

2.0 PURPOSE AND NEED

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The project purpose is: to relocate and consolidate Advanced Scientific Computing Research (ASCR)-funded Lawrence Berkeley National Laboratory (LBNL) programs with other LBNL/University of California (UC) Berkeley programs focusing on computational and computer science research in a new facility on the LBNL site; to enable the continued operation and future advancement of the LBNL National Energy Research Scientific Computing Center (NERSC) high-performance computing (HPC) national user facility and the Computational Research Division (CRD) program; to co-locate a portion of the joint LBNL/UC Berkeley Computational Science and Engineering (CSE) program¹ with NERSC and CRD; to foster interaction and collaboration between the NERSC staff and other LBNL and UC Berkeley researchers; and provide NERSC, CRD, and CSE staff with convenient access to other LBNL scientific facilities, programs, researchers, and services.

The project need is for high performance computing space due to the immediate and projected deficiency in high performance computing space at the existing NERSC HPC facility and to remove the constraints to intellectual exchange and collaboration resulting from the dispersed locations of ASCR-funded and ASCR-related programs and researchers.

2.2 BACKGROUND

The U.S. Department of Energy's (DOE's) overarching mission is to advance the national, economic, and energy security of the United States and to promote scientific and technological innovation in support of that mission. To advance its mission, the DOE has established several national laboratories, including LBNL at the Berkeley site.

The charge of the DOE's ASCR program is to discover, develop, and deploy the computational and networking tools that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex phenomena important to the DOE. ASCR-funded programs at LBNL include (1) the NERSC facility, (2) the Energy Sciences Network (ESnet), and (3) research projects within the CRD. The joint UC Berkeley/LBNL CSE program conducts related research focused on computational and computer science areas. The following discussion presents the mission of each of these programs and their interrelationships with one another.

¹ CSE is a UC Berkeley and LBNL collaborative program that conducts research focused on computational and computer science areas. The program is not ASCR funded but includes some UC Berkeley faculty, students, and postdoctoral researchers who conduct research funded by ASCR.

2.2.1 National Energy Research Scientific Computing Center

NERSC is a premier HPC national user facility currently located in Oakland at the Oakland Scientific Facility (OSF). The DOE Office of Science (SC) relies on NERSC as the primary provider of computing and storage services to the vast majority of computational scientists funded by the DOE SC. NERSC's mission is to accelerate the pace of scientific discovery in the DOE SC community by providing high performance computing, information, data, and communications services.

NERSC provides HPC systems that enable computational science at a scale large enough to meet needs of universities, government laboratories, and international research facilities via extremely fast fiber optics networks. With this capability, national and international interdisciplinary teams of scientists explore fundamental scientific and engineering problems that require massive unclassified scientific computer simulation and data analysis calculation. In November 2003, the DOE SC ranked NERSC as one of its top 11 most important scientific facilities to ensure the U.S. retains its primacy in critical areas of science and technology well into the future.²

In order to meet an ever-increasing demand for such computing capabilities, NERSC must continually upgrade its computing systems in a seamless manner (i.e., with no lengthy downtime between upgrades). NERSC's ongoing operational plan is to replace one of the existing systems approximately every three years while maintaining user access to the other existing systems. To do this, NERSC requires space for at least two fully operational HPC systems to allow one to undergo replacement or upgrade while the other system is used by scientific researchers. To house these two HPC systems, there should be two 10,000-square-foot (sf) column-free spaces flanking a 12,000-sf space, which is required for large amounts of archival data storage, high-performance intermediate storage, smaller computing clusters, and visualization servers. NERSC supercomputers are currently housed in a 19,000-sf computer room in off-site leased space at LBNL's OSF, which also provides limited staff office space. Neither the computer room space, the mechanical equipment space, nor the available electrical power is adequate for future generations of high-performance computers.

2.2.2 Computational Research Division

The DOE SC's computational science mission relies on the basic and applied research within CRD in the development of algorithms, computer systems software, data management tools, and the evaluation of HPC architectures. The CRD mission is to create computational tools and techniques by conducting applied research and development in computer science, computational science, and applied mathematics.

² *Facilities for the Future of Science: A Twenty-Year Outlook*; http://www.er.doe.gov/Scientific_User_Facilities/History/20-Year-Outlook-screen.pdf

CRD is located on the LBNL site. CRD also contains the ESnet department, which provides the high-performance scientific data network across the DOE complex.

CRD and NERSC have a synergistic relationship, with CRD research informing NERSC on what types of systems, software, and algorithms might be effective in future deployments at NERSC, while the experience of users and system support staff at NERSC reveals research challenges in computing and mathematics and suggests new research challenges for CRD. Close collaboration and frequent communication between NERSC and CRD benefits both organizations and thus DOE in the quality and effectiveness of the two programs.

Computational Science and Engineering Program

The CSE program was jointly created by LBNL and UC Berkeley, and is currently located on the UC Berkeley campus. Computational science research in areas like biology, chemistry, energy science, nanotechnology, climate modeling, and physics are interdisciplinary and interactive. Teams of researchers often involve scientists from one of these disciplines along with applied mathematicians and computer hardware and software experts to address the most challenging research questions. The CSE program brings these researchers into a common organizational structure for planning and coordination of research activities, along with a graduate curriculum to train the next generation of scientists.

The CSE program contains computer scientists and applied mathematicians who interact regularly with CRD and NERSC staff and scientists across the UC Berkeley campus who use high-end computing in their daily research. Frequent contact and communication between people working on diverse projects is vital for innovation and the sharing and “cross-fertilization” of ideas.

CSE is a UC Berkeley and LBNL collaborative program, which is not ASCR funded, but includes some UC Berkeley faculty, students, and postdoctoral researchers who conduct research funded by ASCR. By co-locating in one facility, the ASCR-funded CRD and NERSC researchers and CSE researchers would engage in mutually beneficial collaborations that bring large teams together to address important computational and computer science research areas such as climate modeling, computational cosmology, combustion research, and chip design for scientific applications.

Existing and Projected Challenges

While the NERSC computers and staff are located in Oakland, the CRD staff is located on the LBNL site, and CSE researchers are located on the UC Berkeley campus, dispersed in multiple buildings in individual and group workspaces that are inadequate in both size and functionality. This limits the

opportunities for frequent interaction and collaboration. These obstacles to collaboration are anticipated to continue in the future.

As a result of the aforementioned challenges, there is an immediate and long-term need to increase computer floor space, to improve workspace size and functionality for both individual and group efforts, and to co-locate CRD staff and some CSE researchers adjacent or nearby to the NERSC. A facility or facilities that bring people and systems together in space designed for functionality and collaboration would result in improved efficiency and productivity, as well as foster intellectual exchanges. Such a facility or facilities should also provide:

- Integrated and appropriately designed space that houses and enables the continued operation and future advancement of LBNL's NERSC HPC national user facility, CRD, and joint LBNL/UC Berkeley CSE programs;
- Adequate space, chilling capacity, and infrastructure to accommodate next-generation computing equipment allowing for continual future upgrades to such equipment;
- Access to a large, reliable, and economical electrical power source. The power source should be capable of serving both the immediate and potential future needs of LBNL's computing program;
- Ability to connect the facility to modern fiber optics that can economically be connected to the existing high-speed DOE ESnet Bay Area Metropolitan Area Network;
- Convenient access to other LBNL scientific facilities, programs, researchers, and services; a location that fosters interaction and collaboration between the NERSC staff and others, including UC Berkeley researchers.

The DOE therefore proposes to relocate and consolidate ASCR-funded LBNL programs with other LBNL/UC Berkeley programs focusing on computational and computer science research in a new facility on the LBNL site. The Proposed Action includes the relocation of the NERSC HPC national user facility, the relocation, and consolidation of all NERSC and CRD staff, and the creation of a collaborative space for the joint UC Berkeley/LBNL CSE program. Housing these activities in the same new building as the supercomputing systems would centralize and co-locate all similar and related functions and programs to improve efficiency and productivity and foster intellectual exchanges and collaboration. The location for the new building to house these relocated programs and computational systems should be in close proximity to the UC Berkeley campus to enable extensive collaboration of CSE staff with NERSC and CRD staff.