Pegasus WMS: Leveraging Condor for Workflow Management

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http://pegasus.isi.edu
Examples of Applications

- **Providing a service to a community** (Montage project)
  - Data and derived data products available to a broad range of users
  - A limited number of small computational requests can be handled locally
  - For large numbers of requests or large requests need to rely on shared cyberinfrastructure resources
  - On-the-fly analysis generation, portable analysis definition

- **Supporting community-based analysis** (SCEC project)
  - Codes are collaboratively developed
  - Codes are “strung” together to model complex systems
  - Ability to correctly connect components, scalability

- **Processing large amounts of shared data on shared resources** (LIGO project)
  - Data captured by various instruments and cataloged in community data registries.
  - Amounts of data necessitate reaching out beyond local clusters
  - Automation, scalability and reliability

- **Automating the work of one scientist** (SIPHT Project, Broad Institute, Epigenomic project, USC)
  - Data collected in a lab needs to be analyzed in several steps
  - Automation, efficiency, and flexibility (scripts age and are difficult to change)
  - Need to have a record of how data was produced
Reasons to use scripts to represent analysis

- You can script something in an afternoon
- You can submit a job directly to a pbs queue or Condor pool
- You can look at stderr to see what went wrong
- You can add calls to measure performance
- You don’t need to learn another language or system
Why Scientific Workflows?

- Workflows can be portable across platforms and scalable
- Workflows are easy to reuse
- Can be shared with others
  - Gives a leg-up to new staff, GRAs, PostDocs, etc
- Workflow Management Systems (WMS) can help recover from failures and optimize overall application performance
- WMS can capture provenance and performance information
- WMS can leverage debugging and monitoring tools
Workflow Lifecycle

Reuse
- Data Products
- Adapt, Modify
- Workflow and Component Libraries

Creation
- Data, Metadata Catalogs
- Populate with data
- Workflow Instance

Planning
- Resource, Application Component Descriptions

Scheduling/Execution
- Compute, Storage and Network Resources
- Execute
- Map to available resources
Our Philosophy

- Work closely
  - with users to improve software, make it relevant
  - with CS colleagues to develop new capabilities, share ideas, and develop complex systems

- Users
  - Enable them to author workflows in a way comfortable for them
  - Allow users to enter the system at any point
  - Provide reliability, scalability, performance

- Software
  - Be a “good” CI ecosystem member
    - Focus on one aspect of the problem and contribute solutions
    - Leverage existing solutions where possible

- Execution Environment
  - Use whatever we can, support heterogeneity
Our Approach

• **Representation**
  - Support a declarative representation for the workflow (dataflow)
  - Represent the workflow structure as a Directed Acyclic Graph (DAG)
  - Use recursion to achieve scalability

• **System**
  - Layered architecture, each layer is responsible for a particular function
  - Mask errors at different levels of the system
  - Modular, composed of well-defined components, where different components can be swapped in
  - Open—provides a number of interfaces to enter the system, and exposes interfaces to other CI entities
  - Use and adapt existing graph and other relevant algorithms
Our system, Pegasus WMS
Pegasus WMS, layering functionality

- Condor Schedd
  - A robust task management and execution capability
- DAGMan
  - A workflow executor
  - Scalable and reliable execution of an executable workflow, adaptivity
- Pegasus Mapper
  - a workflow “compiler”
  - target language - DAGMan’s DAG and Condor submit files
    - Generated an executable workflow
  - transforms the workflow for performance and reliability
- Abstract Workflows
  - identifies only the computations that a user wants to do
  - devoid of resource descriptions
  - devoid of data locations
Pegasus:
Selects an execution site
Selects a data archive
Creates a workflow that
• Creates a “sandbox” on the execution site
• Stages data
• Invokes the computation
• Stages out data
• Registers data and Cleans up execution site
• Captures provenance information

Perform other optimizations
Populated by user or community
Transformation Catalog

DAX snippet

Populated automatically through pegasus-get-sites* or by the user

*OSG interface provided by Vikas Patel and Sebastian Goasguen
The LIGO example, migrating up the software stack

- LIGO has been using DAGMan for its scientific analysis
- **Issue 1**: LIGO users log onto a particular cluster and launch computations there (no load balance)
- **Issue 2**: Sometimes part of input data is “vetoed” and needs to be eliminated from the analysis, so potentially large amounts of redundant work need to be redone
- **Issue 3**: Some tasks are very short running and incur large overheads
- **Issue 4**: Want to be able to run the same workflow on other Grids (OSG), and share analyses with EU colleagues
- **Issue 5**: Want to be able to keep parts of a pipeline as a DAG—for legacy visualization pipelines
- **Issue 6**: For large workflows, it is difficult to analyze the DAGMan/Condor logs to pinpoint problems
LIGO on OSG and LDG

Total 5402 jobs
~800 CPU hours cumulative
LIGO Issues

- **Issue 1**: LIGO users log onto a particular cluster and launch computations there (no load balance)
  - Pegasus uses information services or user-provided information to schedule an entire workflow onto a single cluster or across clusters
  - Pegasus brings back intermediate and final results to a user-specified location

- **Issue 2**: Sometimes part of input data is “vetoed” and needs to be eliminated from analysis, so potentially large amounts of redundant work need to be redone
  - Pegasus has the concept of “virtual data” where if data are already available it will be reused
  - If the same workflow is re-submitted, and some intermediate data are already available, the executable workflow will reuse it ➔ efficient execution, scientists can start analysis without waiting for final “vetoes”

- **Issue 3**: Some tasks are very short running and incur large overheads
  - Pegasus can automatically cluster tasks together so that they are treated as one by DAGMan, Condor, and the target execution system
● **Issue 4:** Want to be able to run on other Grids, and share analyses with EU colleagues
  
  ● Pegasus DAXes are devoid of resource information, so to run a DAX in a new environment, only “local” info about resources and data locations needs to be given separately, Pegasus will generate the right DAG and Condor Submit files

● **Issue 5:** Want to be able to keep parts of a pipeline as a DAG—legacy visualization pipelines
  
  ● You can embed a DAG into a DAX and this information will be passed through to DAGMan ➔ You can use any DAGMAN features inside a DAX
Issue 6: Difficulty analyzing the DAGMan/Condor logs to pinpoint problems

Developed pegasus-analyzer that can traverse

- the DAGMan.out and Condor's *.err and *.out information

“This is so much easier!” -- Duncan Brown, LIGO

```
===================lalapps_tmpltbank_ID002291===========================
last state: JOB_FAILURE
  site: local
submit file: /usr1/ilya/log/H1L1V1-s6_highmass_ihope-937800015-4197585.3CpZuA/datafind/lalapps_tmpltbank_ID002291.sub
output file: /usr1/ilya/log/H1L1V1-s6_highmass_ihope-937800015-4197585.3CpZuA/datafind/lalapps_tmpltbank_ID002291.out
error file: /usr1/ilya/log/H1L1V1-s6_highmass_ihope-937800015-4197585.3CpZuA/datafind/lalapps_tmpltbank_ID002291.err

------------------------- lalapps_tmpltbank_ID002291.out-------------------------
-------------------------lalapps_tmpltbank_ID002291.err-------------------------
```

XLAL Error - XLALFrNext: gap in frame data
XLAL Error - XLALFrNext: time 941096000.000000 is end of frame 3999 of file URL
  file://localhost/frames/VSR2/HrecOnline/V1/V-HrecOnline-941/V-HrecOnline-941092000-4000.gwf
XLAL Error - XLALFrNext: time 941100000.000000 is start of frame 0 of file URL
  file://localhost/frames/VSR2/HrecOnline/V1/V-HrecOnline-941/V-HrecOnline-941100000-4000.gwf
XLAL Error - XLALFrNext (FrameStream.c:608): Invalid time
Error[2] 8192: function LALFrNext, file FrameStream.c, line 1046, $Id$
ABORT: Gap in the data

```
```

................................
● Developing a browser-based visualization for performance and failure analysis

● “When LIGO inspiral group switched the from DAGs to DAXes—we did not notice, the results were delivered as before” -- Frederique Marion, LIGO-Virgo CBC Group
Challenges in workflow reliability *leveraging the software layers*

- Resources fail
  - Provide a retry mechanism
- Services fail (data movement, data registration)
  - Retry the action, choose a different service
- Computations fail within a workflow
  - Checkpoint the workflow
- Storage gets filled up
  - Analyze the workflow and clean up unneeded data as the workflow execution progresses
NMI Test and Build Lab

Production releases

Nightly builds and tests
3 Pegasus packages
(Mapper, WMS, Worker)
15 platforms
.tar.gz / .deb / .rpm
• Latest code is pulled from the Pegasus SVN, built and tested.
• Generated packages (~50) are automatically pushed back to the Pegasus website

Pinned Condor release build used as input to the WMS package
Future Directions

• Debugging workflows is still difficult
  • Need to be able to interpret errors
  • Analyze what happened
  • Need to be able to provide error information at the level needed by the user

• Online monitoring is still an issue for large workflows (teaming up with Netlogger)

• Automatically exploiting data parallelism, how to subdivide a data set

• Generate computational bundles (data, codes, configurations) – automated boinc
Want to try?
pegasus@isi.edu
● Hands-on help
http://pegasus.isi.edu
● Tutorial materials

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**Related Technologies:** Corral-WMS Th. pm by Mats Rynge