ASCR Leadership Computing Challenge (ALCC)

Program webpage: https://science.osti.gov/bes

BES Mission and Research Priority Areas of Interest:

The mission of the Basic Energy Sciences (BES) program is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. BES also supports world-class, open-access scientific user facilities consisting of a complementary set of intense x-ray sources, neutron sources, and research centers for nanoscale science.

Applicants need to propose computational research that fits within the scope and priorities of research activities within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division, Materials Sciences and Engineering (MSE) Division, and/or Scientific User Facilities (SUF) Division, including optimization of beamline operation and real-time experiment control. Of special interest is modeling and simulation aimed at extending currently attainable length/time scales, accuracy, or increasing complexity that algorithmically match efficiency enhancements offered by ALCC high-end computing resources. Preference will be given across all core research areas to applications that can demonstrate efficient large-scale parallel utilization rates for high end and high performance computing.

Applications and LOIs need to select and address one or more BES research and facilities focus areas given below. Additional technical information and descriptions can be found following the hyperlinks on the BES website <u>https://science.osti.gov/bes</u>:

CSGB Research Focus Areas

Fundamental Interactions

Photochemistry and Biochemistry

Chemical Transformations

MSE Research Focus Areas

Materials Discovery, Design, and Synthesis

Scattering and Instrumentation Sciences

Condensed Matter and Materials Physics

SUF Research and Facilities Focus Areas
Accelerator and Detector Research
Nanoscale Science Research Centers
X-Ray Light Sources
Neutron Scattering Facilities