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Enabling Biology, Chemistry and Other Sciences on Titan through BigPanDA

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The Oak Ridge Leadership Computing Facility (OLCF) is one of the most powerful HPC centers available to researchers from different scientific fields to solve some of the world's most challenging scientific problems. Small scientific groups often need to develop expertise to optimize their applications for running on Titan, and to fit the usage policies of such big machines. We have installed the BigPanDA workload management system at OLCF to simplify the submission of user tasks to Titan. In this talk we will present results of an R&D project to execute workloads from different scientific groups at OLCF. We will describe all steps: starting from deployment of PanDA server as service on demand at OLCF in OpenShift containers, to the adaptation of PanDA client tools for new users. Examples from some of the different scientific fields using this service will include biology/genomics, molecular dynamics, LQCD, solid-state and neutrino physics, and different data science experiments: nEDM, LSST, and IceQube. In more details we will address a "proof of concept" project with BlueBrain. It was conducted jointly by the BigPanDA team and the Blue Brain Project (BBP) of the Ecole Polytechnique Federal de Lausanne (EPFL). This proof of concept project showed the efficient application of the BigPanDA system to support the complex scientific workflow of the BBP using a mix of desktop, cluster and supercomputers to reconstruct and simulate accurate models of brain tissue.

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