HPC-WDR) Action Group* facilitates collaboration among DOE national laboratories and their associated computing communities to share knowledge and insights aimed at creating a diverse, equitable, and inclusive workforce for high-performance computing. This effort focuses on building a community and gathering proven tools and best practices. Initially, representatives from ten national laboratories convened regularly to exchange ideas and develop recommendations and strategies for building supportive workforce cultures. The first two activities undertaken by HPC-WDR have been organizing a quarterly webinar series on HPC workforce topics[20] and establishing a dedicated website that focuses on fostering a diverse and inclusive HPC workforce culture as well as addressing workforce retention.

The webinars have explored topics such as effective mentoring practices and the significance of embracing diversity for inclusion. Since their inception in May 2022, seven webinars in the series have garnered participation from 672 individuals, representing 10 national laboratories, 38 universities, and 22 businesses, with speakers drawn from the scientific computing community; recordings enable even broader reach.

The HPC-WDR website[21] serves as a repository

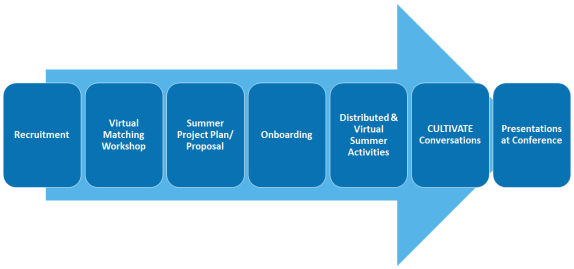

FIGURE 6. Components of the SRP program engage students to promote multifaceted learning and community building across a broad timeline before, during, and after the summer internship experience.

[19] https://extremecomputingtraining.anl.gov

[20] https://www.exascaleproject.org/workforce-development-seminar-series

[21] https://hpc-workforce-development-and-retention.github.io/hpc-wdr

for webinar recordings and provides announcements of computing workforce events. Moreover, the website houses a growing collection of best practices on HPC workforce issues, often presented in blog posts. For instance, one blog discusses the adoption of "inclusive minutes" during team meetings.[22] In this practice, teams allocate a minute during their meetings to exchange insights on integrating inclusive and culturally aware practices into their work areas, with a goal of improving communication and fostering mutual respect.

Recognizing that changing workplace culture is a complex problem with long timescales, our ongoing objective is to maintain the website as a living community resource and to steward and advance our community's presence. We intend to continue hosting webinars and workforce community meetings, recognizing these activities as vital for assisting the DOE labs' computing community in intentionally identifying and implementing best practices in workforce development and retention. Our initial efforts focused on establishing the working group. With a gratifying response from webinar attendees, our next focus is to develop a mixture of qualitative and quantitative methods for capturing impacts and to establish data collection points to measure changes over time, thereby motivating further work and study.

Future directions

The ECP Broadening Participation Initiative has established a strong foundation for collaborating and innovating as a multilab community to address challenges in the complete life cycle of the DOE HPC workforce. Early successes include an overwhelming response to the call for participation in the innovative energy justice project-based HPC bootcamp; phenomenal SRP growth from a single lab to a multi-lab initiative that fostered nearly 200 collaborations across 10 labs in the summer of 2023; and the establishment of a highly collaborative group of laboratory, academic, and industrial HPC professionals who have shared best practices, established a repository of materials, and facilitated webinars attended by nearly 700 people.

The three thrusts—the Intro to HPC Bootcamp, Sustainable Research Pathways, and the HPC Workforce Development and Retention Action Group—provide different entry points onto what we imagine as the fast-paced, exciting, multi- and interdisciplinary HPC career superhighway. Through this multipronged approach, we can attract students of varied backgrounds, experience levels, and interests, wherever they are in their journeys. We further invite them to join us as we work toward a HPC community where everyone can reach their potential, be their full selves, and contribute to a more innovative mission-driven team science enterprise.

Together, as we plan for the next phases of work to broaden the participation of underrepresented groups, we are working to realize a sustainable strategy to recruit and retain a diverse HPC workforce by fostering a supportive and inclusive culture within the computing sciences at DOE national laboratories. The exciting and complex era of next-generation computational science demands a multidisciplinary workforce whose members provide a diversity of technical expertise *and* are fully representative of our whole population. This diversity across many axes will inspire innovation, provide new perspectives, and enable us to tackle big problems through HPC team science.

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[22] https://hpc-workforce-development-and-retention.github.io/hpc-wdr/jekyll/update/2023/04/08/inclusive-minute.html

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