

I would like to offer my special invitation for you to participate in a workshop on "Large Scale Production Computing Requirements for Biological and Environmental Research." The workshop will be held at Hilton Rockville (in front of the Twinbrook Metro Station on the Red Line) in Maryland on May 7-8, 2009. Please respond to BER-workshop-committee@nersc.gov by **COB March 9, 2009 (note the new due date)**, confirming your participation.

The goal of this workshop is to accurately characterize the High Performance Computing (HPC) requirements of current and future work funded by the Office of Biological and Environmental Research (BER). These requirements will serve as input to the NERSC architecture and planning processes, and will help ensure that NERSC continues to provide world-class support for scientific discovery for DOE scientists and their collaborators. The tangible outcome of the workshop will be a document that includes both HPC requirements and a supporting narrative.

The mission of the NERSC Facility is to accelerate the pace of scientific discovery by providing HPC, information, data, and communications services for research sponsored by the Office of Science (SC). NERSC is the principal provider of production HPC services for SC Programs. NERSC has been serving a large number of "broad impact" computational science users as well as a smaller number of "high impact" scientific users.

NERSC regularly updates and refreshes its understanding of the HPC requirements of the science programs in Greenbook and other user-driven or LBNL NERSC-driven documents every three-four years. NERSC also publishes "Science-Driven Computing: NERSC's Plan." This plan document is the closest to capture SC's needs, and has been published every 5 years. Since science needs are changing very rapidly, the five-year cycle does no longer capture the changing needs very effectively. NERSC also needs more computation-oriented data than those currently collected using the existing mechanisms. To fill the gap of accurately characterize science and computation-centric needs for NERSC resources from the Headquarters' perspective, ASCR Associate Director recognized the need for a new mechanism to gather HPC resource needs.

The mechanism by which NERSC obtains this information is by holding a workshop with each Program Office in the Office of Science every 3 years. The first workshop is with the BER Program, which is supported by the BER Associate Director. The workshop will be conducted tailoring the format developed by ESnet, which conducted similar workshops in the past.

Among the specific goals of the workshop are: (i) identifying the leading current and upcoming DOE research imperatives in biological, climate, and environmental science that require or will soon require large-scale computing resources such as those offered by NERSC; (ii) understanding the associated underlying algorithms and applications that will be used to address those imperatives; (iii) clarifying what model parameters are typical for today's science simulations and how those might change; (iv) exploring what new science results might be afforded by improvements in NERSC computing hardware, software and services; (v) providing a forum for discussion of NERSC system and service attributes expected to have the greatest impact on existing and developing science applications over the next five years. Of particular importance are challenges that arise from the intersection of high end production computing needs and system architectural constraints as we currently understand them, especially multi-core parallelism. A "case study" template to capture the above will be available from the workshop organizer.

Those case studies and your discussions at the workshop will become the input to a written report representing the results of the workshop, which will be prepared by NERSC and submitted to DOE. The report should address the areas noted above in a "case study" format that (i)

summarizes the specific scientific endeavor; (ii) presents a computing-centric view of the process by which the science is done; and (iii) describes how science demands for higher physical model fidelity, numerical algorithm improvement, data analytics and work flow are likely to evolve. A preliminary version of the report should be available for a brief DOE and user comment period in June 2009, and the final report is to be available six weeks after the conclusion of the comment period.

The case study template form and instructions, other pertinent information, hotel information, and reference materials will be available from the workshop URL at:

http://www.nersc.gov/projects/science_requirements/workshops.php

We believe that this workshop will help NERSC maintain its reputation as the flagship production computing facility for SC and will enhance scientific productivity in the solution of biological, climate, and environmental research problems over the course of the next decade. Thank you again for your participation.

Best,

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