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**BEAM: An HPC Pipeline for Nanoscale Materials Analysis and Neutron Data Modeling** ERIC LINGERFELT, EIRIK ENDEVE, YAWEI HUI, CHRIS SMITH, SUHAS SOMNATH, NATHAN GRODOWITZ, JOSE BORREGUERO, Oak Ridge National Laboratory, FENG BAO, University of Tennessee at Chattanooga, JENNIFER NIEDZIELA, DIPANSHU BANSAL, Oak Ridge National Laboratory, OLIVIER DELAIRE, Duke University, RICHARD ARCHIBALD, ALEX BELIANINOV, MALLIKARJUN SHANKAR, STEPHEN JESSE, Oak Ridge National Laboratory — The Bellerophon Environment for Analysis of Materials (BEAM) enables scientists at ORNL’s Center for Nanophase Materials Sciences and Spallation Neutron Source to leverage the computational power of ORNL’s Compute And Data Environment for Science (CADES) and the Oak Ridge Leadership Computing Facility (OLCF) to perform near real-time scalable analysis and modeling. At the core of this computational workflow system is a web and data server located at CADES that enables multiple, concurrent users to securely upload and manage data, execute materials science analysis and modeling workflows, and interactively explore results. BEAM’s data management capabilities utilize a petabyte-scale file system and enable users to easily manipulate remote directories and uploaded data. The framework facilitates user workflow needs by enabling integration of advanced data analysis algorithms and push-button execution of dynamically generated HPC workflows employing these algorithms. We will present features of the system which include HPC analysis of SPM and STEM data and automated workflows for the optimization of inelastic and quasi-elastic neutron scattering data.

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