Pegasus WMS: Enabling Large Scale Workflows on National Cyberinfrastructure

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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 different execution environments such as XSEDE, OSG, commercial and academic clouds, campus grids, and clusters.
- Pegasus Workflow Management System (WMS) consists of three main components: the Pegasus Mapper, HTCondor DAGMan, and the HTCondor Schedd.

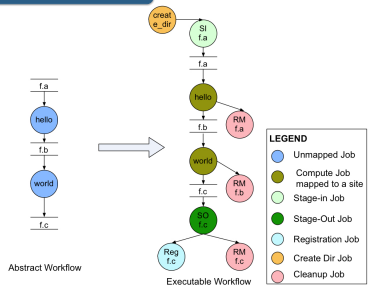
Features

- **Portability / Reuse** - User created abstract workflows can easily be run in different environments without alteration. The same workflow can run on a single system or across a heterogeneous set of resources.
- **Performance -** The Pegasus Mapper can reorder, group, and prioritize tasks in order to increase the overall workflow performance.
- **Scalability** - 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.
- **Data Management** - Pegasus handles replica selection, data transfers and output registrations in data catalogs. These tasks are added to a workflow as auxiliary jobs by the Pegasus Mapper.
- **Reliability** - Jobs and data transfers are automatically retried in case of failures. When errors occur, Pegasus tries to recover when possible by retrying tasks, by retrying the entire workflow and by providing workflow-level checkpointing, by re-mapping portions of the workflow
- **Monitoring and Debugging–** Command line monitoring and debugging tools to debug large scale workflows. Debugging tools such as *pegasus-analyzer* helps the user to debug the workflow in case of non-recoverable failures.
- **Workflow and Task level notifications** (email, instant messenger, user defined script callout)

Workflow Design and Mapping

```
#!/usr/bin/env python

from Pegasus.DAX3 import *
import sys
import os

# Create a abstract dag
dax = ADAG("hello_world")

# Add the hello job
hello = Job(namespace="hello_world",
            name="hello", version="1.0")
b = File("f.b")
hello.uses(a, link=Link.INPUT)
hello.uses(b, link=Link.OUTPUT)
dax.addJob(hello)

# Add the world job (depends on the hello job)
world = Job(namespace="hello_world",
            name="world", version="1.0")
c = File("f.c")
world.uses(b, link=Link.INPUT)
world.uses(c, link=Link.OUTPUT)
dax.addJob(world)

# Add control-flow dependencies
dax.addDependency(Dependency(parent=hello,
                             child=world))

# Write the DAX to stdout
dax.writeXML(sys.stdout)
```

```
<?xml version="1.0" encoding="UTF-8"?>

<!-- generator: python -->
<adag xmlns="http://pegasus.isi.edu/schema/DAX"
      version="3.4" name="hello_world">

    <!-- describe the jobs making
         up the hello world pipeline -->
    <job id="ID0000001" namespace="hello_world"
         name="hello" version="1.0">

        <uses name="f.b" link="output"/>
        <uses name="f.a" link="input"/>
    </job>

    <job id="ID0000002" namespace="hello_world"
         name="world" version="1.0">

        <uses name="f.b" link="input"/>
        <uses name="f.c" link="output"/>
    </job>

    <!-- describe the edges in the DAG -->
    <child ref="ID0000002">
        <parent ref="ID0000001"/>
    </child>
</adag>
```



DAX Generator API

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)

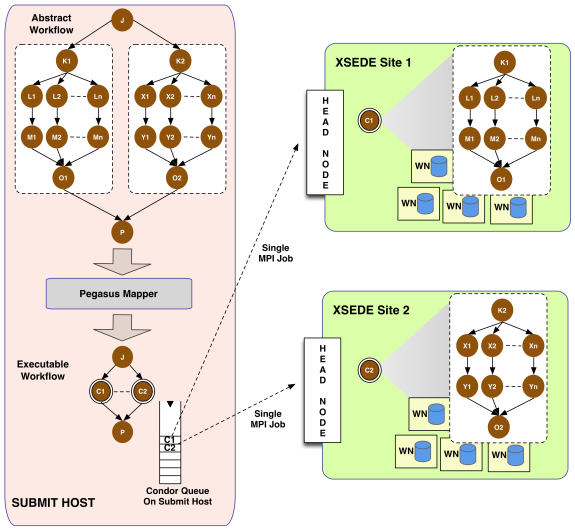
The abstract workflow rendered as XML . It only captures the computations the user wants to do and is devoid of any physical paths. Input and output files are identified by logical identifiers. This representation is portable between different execution environments.

Abstract to Executable Workflow Mapping

The DAX is passed to the Pegasus Mapper and it generates an executable 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.

Fine-grained Workflows on XSEDE Using MPI Clustering



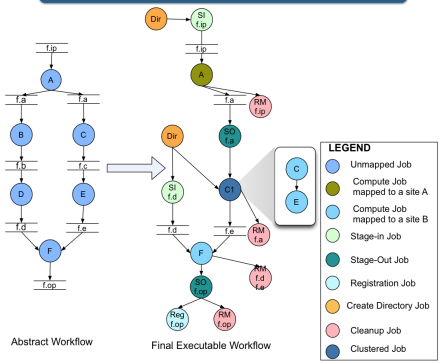
Problem: How can you efficiently execute fine-grained workflows on HPC resources? These workflows can have a large number of tasks which cannot all be submitted to the HPC resource's queue, and the tasks can have a mix of different core and memory requirements.

Solution: The workflow is partitioned into independent sub graphs, which are submitted as self-contained Pegasus MPI Cluster (PMC) jobs to the remote sites.

A PMC job is expressed as a DAG and PMC uses the master-worker paradigm to farm out individual tasks to worker nodes. PMC acts a scheduler and considers core and memory requirements of the tasks when making scheduling decisions.

PMC can be easier to setup than pilot jobs / glideins as no special networking is required. PMC relies on standard MPI constructs.

Canonical Workflow 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.

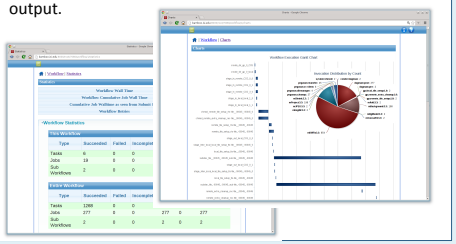
Job Clustering: Jobs C and E are clustered together into a single clustered job.

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 jobs status and output.



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http://pegasus.isi.edu