

Extended Collaborative Support to optimize codes and build Science Gateway workflow infrastructure for Dark Energy Survey Simulation Working Group

Principal Investigators: Prof. Andrey Kravtsov (University of Chicago), Prof. August Evrard (University of Michigan)

Description: The Dark Energy Survey (DES) is an upcoming international experiment that aims to constrain the properties of dark energy and dark matter in the universe using a deep, 5000-square degree survey in five optical bands. The production of a suite of large N-body simulations will allow the development of a Blind Cosmology Challenge (BCC) process for the DES collaboration. IU XSEDE Extended Collaborative Support Services team members Raminder Singh and Suresh Marru are collaborating with Prof. Evrard and his graduate students to build science gateway building blocks, in particular, workflow infrastructure to implement DES automated workflows that will be used to generate synthetic data sets and perform post-processing. The gateway tools accept user-defined cosmology as workflow input files and pipes through pre-processing components of computing power spectrum using CAMB application and generates initial conditions using 2LPTic applications. The workflow then executes the L-GADGET simulation code (which performs the N-Body simulations), verifies correct execution, archives output, re-submits and verifies until the code terminates successfully. The Extended Collaborative Support focuses on building workflow infrastructure to interact with XSEDE job management and data movement components. The collaboration intends to build on these building blocks to deploy a production science gateway with a portal interface targeting the DES Simulation Working Group members. The workflow is currently executed on TACC's Ranger through GRAM5 invocations using the workflow composer tool (Figure 1) and supporting services from the Open Gateway Computing Environments (OGCE) tool suite, which were hosted on the XSEDE Gateway Hosting Environment at IU. Currently running workflow tests will execute three 512 node jobs for validation, as we prepare for full simulations (requiring 1000 nodes and approximately five days to execute). TACC's Dr. Warren Smith provided significant assistance resolving GRAM5 deployment problems on Ranger. In the next quarter, IU will work with Prof. Evrard's team to develop and deploy a second workflow for post-processing runs (extending the current workflow). These will execute the codes ROCKSTAR and RNN(halo) and will generate galaxy catalogs using ADDGALS applications. These codes are currently being ported to Ranger by Evrard's team in collaboration with TACC's Dr. Lars Koesterke. Dr. Koesterke contributes his time from Extended Collaborative Support Services and is benchmarking and optimizing the ADDGALS and L-Gadget applications.

The Workflow Infrastructure supported by the ECSS and OGCE projects are made available to the community at large through the Apache Airavata Science Gateway Framework currently incubating at the Apache Software Foundation.

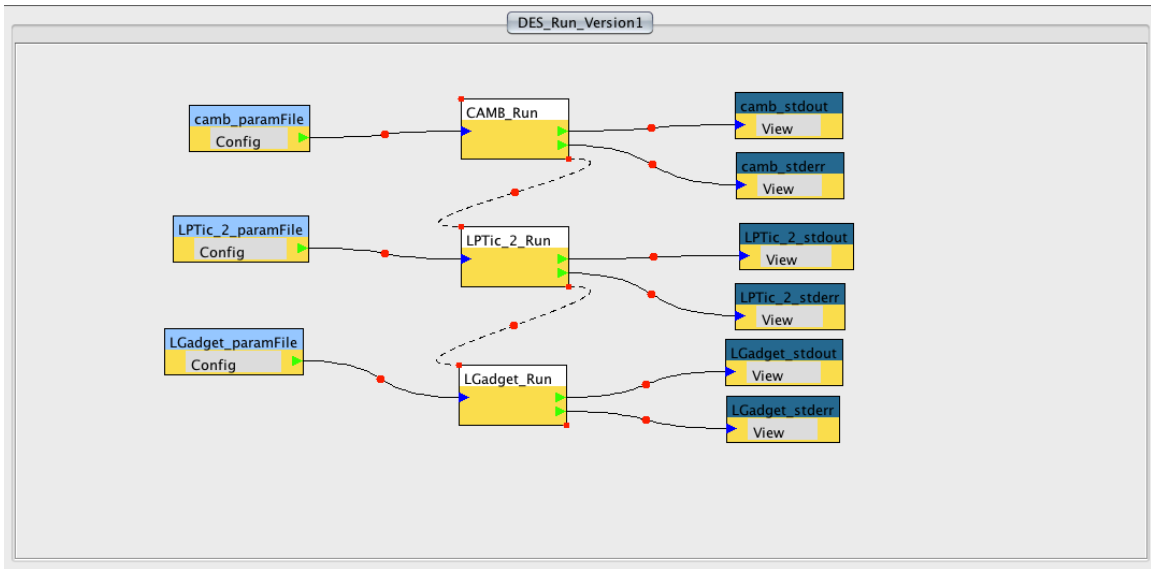


Figure 1 DES Simulation Working Group's initial workflow running in the OGCE's XBay workflow composition tool. Central boxes represent services for remotely executing 2LPT and L-GADGET applications on Ranger. Inputs are expressed on the left and outputs are listed on the right.