Pegasus WMS – Automated Data Management in Shared and Nonshared Environments

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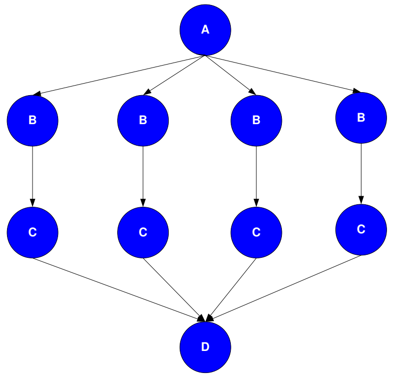
Pegasus Workflow Management System

- NSF funded project and developed since 2001 as a collaboration between USC Information Sciences Institute and the HTCondor Team at UW Madison

- Builds on top of HTCondor DAGMan.

- Abstract Workflows - Pegasus input workflow description
  - Workflow "high-level language"
  - Only identifies the computation, devoid of resource descriptions, devoid of data locations

- Pegasus is a workflow "compiler" (plan/map)
  - Target is DAGMan DAGs and HTCondor submit files
  - Transforms the workflow for performance and reliability
  - Automatically locates physical locations for both workflow components and data
  - Collects runtime provenance

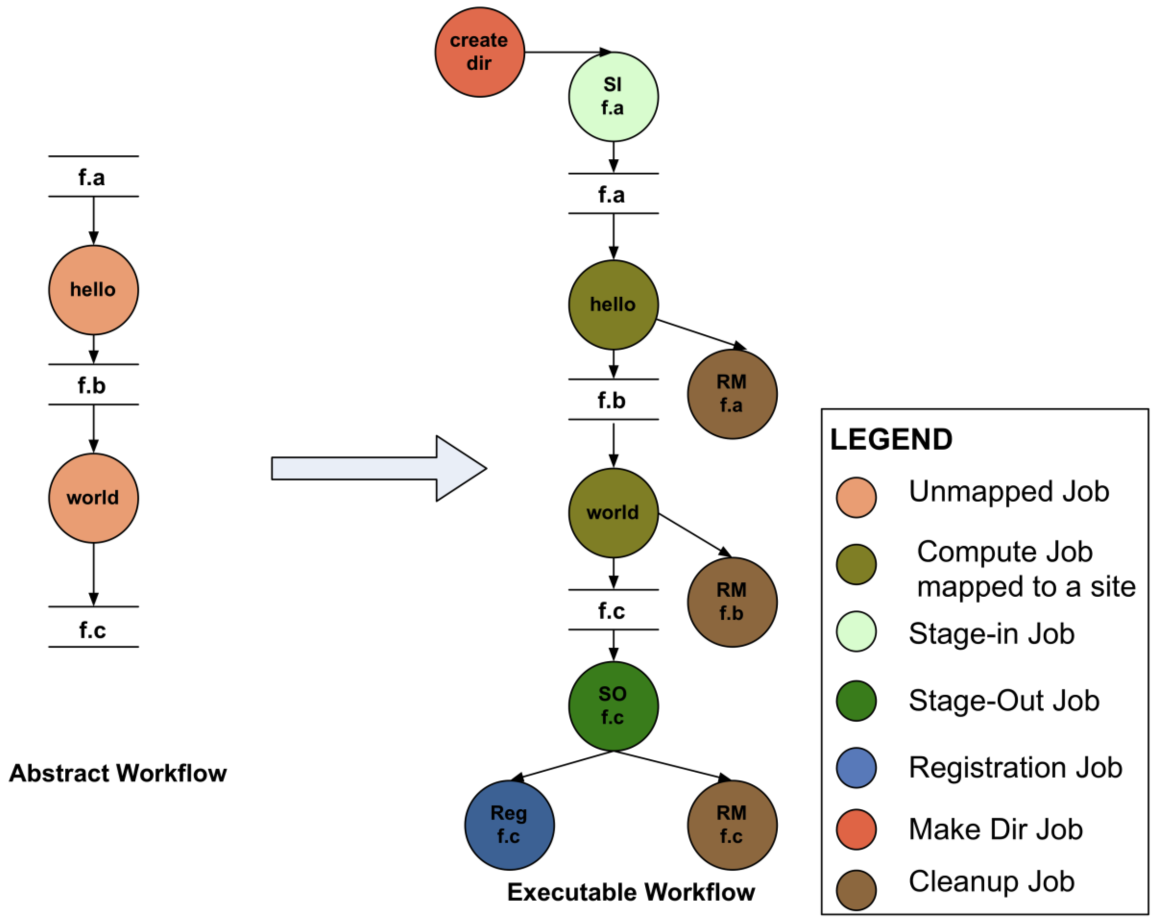


Abstract Workflow

```python
#!/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
<?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>
```

Abstract to Executable Workflow Mapping



- **Abstraction provides**
  - Ease of Use (do not need to worry about low-level execution details)
  - Portability (can use the same workflow description to run on a number of resources and/or across them)
  - Gives opportunities for optimization and fault tolerance
    - automatically restructure the workflow
    - automatically provide fault recovery (retry, choose different resource)

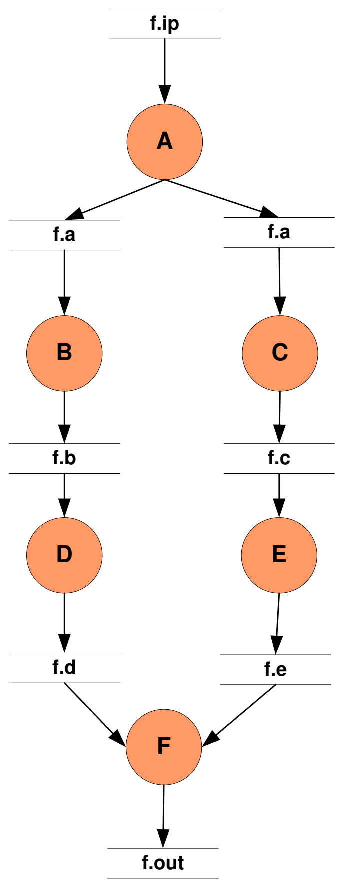
Supported Data Staging Approaches

- Shared Filesystem setup (typical of XSEDE and HPC sites)
  - Worker nodes and the head node have a shared filesystem, usually a parallel filesystem with great I/O characteristics

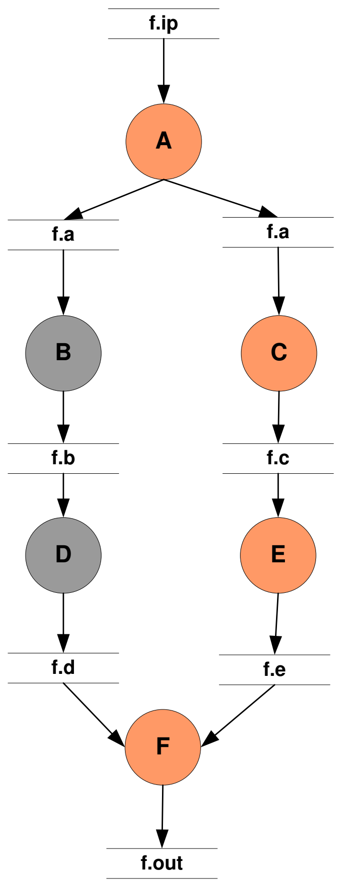
- Condor IO
  - Worker nodes don't share a filesystem
  - Data is pulled from / pushed to the submit host via Condor file transfers

- NonShared filesystem setup using an existing storage element for staging (typical of OSG and campus Condor pools)
  - Worker nodes don't share a filesystem.
  - Data is pulled from / pushed to the existing storage element.

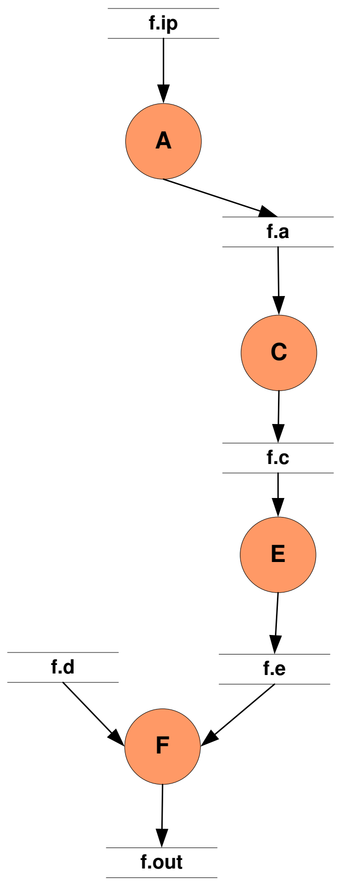
Workflow Reduction (Data Reuse)



Abstract Workflow

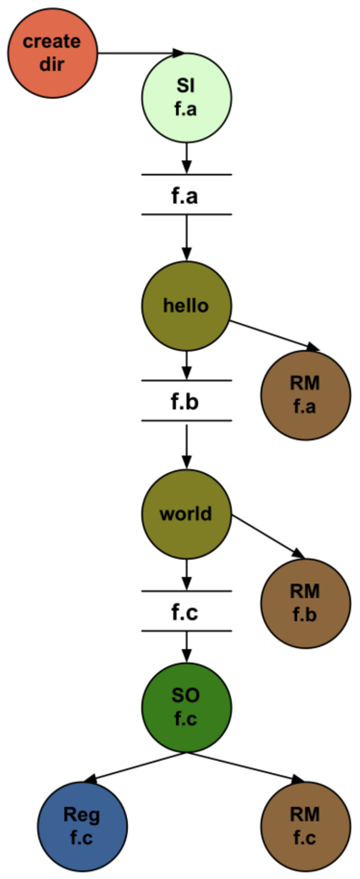


File f.d exists somewhere.
Reuse it.
Mark Jobs D and B to delete

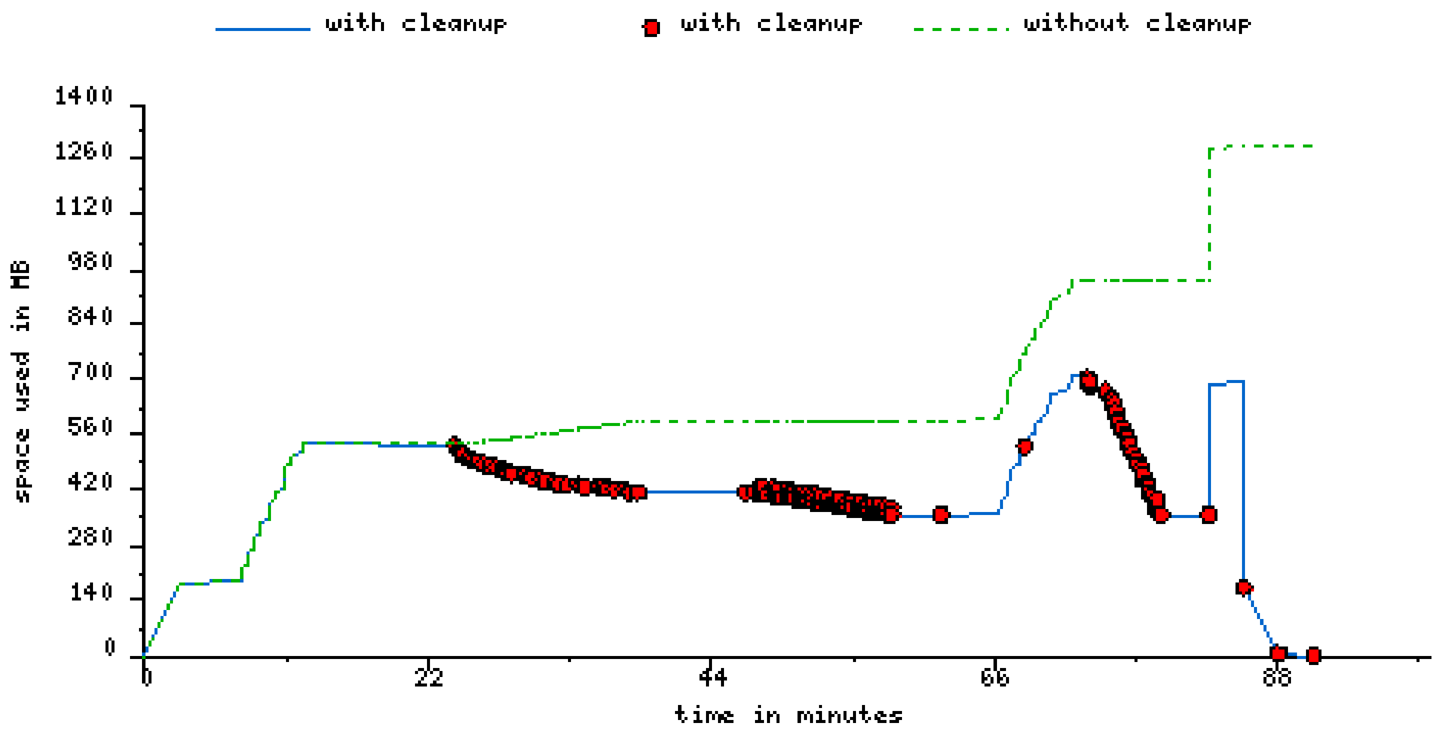


Delete Job D and Job B

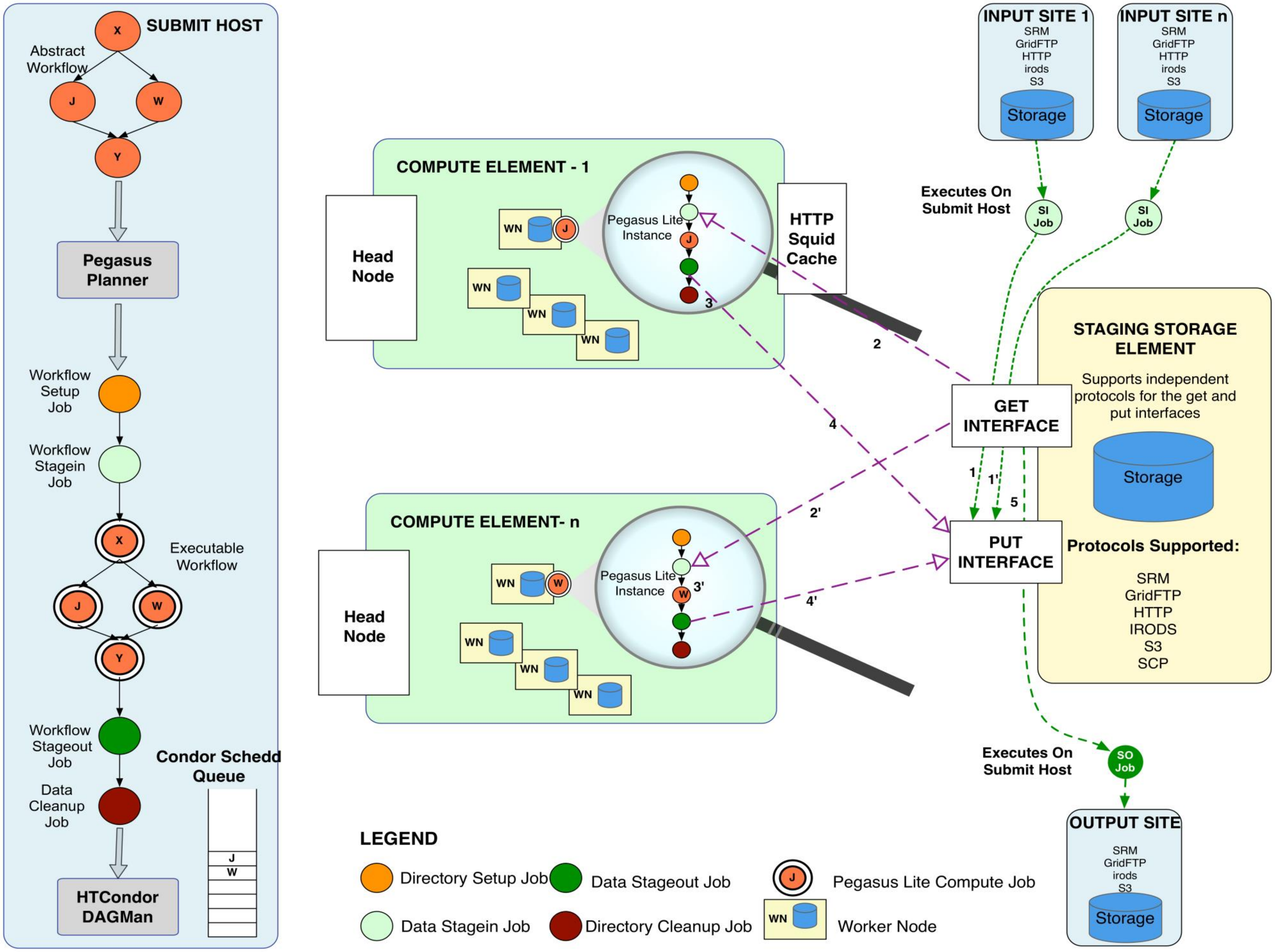
File cleanup (cont)

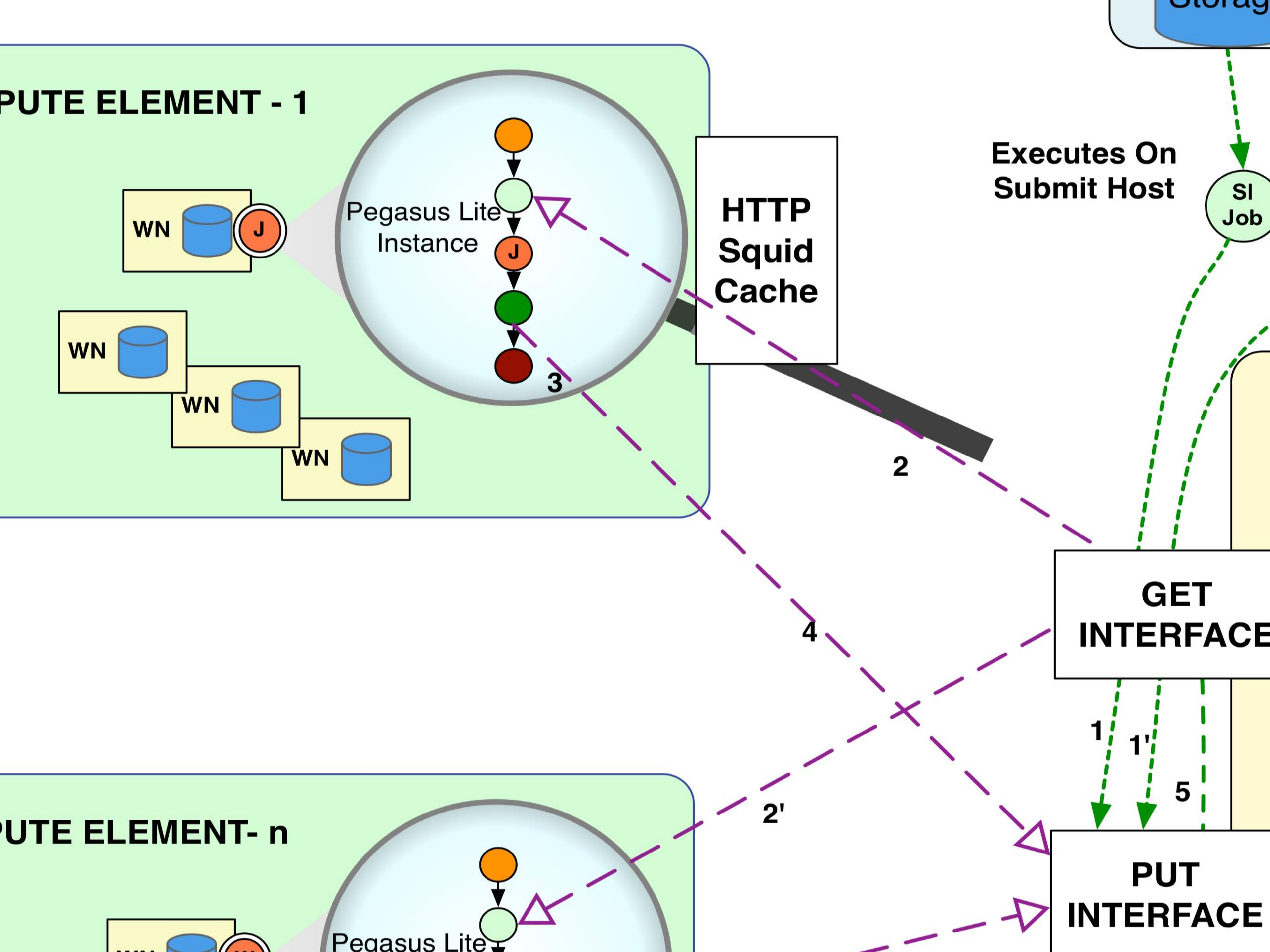


Executable Workflow



Montage 1 degree workflow run with cleanup


SUBMIT HOST
Abstract Workflow
X
J
W
Y
Pegasus Planner
Workflow Setup Job
Workflow Stagein Job
Executable Workflow
Workflow Stageout Job
Data Cleanup Job
Condor Schedd Queue
HTCondor DAGMan
COMPUTE ELEMENT - 1
COMPUTE ELEMENT- n
Head Node
WN
Pegasus Lite Instance
HTTP Squid Cache
INPUT SITE 1
INPUT SITE n
SRM
GridFTP
HTTP
irods
S3
Storage
Executes On Submit Host
SI Job
STAGING STORAGE ELEMENT
Supports independent protocols for the get and put interfaces
GET INTERFACE
PUT INTERFACE
Protocols Supported:
SRM
GridFTP
HTTP
IRODS
S3
SCP
1
1'
2
2'
3
3'
4
4'
5
SO Job
OUTPUT SITE
LEGEND
Directory Setup Job
Data Stageout Job
Pegasus Lite Compute Job
Data Stagein Job
Directory Cleanup Job
Worker Node


PUTE ELEMENT - 1
Pegasus Lite Instance
J
WN
WN
WN
WN
3
HTTP Squid Cache
2
4
Executes On Submit Host
SI Job
GET INTERFACE
1
1'
5
2'
PUTE ELEMENT- n
Pegasus Lite
PUT INTERFACE

pegasus-transfer subsystem

- Command line tool used internally by Pegasus workflows
- Input is a list of source and destination URLs
- Transfers the data by calling out to tools – provided by the system (cp, wget, …) Pegasus (pegasus-gridftp, pegasus-s3) or third party (gsutil)
- Transfers are parallelized
- Transfers between non-compatible protocols are split up into two transfers using the local filesystem as a staging point
  - for example: GridFTP->GS becomes GridFTP->File and File->GS

Supported URLs

GridFTP
SRM
iRods
S3
GS
SCP
HTTP
File
Symlink

Relevant Links

http://pegasus.isi.edu

Tutorial and documentation:

http://pegasus.isi.edu/wms/docs/latest/

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Catalogs

- Pegasus uses 3 catalogs to fill in the blanks of the abstract workflow
- Site catalog
  - Defines the execution environment and potential data staging resources
  - Simple in the case of Condor pool, but can be more complex when running on grid resources
- Transformation catalog
  - Defines executables used by the workflow
  - Executables can be installed in different locations at different sites
- Replica catalog
  - Locations of existing data products – input files and intermediate files from previous runs