Using Pegasus 3.0 for data-based workflows on the OSG

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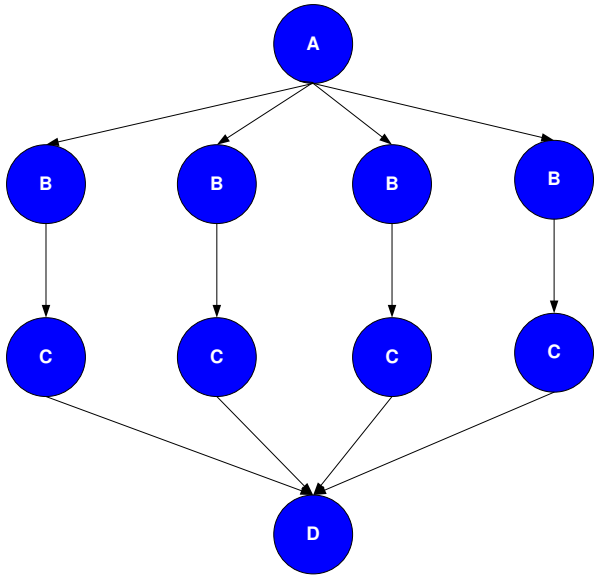
Pegasus: Planning for Execution in Grids

- Abstract Workflows - Pegasus input workflow description
  - Workflow "high-level language"
  - Only identifies the computation, devoid of resource descriptions, devoid of data locations
- Pegasus
  - Workflow "compiler" (plan/map)
  - Target is DAGMan DAGs and Condor submit files
  - Transforms the workflow for performance and reliability
  - Automatically locates physical locations for both workflow components and data
  - Provides runtime provenance



How to generate a DAX

- Use the Pegasus Java, Perl, Python APIs
- Use Wings for semantically rich workflow composition (http://www.isi.edu/ikcap/wings/)
- Write the XML directly

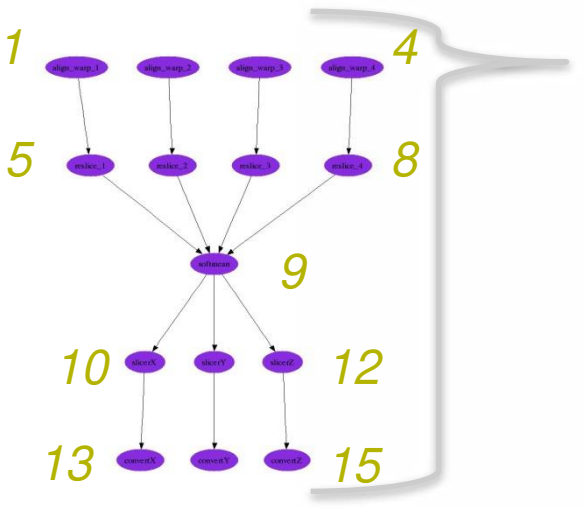
```
<!-- part 1: list of all files used (may be empty) -->
  <filename file="f.input" link="input"/>
  <filename file="f.intermediate" link="input"/>
  <filename file="f.output" link="output"/>

<!-- part 2: definition of all jobs (at least one) -->
  <job id="ID000001" namespace="pegasus" name="preprocess" version="1.0" >
          <argument>-a top -T 6  -i <filename file="f.input"/>  -o <filename file="f.inter
          </argument>
          <uses file="f.input" link="input" dontRegister="false" dontTransfer="false"/>
          <uses file="f.intermediate" link="output" dontRegister="true" dontTransfer="
```

Basic Workflow Mapping

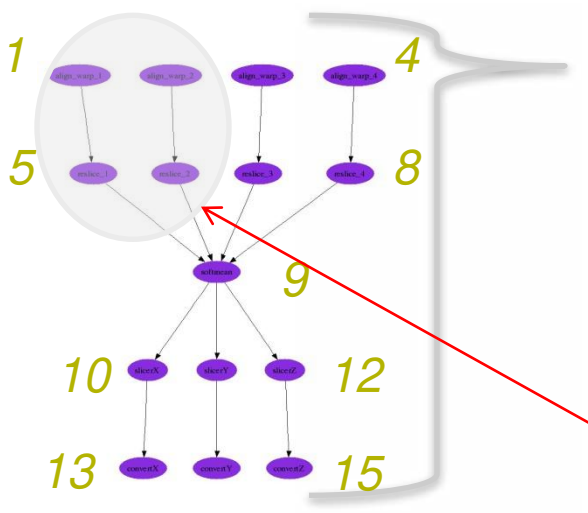
- Select where to run the computations
  - Change task nodes into nodes with executable descriptions
    - Execution location
    - Environment variables initializes
- Select which data to access
  - Add stage-in nodes to move data to computations
  - Add stage-out nodes to transfer data out of remote sites to storage
  - Add data transfer nodes between computation nodes that execute on different resources

Additional Mapping Elements

- Add data cleanup nodes to remove data from remote sites when no longer needed
  - reduces workflow data footprint
- Cluster compute nodes in small computational granularity applications
- Add nodes that register the newly-created data products
- Provide provenance capture steps
  - Information about source of data, executables invoked, environment variables, parameters, machines used, performance
- Scale matters - today we can handle:
  - 1 million tasks in the workflow instance (SCEC)
  - 10TB input data (LIGO)

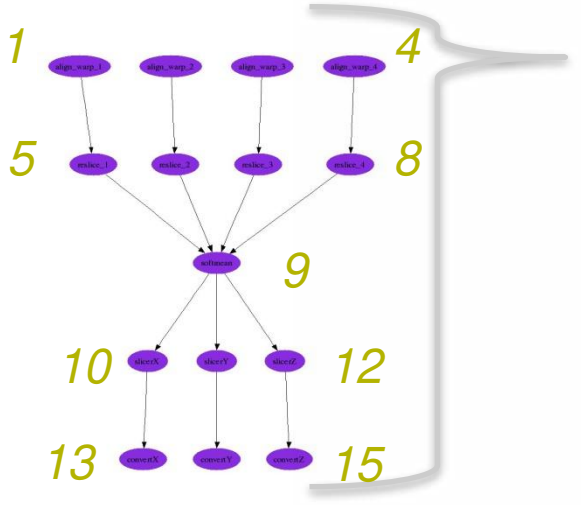


Original workflow: 15 compute nodes devoid of resource assignment



Original workflow: 15 compute nodes devoid of resource assignment

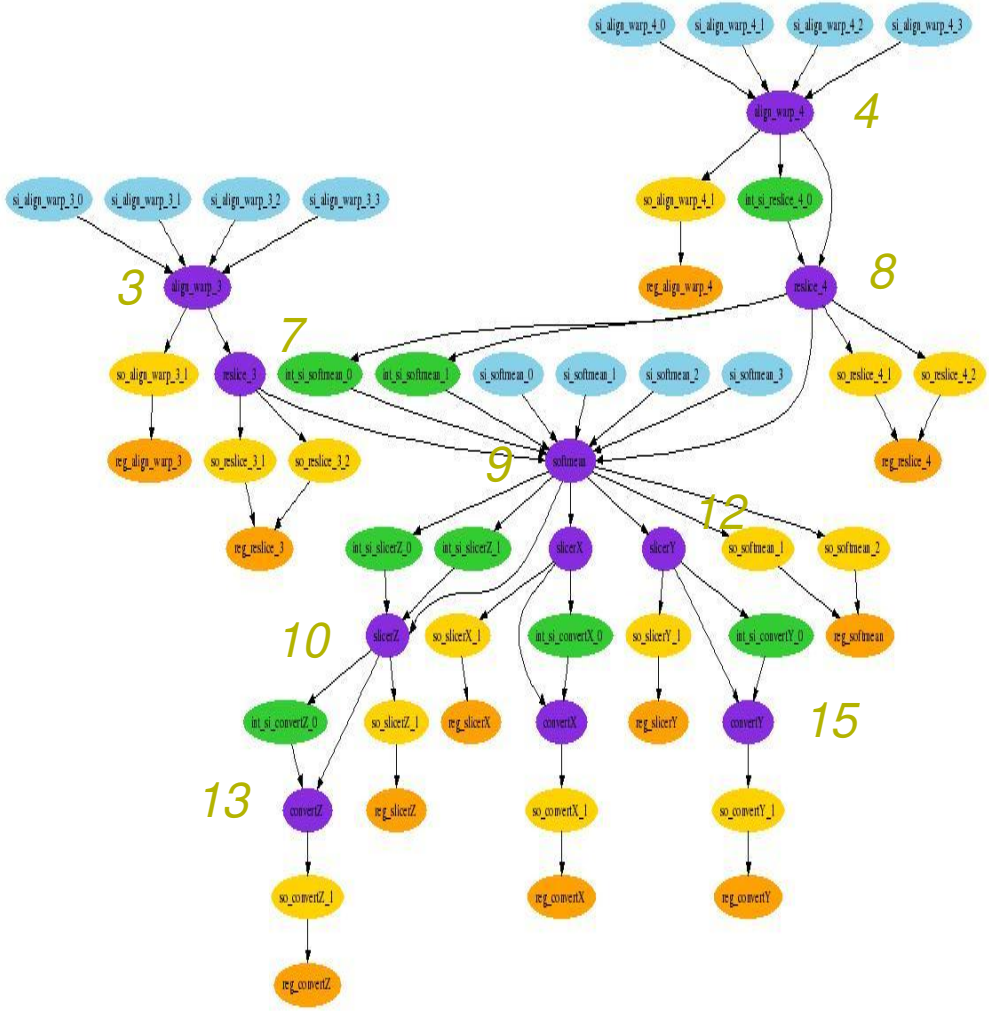
Assume the results of these computations are already available



Original workflow: 15 compute nodes devoid of resource assignment

Resulting workflow mapped onto 3 Grid sites:

13 data stage-in nodes
11 compute nodes (4 reduced based on available intermediate data)
8 inter-site data transfers
14 data stage-out nodes to long-term storage
14 data registration nodes (data cataloging)



Catalogs used for discovery

- To execute in a distributed environment Pegasus needs to discover
  - Data (the input data that is required by the workflows)
    - Replica catalog, data registry, db, dax
  - Executables (application executables already installed or can that be dynamically staged)
    - Transformation catalog, dax
  - Site Layout (site services and environment)
    - Site catalog

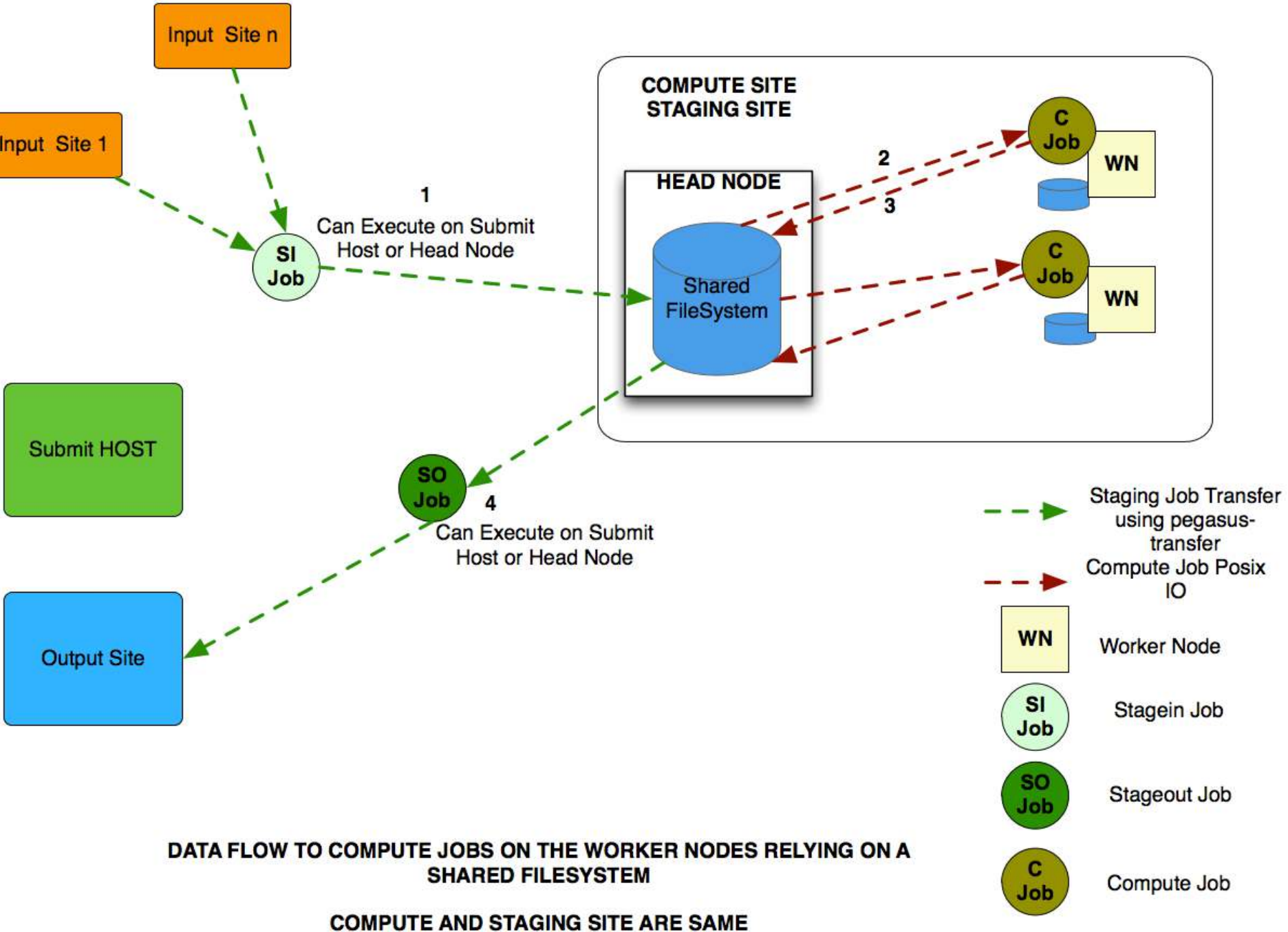
Discovery of Data

- Replica Catalog stores mappings between logical files and their target locations.
- Interfaces with a variety of replica catalogs
  - File based Replica Catalog
    - useful for small datasets
    - cannot be shared across users
  - Database based Replica Catalog
    - useful for medium sized datasets.
    - can be used across users

Discovery of Site Layout

- Pegasus queries a site catalog to discover site layout
  - Job submission points for different types of schedulers
  - Data transfer servers
  - Local Replica Catalogs where data residing in that site has to be catalogued
  - Site Wide Profiles like environment variables
  - Work and storage directories

The pegasus-sc-client can pull the site information from ReSS or OSGMM



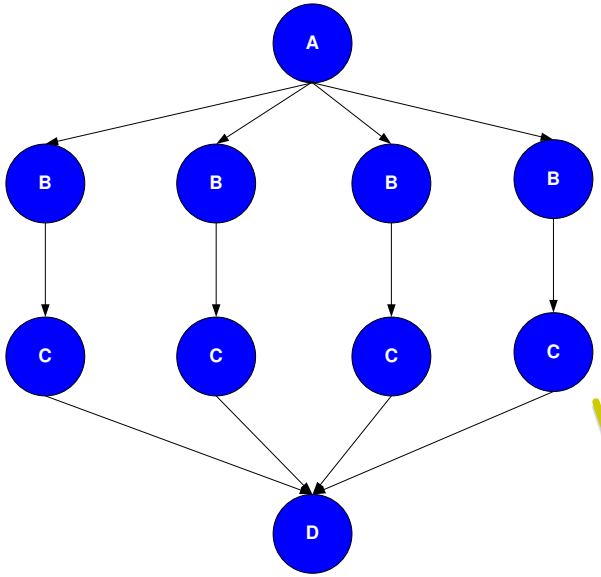
DATA FLOW TO COMPUTE JOBS ON THE WORKER NODES RELYING ON A SHARED FILESYSTEM

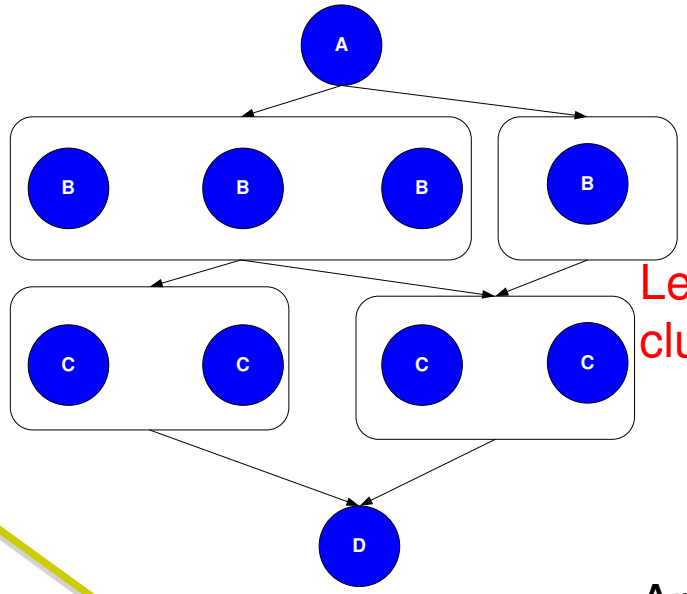
COMPUTE AND STAGING SITE ARE SAME

Optimizations during Mapping

- Node clustering for fine-grained computations
  - Can obtain significant performance benefits for some applications (in Montage ~80%, SCEC ~50%)
- Data reuse in case intermediate data products are available
  - Performance and reliability advantages—workflow-level checkpointing
- Data cleanup nodes can reduce workflow data footprint
  - by ~50% for Montage, applications such as LIGO need restructuring

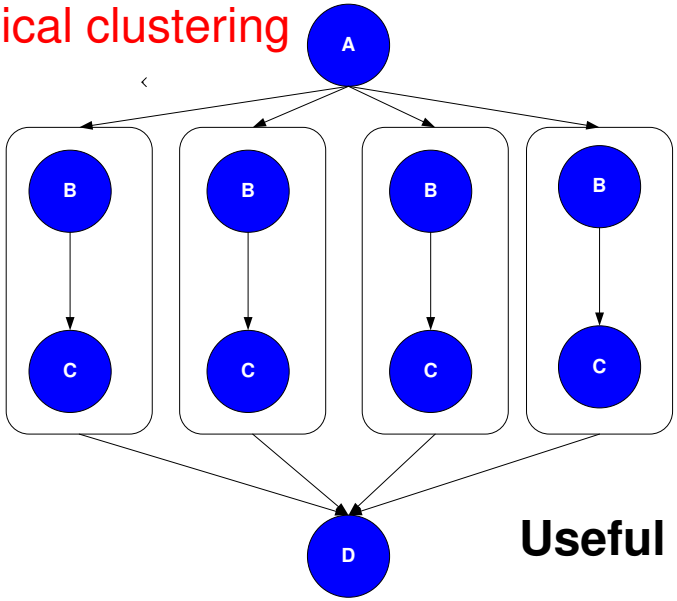
Job clustering



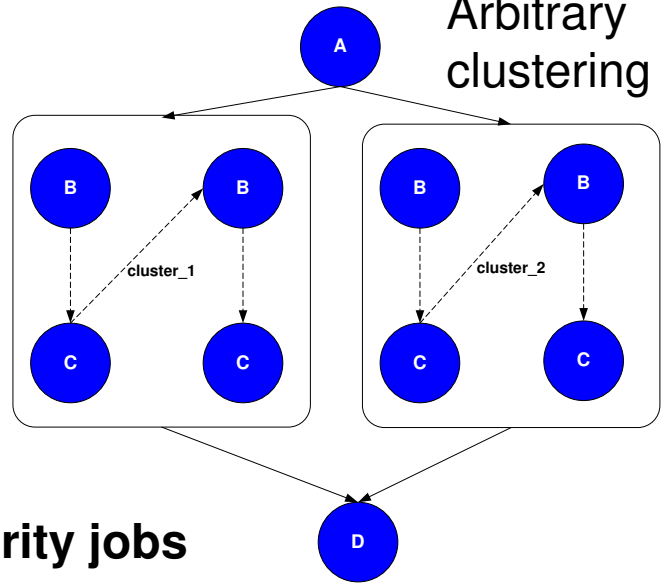


Level-based clustering

Vertical clustering

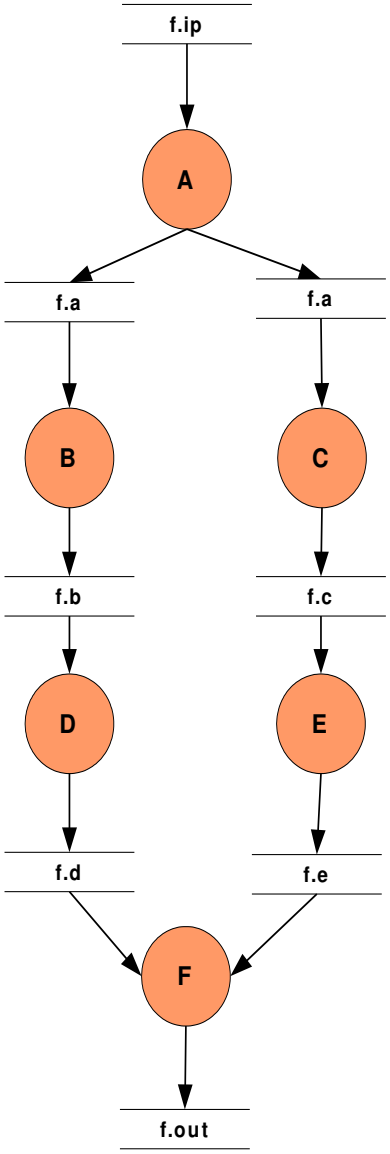


Arbitrary clustering

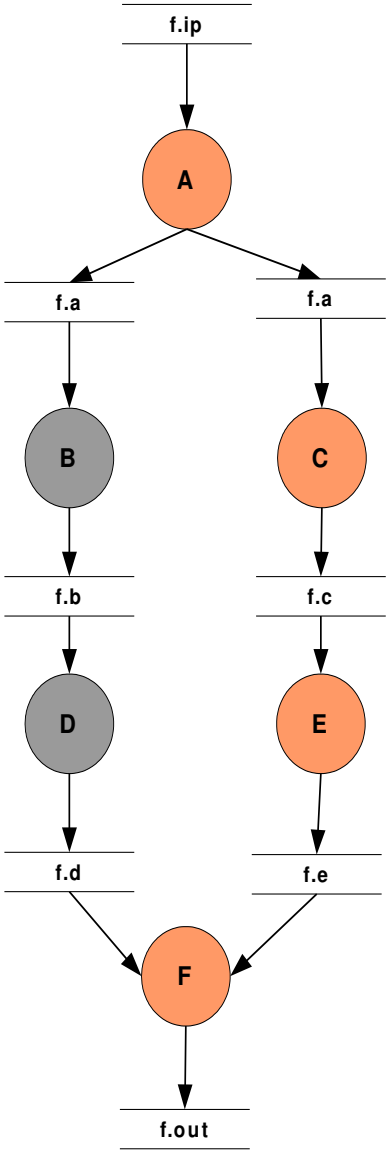


Useful for small granularity jobs

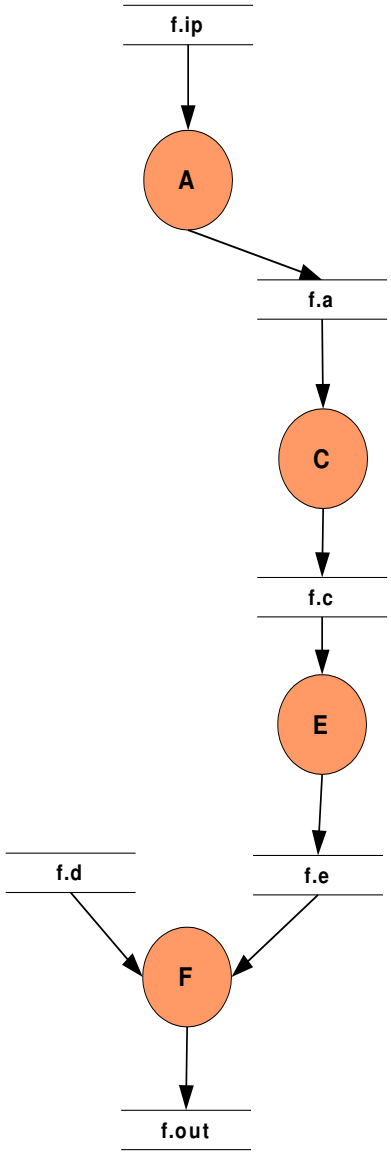
Workflow Reduction (Data Reuse)



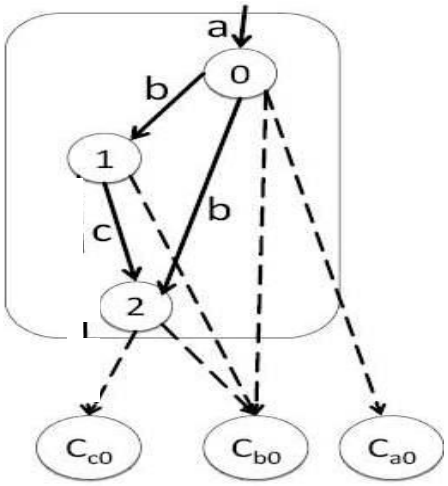
Abstract Workflow



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

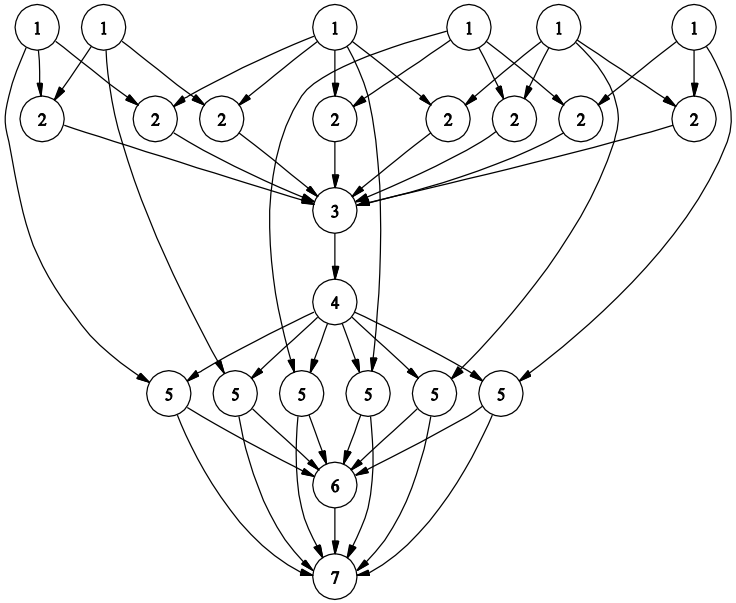


Delete Job D and Job B

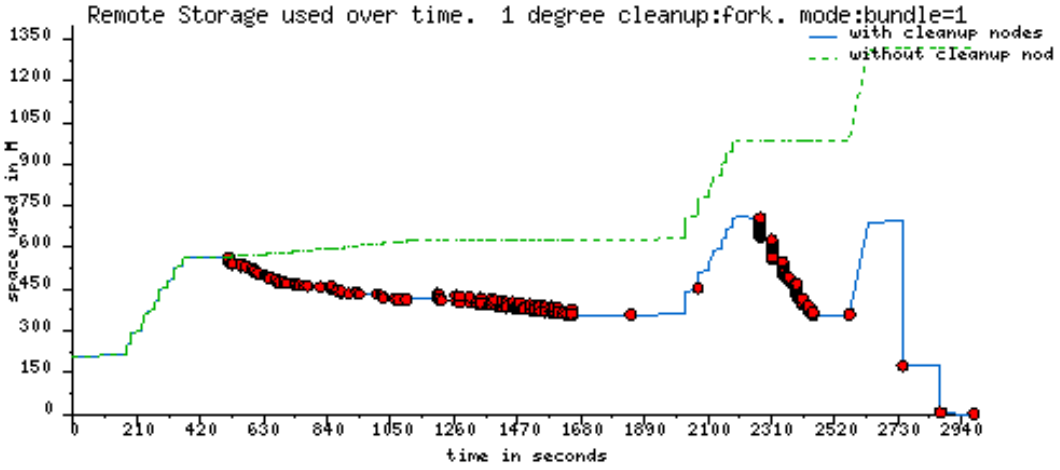


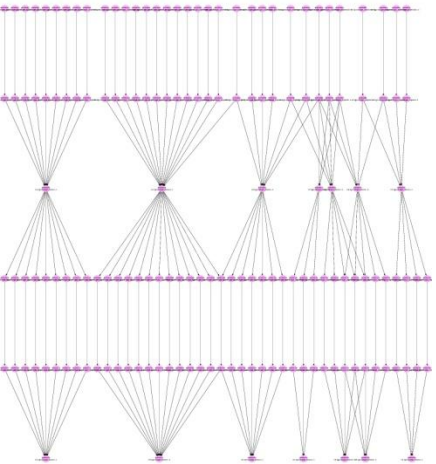
Data Cleanup

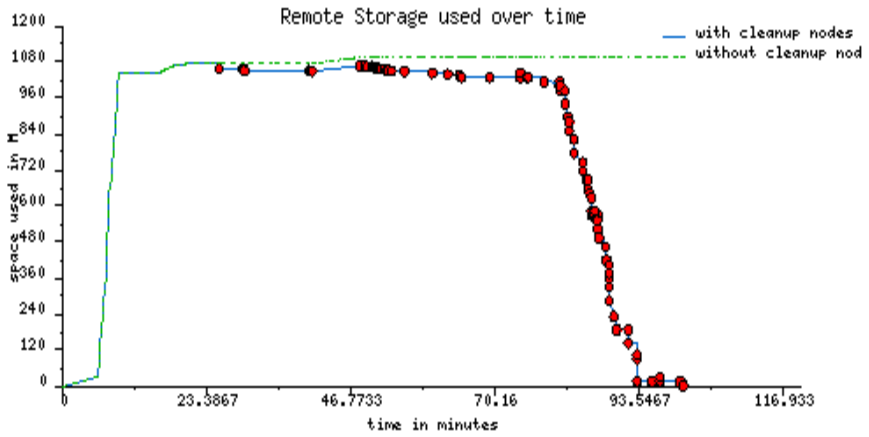
Adding cleanup nodes to the workflow



1.25GB versus 4.5 GB

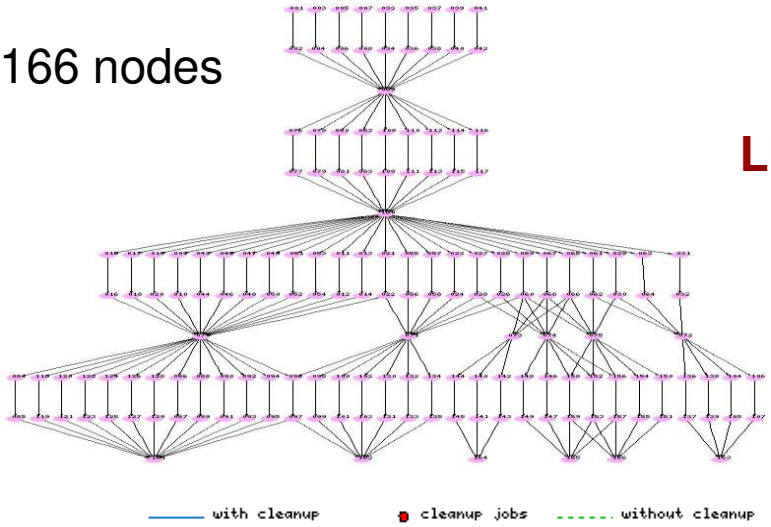




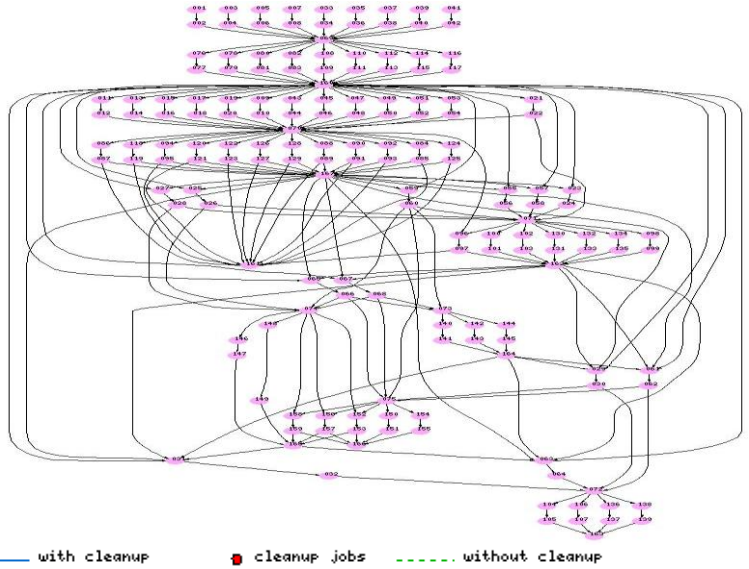


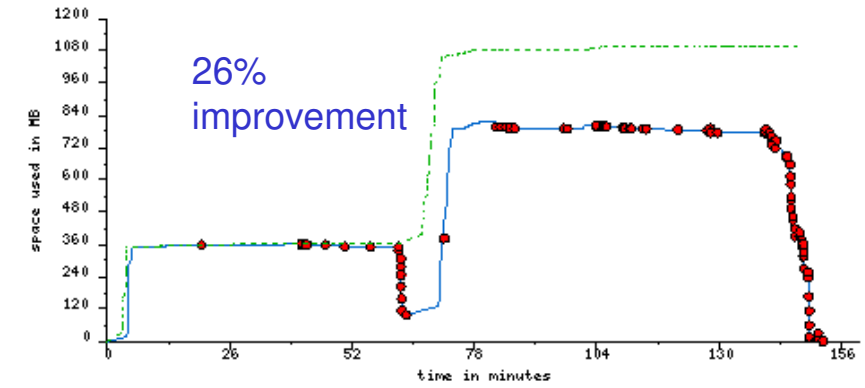
Full workflow:
185,000 nodes
466,000 edges
10 TB of input data
1 TB of output data.

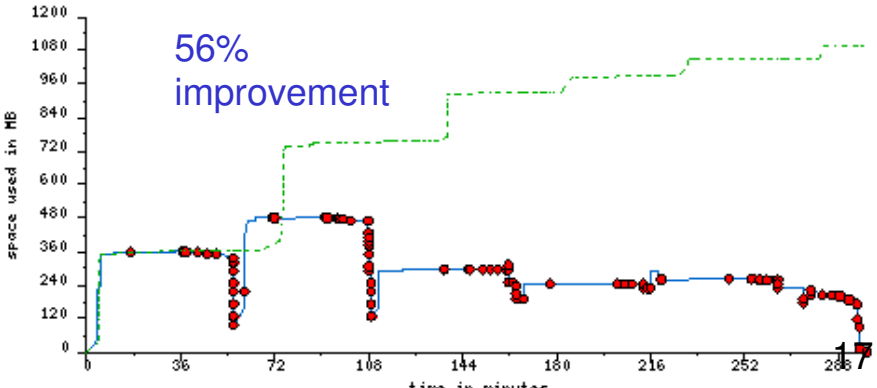
166 nodes



LIGO Workflows







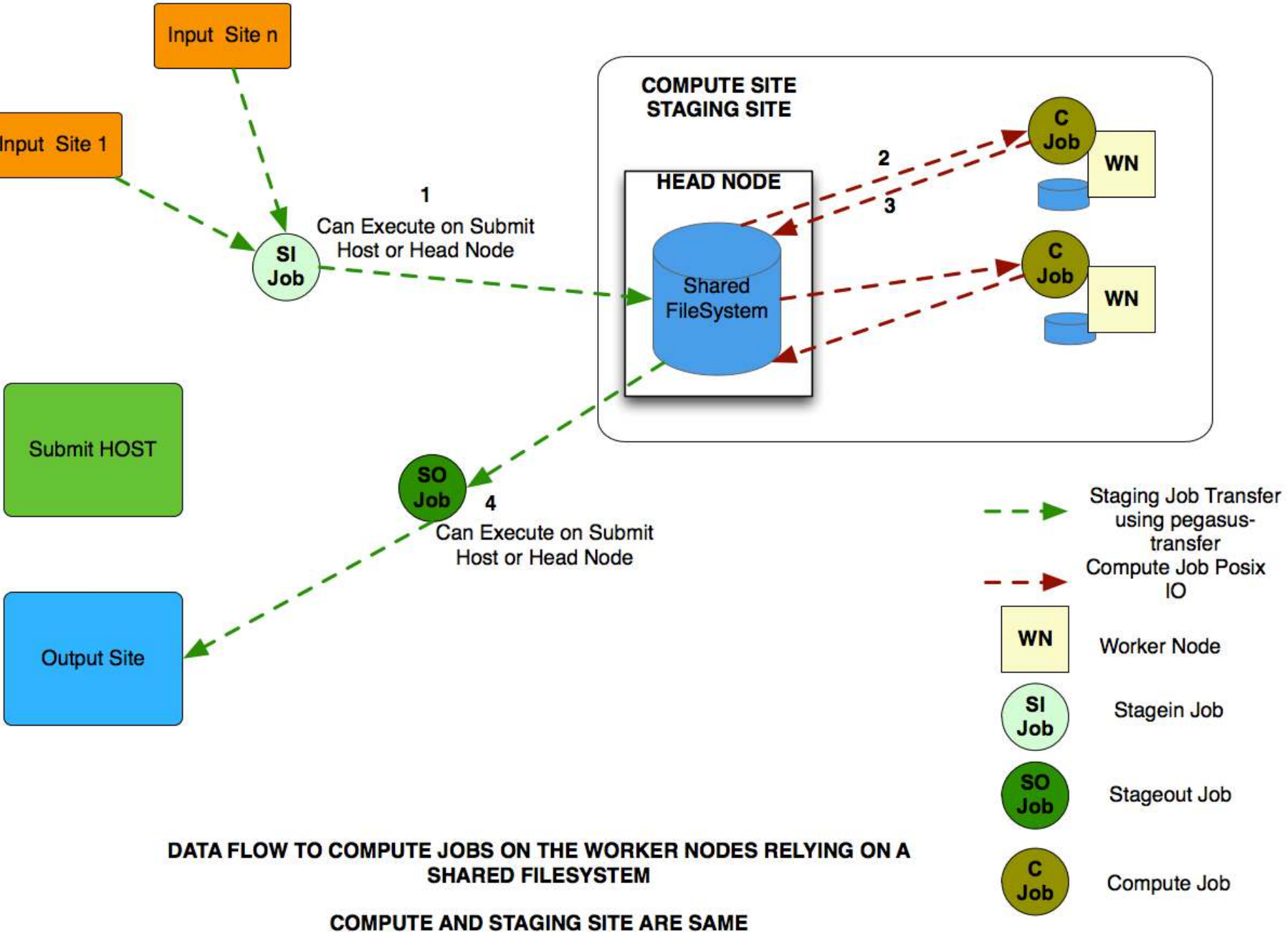
Job Priorities – Overlapping Data Staging and Computations

- Pegasus assigns default priorities to jobs (new feature in 3.0)
- Compute jobs
  - Based on what level the job is in the workflow (10, 20, …)
  - Useful when running multiple workflows
- Auxiliary jobs
  - Create dir – 800
  - Stage in – 700
  - Stage out – 900
  - Cleanup – 1000

Jobs belonging to the same workflow can run in different universes. For example: compute jobs in “grid” and staging jobs in “local”

Pegasus 3.1 Upcoming Features

- Advanced transfer features with Storage Servers
  - Allows to share intermediate advanced storage infrastructure with several remote sites
  - No need for shared file system on local site
  - Can be enabled or disabled based on compute site as well as file level.
- Define metadata in DAX and populate automatically to a given metadata server
- Notification hooks on tasks, DAX, DAGs events (maybe!)



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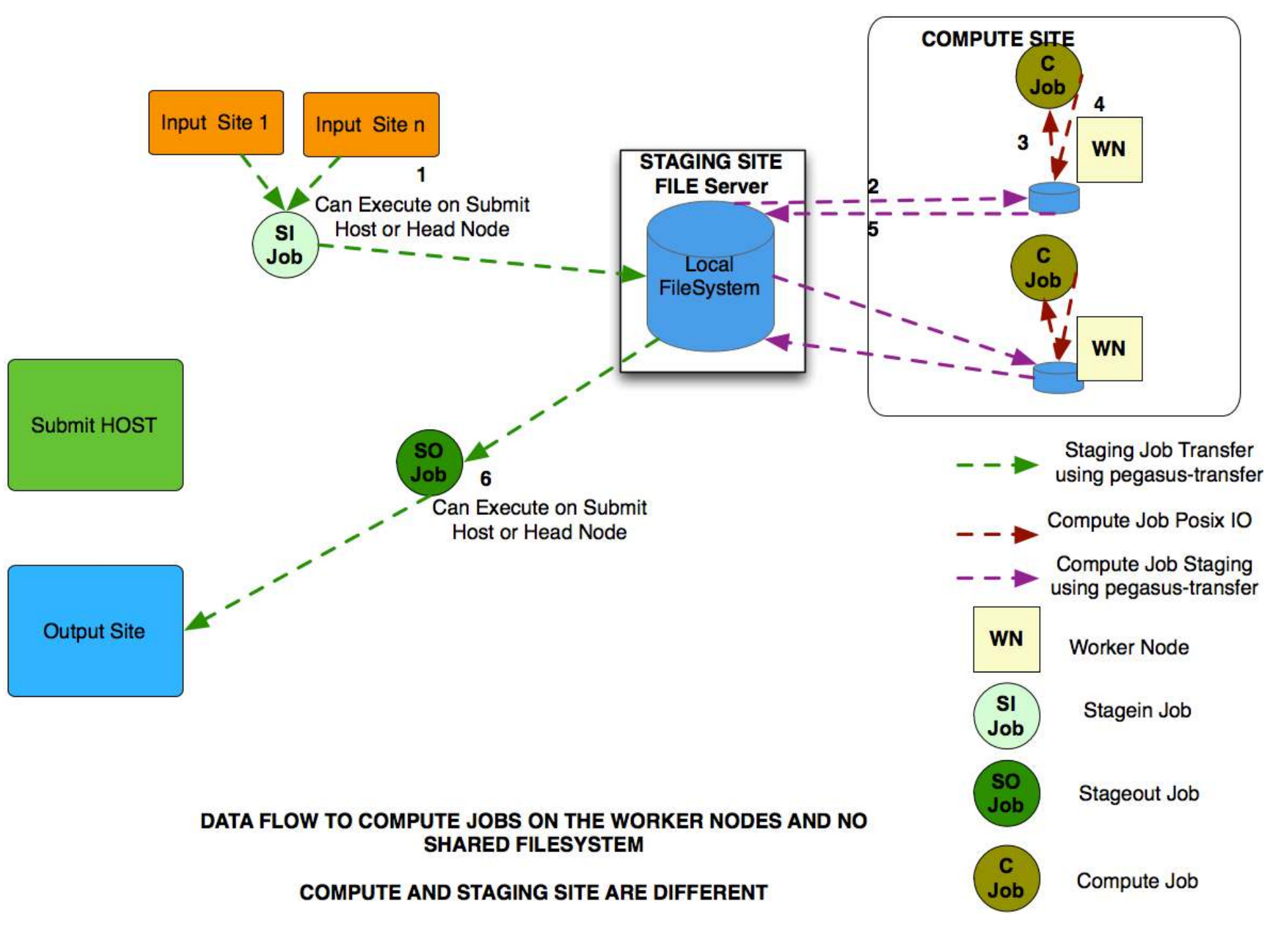
COMPUTE SITE
C Job
4
3
WN
Input Site 1
Input Site n
1
STAGING SITE
FILE Server
2
5
Can Execute on Submit Host or Head Node
SI Job
Local FileSystem
C Job
WN
Submit HOST
SO Job
6
Can Execute on Submit Host or Head Node
Output Site
Staging Job Transfer using pegasus-transfer
Compute Job Posix IO
Compute Job Staging using pegasus-transfer
WN
Worker Node
SI Job
Stagein Job
SO Job
Stageout Job
C Job
Compute Job
DATA FLOW TO COMPUTE JOBS ON THE WORKER NODES AND NO SHARED FILESYSTEM
COMPUTE AND STAGING SITE ARE DIFFERENT

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QUESTIONS?