Adding Workflow Management Flexibility to LSST Pipelines Execution

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Abstract. Data processing pipelines need to be executed at scales ranging from small runs up through large production data release runs resulting in millions of data products. As part of the Rubin Observatory’s pipeline execution system, BPS is the abstraction layer that provides an interface to different Workflow Management Systems (WMS) such as HTCondor and PanDA. During the submission process, the pipeline execution system interacts with the Data Butler to produce a science-oriented execution graph from algorithmic tasks. BPS converts this execution graph to a workflow graph and then uses a WMS-specific plugin to submit and manage the workflow. Here we will discuss the architectural design of this interface and report briefly on the recent production of the Data Preview 0.2 release and how the system is used by pipeline developers.

1. Introduction

A large number of images will be taken during the 10-year Legacy Survey of Space and Time (LSST; [Ivezić et al. 2019], [O’Mullane et al. 2023]). Processing of this data will be done at scales ranging from small runs up through large production data release runs. Data processing will be done using data management and execution systems for the Rubin Observatory LSST Science Pipelines with the Data Butler and science-oriented execution graphs ([Lust et al. 2023], [Jenness et al. 2022]).

The Data Butler is the system that abstracts the data access details from the pipeline developers. A Quantum is the work to be done on a single set of inputs (e.g., remove instrument signature on the raw image for detector 3 of exposure 12345). These Quanta take inputs and produce outputs which affect the order in which they can be executed. This science-oriented execution directed acyclic graph is called a Quantum-Graph.

This QuantumGraph is executable by LSST middleware on a single machine. At this point, the graph has no runtime information (such as command lines or required memory) that would be needed to run jobs via a workload management system (e.g., Slurm). BPS is the middleware that converts the Quantum Graph into a workflow by adding the runtime information. It provides a layer of abstraction so different WMS
can be used with minimal user-facing changes in either commands or configuration as it was quickly apparent that LSST needs to have the flexibility to use different WMS. For example, users at different sites want to use the WMS they are familiar with or the release processing would like to try a new WMS.

2. Submission

Users interact with BPS using the same middleware terminology as used in notebooks and single machine execution to define the input data and pipeline. The submission process is broken up into phases:

1. acquire: Create the QuantumGraph or read an existing one.
2. cluster: Group Quanta into clusters for efficiency (see subsection 2.1 for more details).
3. transform: Create a generic workflow graph from the clustered QuantumGraph (see §2.2 for more details).
4. prepare: Convert the generic workflow graph into the representation required by the workflow management system. Being able to save this representation to disk is especially helpful for debugging submission issues.
5. submit: Finally submit the workflow representation for execution.

2.1. Clustering

Early running of pipelines showed that many of the Quanta were executed very quickly, for example in less than a minute. The job overhead would be too large for efficient running of those quick jobs and many batch schedulers do not handle well thousands of minute long jobs. We added an option for the BPS submission process to group Quanta into clusters and then each cluster corresponds to a compute job.

The disadvantages of clustering is that the clusters are black boxes to the workflow and batch services. This means that workflow and batch services cannot monitor or retry at the Quantum level. The LSST execution middleware can skip Quanta that have already successfully run, and more work is planned on Quantum-level reporting and real-time logging. The bigger disadvantage is that workflows generally stop execution downstream of a failed job. This means a single Quantum failure could keep many other Quanta from running that could actually be run just because of the way they were clustered.

The method used to perform the clustering is a submit time configuration. Clustering is independent of the workflow management system. There are currently two clustering methods supported: the original behavior where each Quantum is its own cluster and a user-specified clustering. The user-specified clustering is done by common data values (e.g., same detector) to help maximize the execution of Quanta in the workflow.

2.2. Generic Workflow

The generic workflow is a directed acyclic graph containing runtime information needed to submit to a workflow management system. Each cluster becomes a job in the
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3. After Submission

There are a few actions users want to take on submitted workflows. The ones implemented so far include report, cancel, and restart. report gets the workflow and job status and summarize the results using LSST labels. Internally this uses the WMS plugin to ask for the statuses. cancel aborts a submitted workflow killing any running jobs. The final job for the canceled workflow should still run to ensure the consistency of the central repository state. Internally this uses the WMS plugin to abort the workflow and its jobs. restart has two modes. As-is restart can be used if a workflow died due to infrastructure issues to retry the failed jobs as is and continue the workflow. This requires support from the workflow system. Re-submission could add a couple of options to the BPS configuration as well as other changes, including software version, and submit again which would produce a new QuantumGraph without the Quanta successfully completed. This does not require restart support from the workflow system.

4. Notable Workflow Needs

There have been a few workflow features that LSST workflows need that cause difficulties for various workflow management systems.

The Butler abstracts the data location from the code. It can directly read and write files in the repository making local cached copies when needed. Therefore, the science inputs and outputs are currently not included in the workflow, and the workflow system can expect the data to be in place when the jobs run. This means that the workflow system needs to support job dependencies without data dependencies or the plugin will need to fake the data dependencies.

There is the final job (see subsection 2.2) that should be executed regardless of whether a job failed. This is not typical behavior for jobs in most workflow systems, so the workflow system needs to have special support for this kind of job.

In order to efficiently share compute resources, many workload schedulers require knowing how much memory a job will need. Different input data can cause a particular job to require more memory than expected especially during development. Having the job automatically retry with a larger memory request if it was killed for memory is a desired feature.

5. Existing Plugins and Future Work

BPS was primarily constructed using HTCondor’s (Thain et al. 2005) DAGMan on a native HTCondor pool at NCSA. During the project’s construction period, pipeline...
developers also used this to run tests. Mini processing campaigns were also run every few weeks as larger scale tests.

Data Preview 0.2 (DP0.2; Yanny et al. [2022]), was generated by executing the workflows via a BPS plugin for the PanDA workflow system (Maeno et al. [2011]). This processing was done on the Interim Data Facility in a Google Cloud environment (O’Mullane et al. [2021]). While not currently officially maintained and supported by the core team, there is also a Pegasus (Deelman et al. [2015]) plugin and a Parsl (Babuji et al. [2019]) plugin.

Development is ongoing across the entire middleware. Besides updating for these changes and making plugin improvements, there are a few areas where work is planned. While still overall useful, BPS’s report has become less informative for the user with clustering. They want to know which Quanta failed and for what reason. Clustering also has caused problems with the current command lines. Work is ongoing for a special job runner that will solve the long command line issue as well as open avenues for other job-related functions across multiple workflow management systems such as sending output to real-time log aggregators.

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