Compute Pipelines with Advanced Data Management using Pegasus WMS
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Overview

- Pegasus is a system for mapping and executing abstract application workflows over a range of execution environments.
- The same abstract workflow can, at different times, be mapped to different execution environments such as XSEDE, OSG, commercial and academic clouds, campus grids, and clusters.
- Pegasus can easily scale both the size of the workflow, and the resources that the workflow is distributed over. Pegasus runs workflows ranging from just a few computational tasks up to 1 million.
- Pegasus Workflow Management System (WMS) consists of three main components: the Pegasus Mapper, HTCondor DAGMan, and the HTCondor Schedd.

Example: Montage Galactic Plane

- Generates mosaics from existing IPAC datasets
- Used to generate tiles 360 x 40 around the galactic equator
- Tiles are 5" x 5" with 1" overlap with neighbors
- One workflow for each of 17 bands (wavelengths)
- Each workflow uses 3.5TB of input imagery (1.6 million files)
- Each workflow consumes 30K CPU hours and produces 1,001 files in FITS format – data to be published publically in Amazon S3

Workflow Design and Mapping

- DAX Generator (DAGX)
- Easy to use APIs in Python, Java and Perl to generate an abstract workflow describing the users computation.
- Above is a simple two node hello world example.

Abstract Workflow (DAX)

- The abstract workflow rendered as XML. It only captures the computations the user wants to do and is devoid of any physical paths. Input and output files are identified by logical identifiers. This representation is portable between different execution environments.

Abstract to Executable Workflow (Condor DAG) Mapping

- The DAX is passed to the Pegasus Mapper and it generates a HTCondor DAGMan workflow that can be run on actual resource.
- The above example highlights addition of data movement nodes to staging in the input data and stage out the output data; addition of data cleanup nodes to remove data that is no longer required; and registration nodes to catalog output data locations for future discovery.

Data Flow For Pegasus Workflows at Runtime

- Data Flow for a Workflow with Pegasus
  1. Stagein jobs transfer input data for the workflow to the staging site
  2. Pegasus Lite wrapped jobs , when they start on compute worker nodes, pull in the input data from staging site
  3. The compute job executes on a local directory on the worker node.
  4. The PegasusLite wrapper pushes the output data from the worker node back to the staging site
  5. The Stageout jobs transfer the relevant output data out to the output site from staging site

Data Reuse Example

- Additional Capabilities Highlighted
  - Data Reuse: Jobs B and D are removed from the workflow as file f.d already exists. The f.d is staged in , instead of regenerating it by executing jobs B and D.
  - Job Clustering: Jobs C and E are clustered together into a single clustered job.
  - Cross Site Run: Single Workflow can be executed on multiple sites, with Pegasus taking care of the data movement between the sites.

Monitoring and Debugging

- At runtime, a database is populated with workflow and task runtime provenance, including which software was used and with what parameters, execution environment, runtime statistics and exit status.
- Pegasus comes with command line monitoring and debugging tools. A web dashboard now allows users to monitor their running workflows and check job status and output.

Pegasus Data Staging Configuration

- Non Shared Filesystem with Staging Site : Data is staged by Pegasus Lite at runtime from an external staging site. Popular on OSG with SRM as data staging server.
- CondorIO Data is staged using Condor File Transfers from submit node. Popular on OSG and Cloud Environments.
- Shared Filesystem (Head Node and the worker nodes of execution sites share a filesystem ). Popular on XSEDE and clusters.

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http://pegasus.isi.edu