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Custom Execution Environments with Containers in Pegasus-enabled Scientific Workflows

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Outline

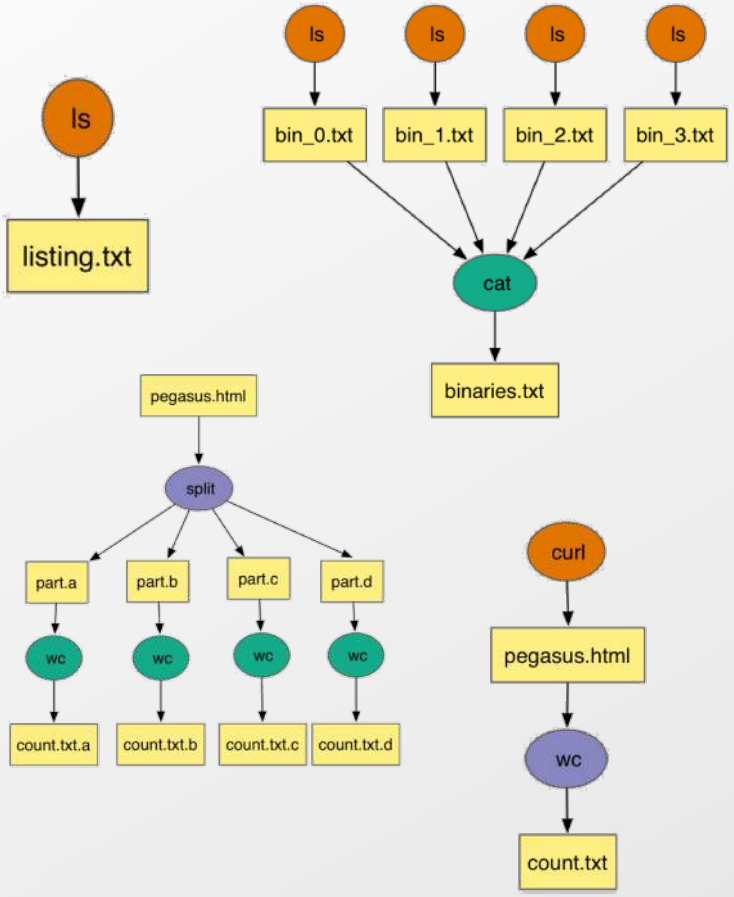
Motivation *Reproducibility for Workflows*

Containers *Solution for Reproducibility*
Challenges deploying for Distributed Workflows
Design Considerations

Pegasus *Introduction*
Container Support

Experiments *Setup*
Results

What are workflows?



- Allows scientists to connect different codes together and execute their analysis
- Workflows can be very simple (independent or parallel) jobs or complex represented usually as DAG's
- Workflows are DAGs
  - Nodes: jobs, edges: dependencies
  - No while loops, no conditional branches
  - Jobs are standalone executables
- Helps users to automate scale up

Reproducibility in Scientific Workflows

- Why?
  - Ease of Use and Portability
    - Don’t limit the execution environments
    - Ideally, users can reliably recreate your analysis on varied execution environments
      - Local Desktop (Windows, Linux, MACOS)
      - Local HPC Cluster (Mainly Linux oriented)
      - Computing Grids (Collection of University HPC clusters, such as OSG)
      - Leadership Class HPC Systems (Linux variants like Cray)
      - Cloud Environments (Choice of OS and architectures available)

Challenges to Reproducibility?

Custom Execution Environments

- When you start using shared resources you loose control over the hardware and OS
- Hard to ensure homogeneity: Users will run your code on same platform/OS it was developed on.
- Some dependent libraries required for your code may conflict with system installed versions
    - TensorFlow requires specific python libraries and versions.
    - Some libraries maybe easy to install on latest Ubuntu, but not on EL7

- If running on shared computing resources such as computational grids
    - you run on a site with heterogeneous nodes and your job lands on a node where OS is incompatible with your executable

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Solutions: Containers

- Virtualizes the OS instead of the Hardware
  - Sits on top of the physical server and the host OS
  - Each container shares the Host kernel and binaries and libraries
- Separates the application from the node OS.
- Lightweight
  - Instead of GB's size is on order of MB's
  - Take seconds to start instead of minutes
  - Can pack more applications on the same node compared to Virtual Machines

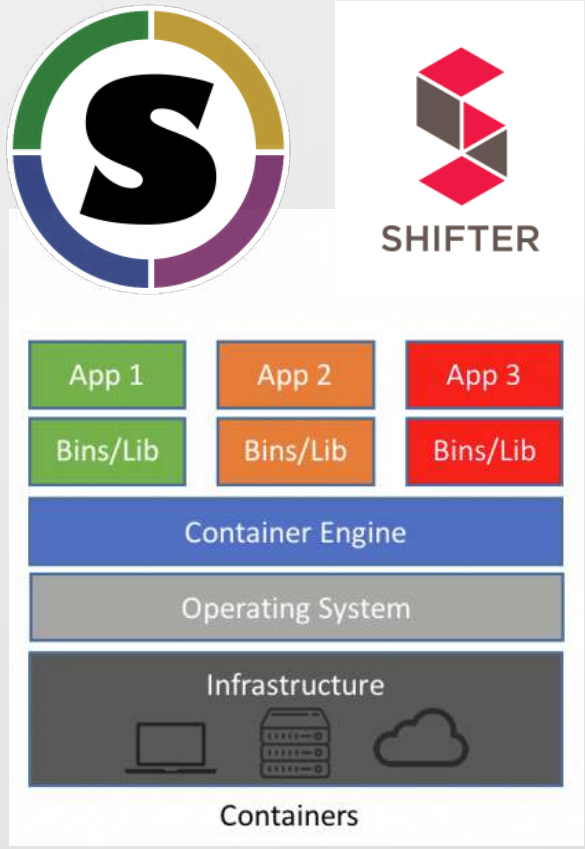

Image Source: https://blog.netapp.com/wp-content/uploads/2016/03/Screen-Shot-2018-03-20-at-9.24.09-AM-935x500.png

Solutions: Why Containers?

- Reproducibility
  - Supply a fully defined and reproducible environment
  - Usually described as a recipe file that captures the steps to configure and setup the container
- Ability to provide a flexible user controlled environment that underlying compute cluster cannot
  - Administrators main goal is to provide a stable, slow moving, multi-user environment
  - Cannot provide all combinations of development libraries and tools for their user community
- Perfect for deploying on demand.
  - Also seamlessly transfer to another compute environment

However: Challenges deploying Containers for Distributed Workflows

- How to distribute container images and make them available to compute jobs
  - Pegasus workflows contain thousands or millions of jobs simultaneously running
- Container Technologies are fragmented
  - One size fits all approach does not work

Design Considerations

- Support for different container technologies
  - Docker popular in traditional corporate computing environment.
    - By default jobs run as root!
  - Singularity preferred in HPC as allows jobs to run in user space
  - Some HPC centers support custom solutions such as Shifter to run Docker images

- Work in Distributed Environments
  - Users don't know a-priori which node or cluster a job lands on.
  - OSG is dynamic computing environment

- Easy Configuration and Representation
  - Easy for users to configure which container and type of container required by their jobs

- Support for Public Registries
  - Lot of popular images available. Have ability to retrieve them

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Pegasus Workflow Management System

Automates complex, multi-stage processing pipelines

Enables parallel, **distributed computations**

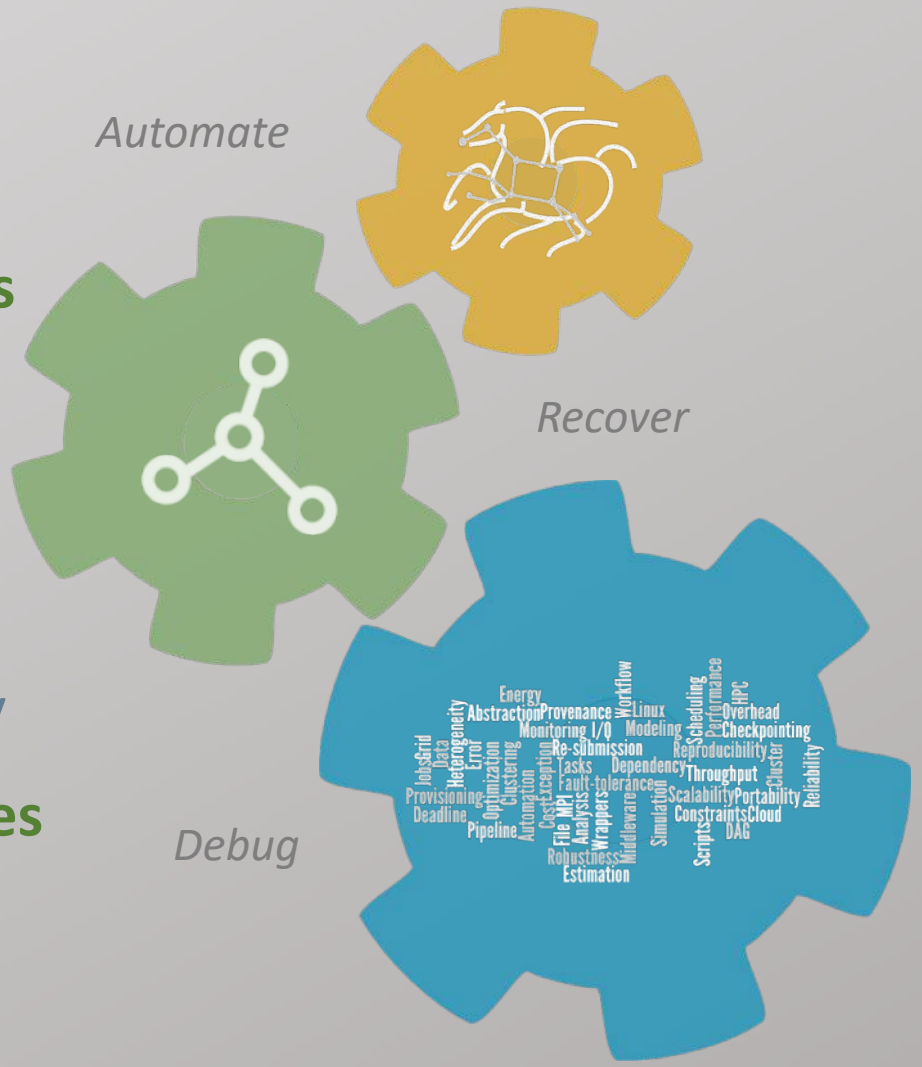
Automatically executes data transfers

Reusable, aids **reproducibility**

Records how data was produced (**provenance**)

Handles **failures** with to provide reliability

Keeps track of data and **files**



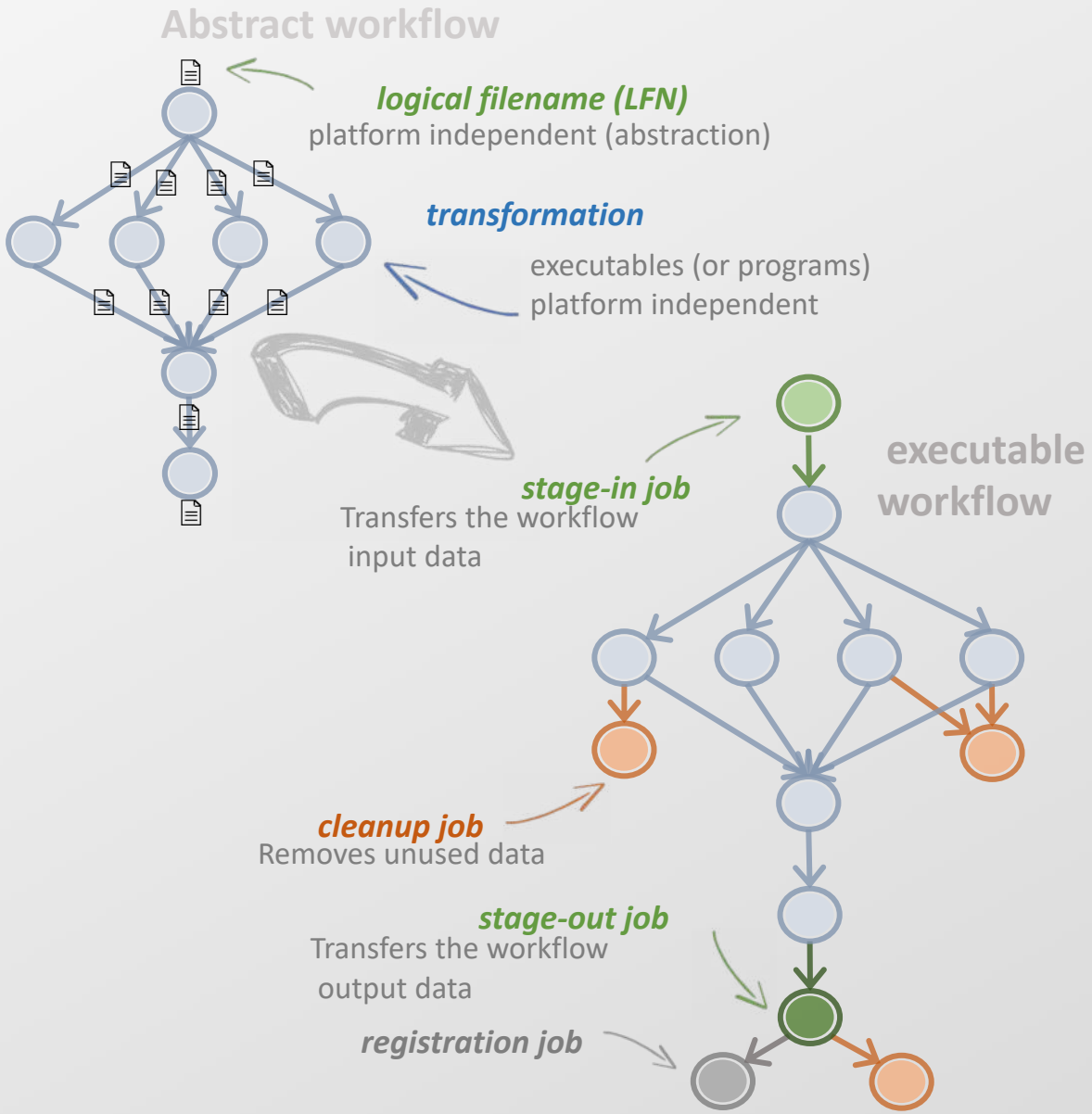
HTCondor High Throughput Computing

NSF funded project since 2001, with close collaboration with HTCondor team

Pegasus

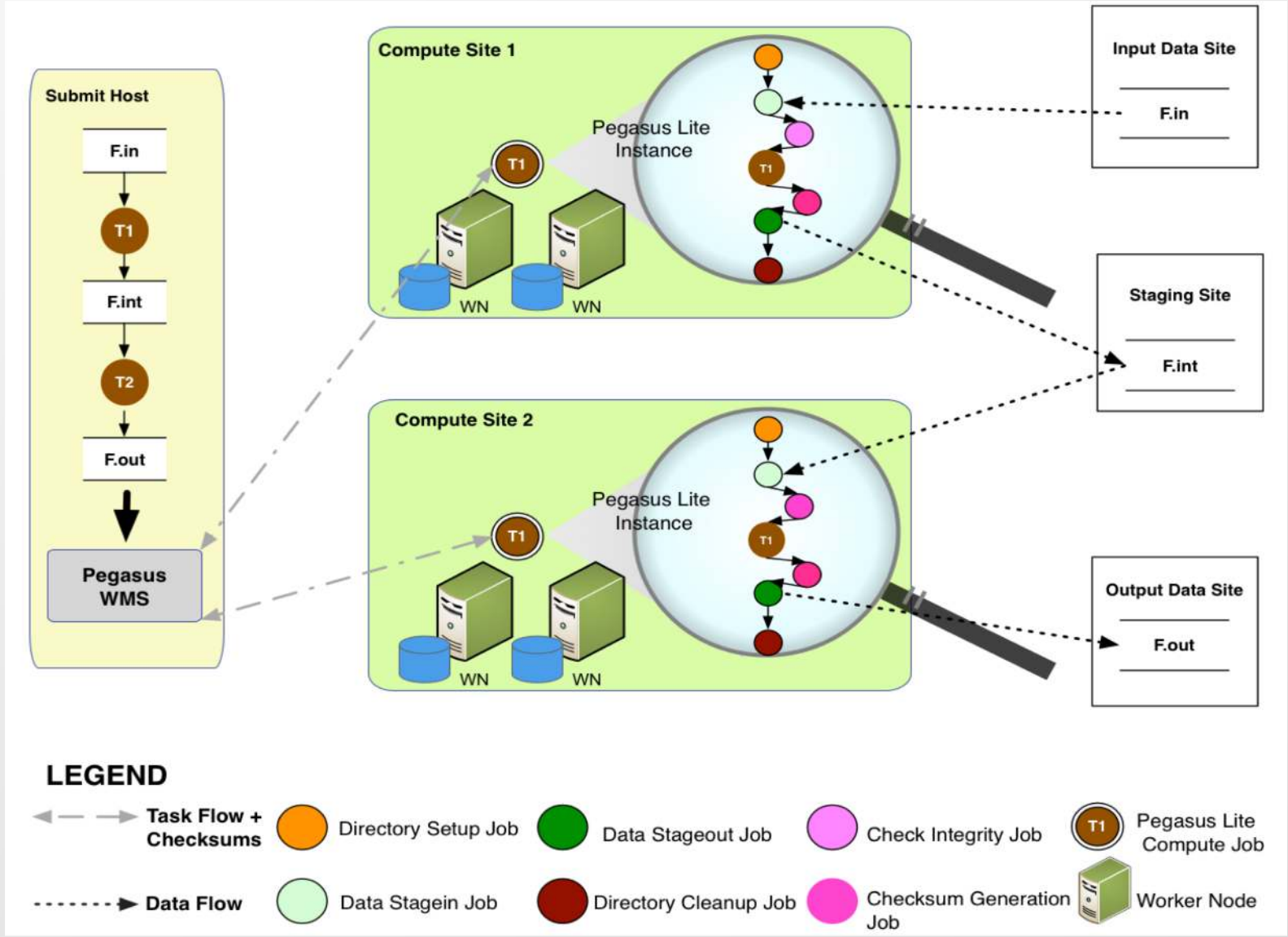
- Users describe their pipelines in a portable format called Abstract Workflow, without worrying about low level execution details.

- Pegasus takes this and generates an executable workflow that
  - has data management tasks added
  - transforms the workflow for performance and reliability



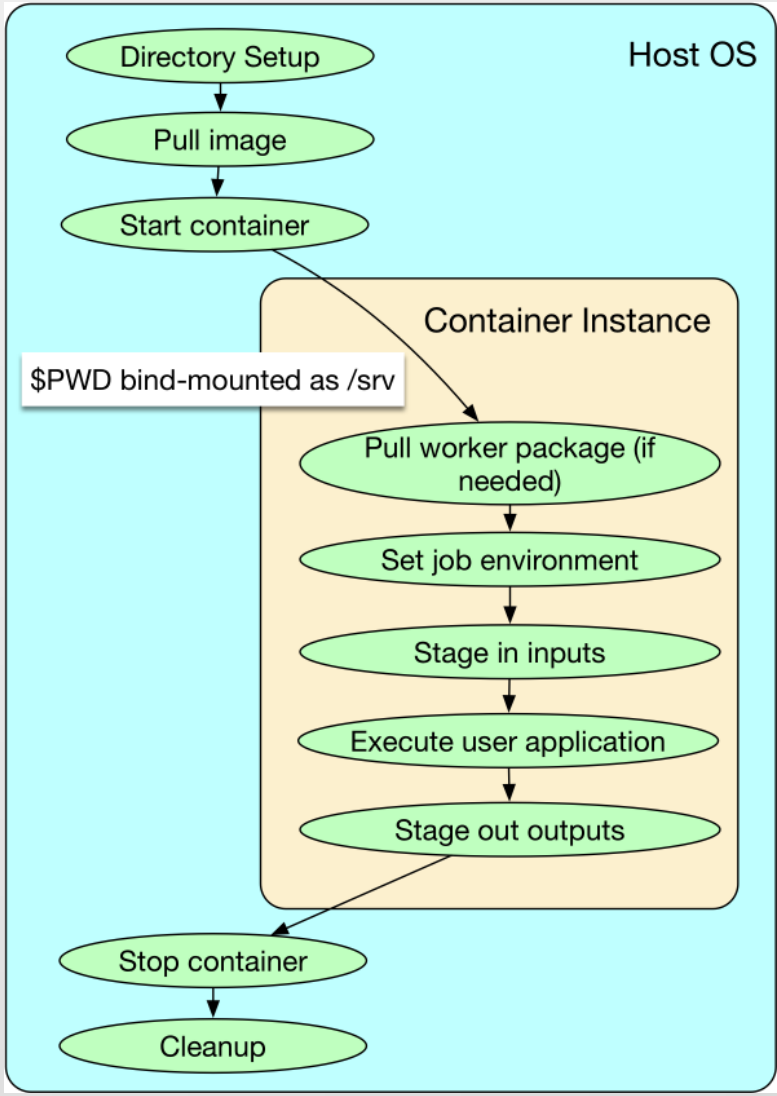
Pegasus Deployment

- Workflow Submit Node
  - Pegasus WMS
  - HTCondor
- One or more Compute Sites
  - Compute Clusters
  - Cloud
  - OSG
- Input Sites
  - Host Input Data
- Data Staging Site
  - Coordinate data movement for workflow
- Output Site
  - Where output data is placed



Pegasus: Container Execution Model

- Containerized jobs are launched via Pegasus Lite
  - Container image is put in the job directory along with input data.
  - Loads the container if required on the node (applicable for Docker)
  - Run a script in the container that sets up Pegasus in the container and job environment
  - Stage-in job input data
  - Launches user application
  - Ship out the output data generated by the application
  - Shut down the container (applicable for Docker)
  - Cleanup the job directory



Pegasus: Data Management

- Treat containers as input data dependency
  - Needs to be staged to compute node if not present
- Users can refer to container images as
  - Docker Hub or Singularity Library URL's
  - Docker Image exported as a TAR file and available at a server , just like any other input dataset.
- If an image is specified to be residing in a hub
  - The image is pulled down as a tar file as part of data stage-in jobs in the workflow
  - The exported tar file is then shipped with the workflow and made available to the jobs
  - Motivation: Avoid hitting Docker Hub/Singularity Library repeatedly for large workflows
- Symlink against a container image if available on shared fileystem
  - For e.g. CVMFS hosted images on Open Science Grid

Pegasus: Container Representation

Described in Transformation Catalog

- Maps logical transformations to physical executables on a particular system

container

Reference to the container to use. Multiple transformation can refer to same container

type

Can be either docker or singularity or shifter

image

URL to image in a docker|singularity hub OR to an existing docker image exported as a tar file or singularity image

mount

Mount information to mount host directories into container

```
- transformations
    - namespace: "example"
      name: "keg"
      version: 1.0
    site:
    - name: "isi"
      arch: "x86
      os "linux"
      pfn "/usr/bin/pegasus-keg
      container "centos-pegasus"

      # INSTALLED means pfn refers to path in the container.
      # STAGEABLE means the executable can be staged into the container
      type "INSTALLED"

- cont:
    - name: "centos-pegasus"

      # can be docker, singularity or shifter
      type: "docker"

      # URL to image in docker|singularity hub or shifter repo URL or
      # URL to an existing image exported as a tar file or singularity image file
      image: "docker:///centos:7"

      # mount information to mount host directories into
      # container format src-dir:dest-dir[:options]
      mount:
         - "/Volumes/Work/lfs1:/shared-data/:ro"

      # environment to be set when the job is run in the container
      # only env profiles are supported
      profile:
      - env:
            "JAVA_HOME" "/opt/java/1.6"
```

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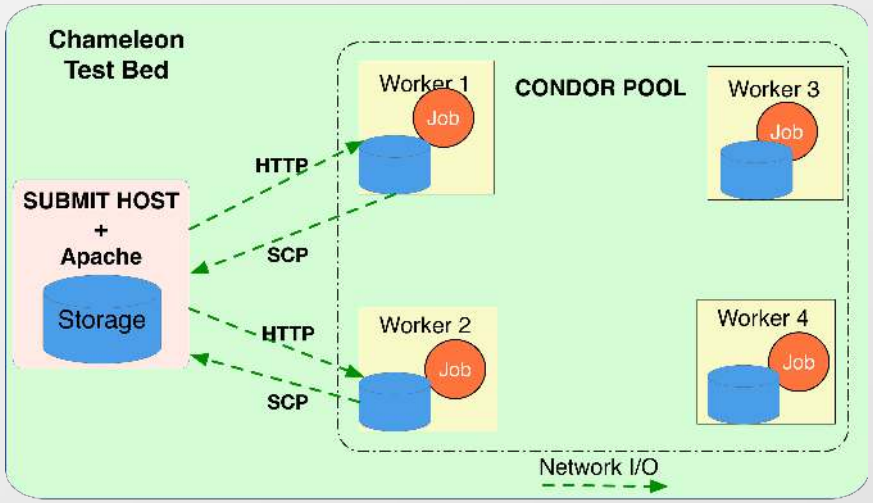
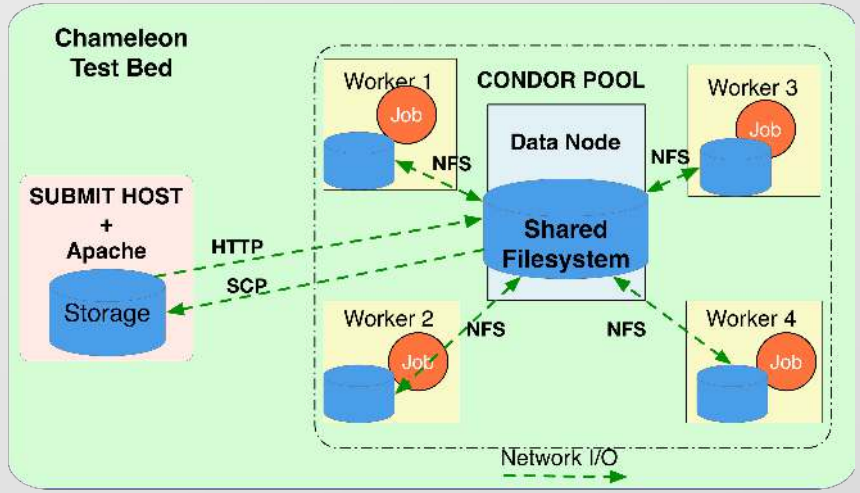
Experiments: Setup

- Used Chameleon Testbed in TACC
  - 1 workflow submit node
  - 1 NSF server node
  - 4 worker nodes
  - All nodes were bare metal with 24 physical cores, 128GB RAM
  - 10 Gbps network connection
    - Network capped at 1Gbps
- Test Workflow
  - CASA workflow with 63 compute jobs and 10 additional data transfer and auxiliary tasks



Non Shared Filesystem Setup



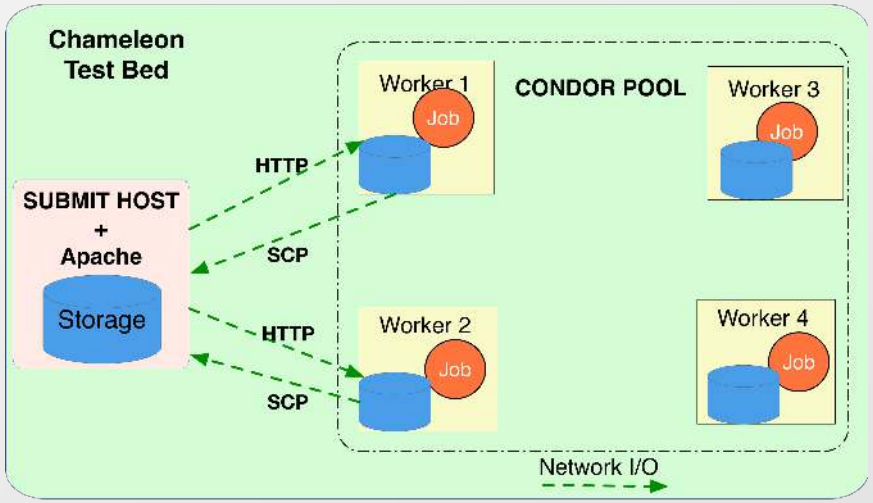
Shared Filesystem Setup

Experiments:

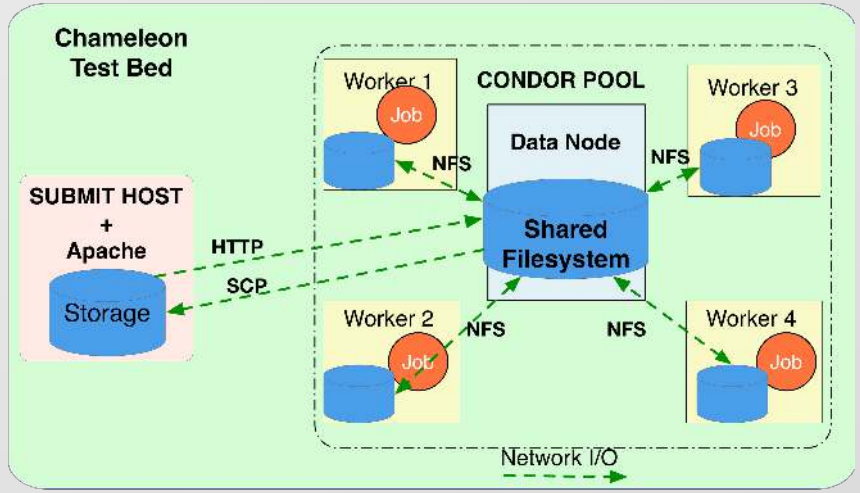
- Base experiment
  - Run CASA workflow without any containers in the non shared filesystem setup
- Experiment 2
  - Executing workflow with Docker and Singularity containers in non shared filesystem setup
- Experiment 3
  - Staged input data to NFS and have compute jobs symlink against it

Goals

- Demonstrate increase in walltime due to staging of containers and how job clustering helps
- Show staging of containers can saturate network and disk IO



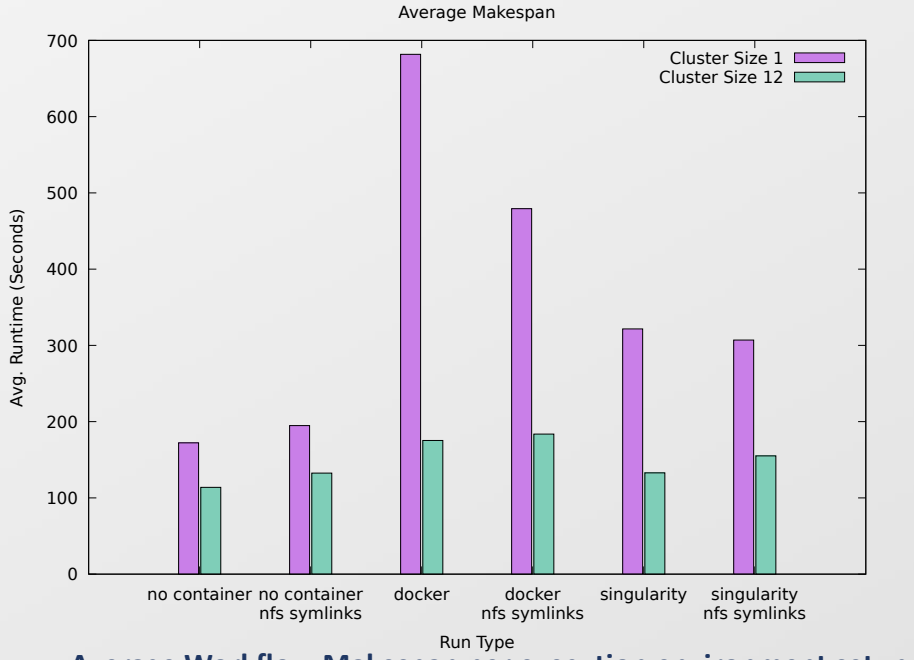
Non Shared Filesystem Setup



Shared Filesystem Setup

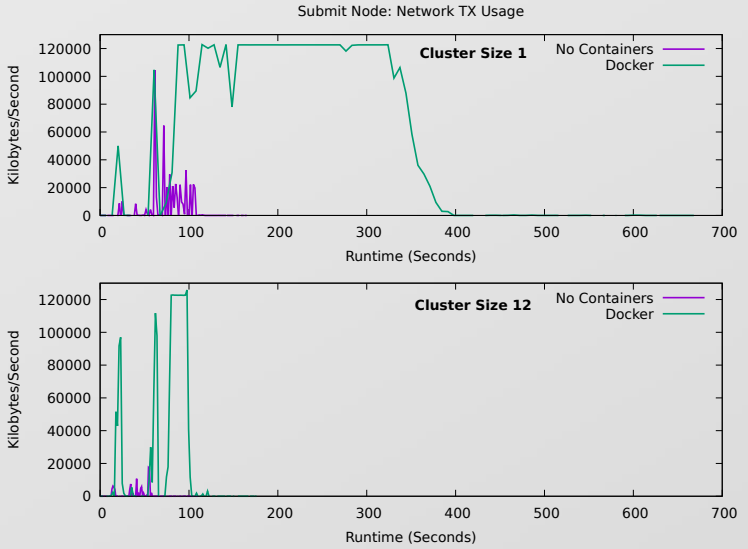
Results:

- Workflow Makespan Per Execution Setup
  - Increase from 172.2 seconds to 681.7 and 321.6 for Docker and Singularity Containers with no job clustering.
  - Clustering decreases the overhead, as container is staged once per 12 tasks.
  - Docker image size 488MB vs 153 MB for Singularity image file.



Average Workflow Makespan per execution environment setup

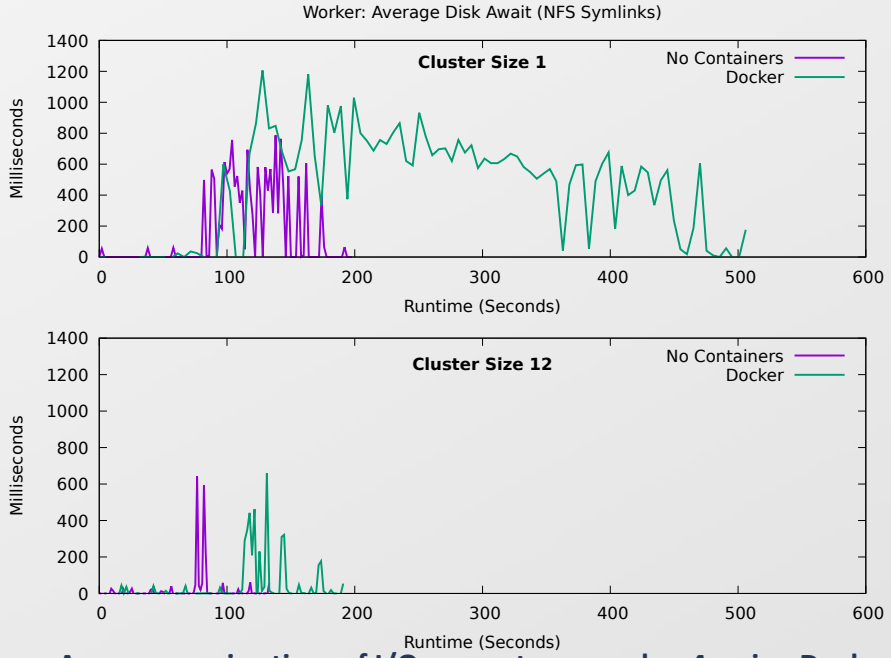
- Egress Traffic on the Submit Node
  - Submit host is data staging site for the non shared filesystem setup.
  - Hight because of transfer of associated data transfers of containers per job.



Egress network traffic on submit node , without use of containers and using Docker. NO NFS

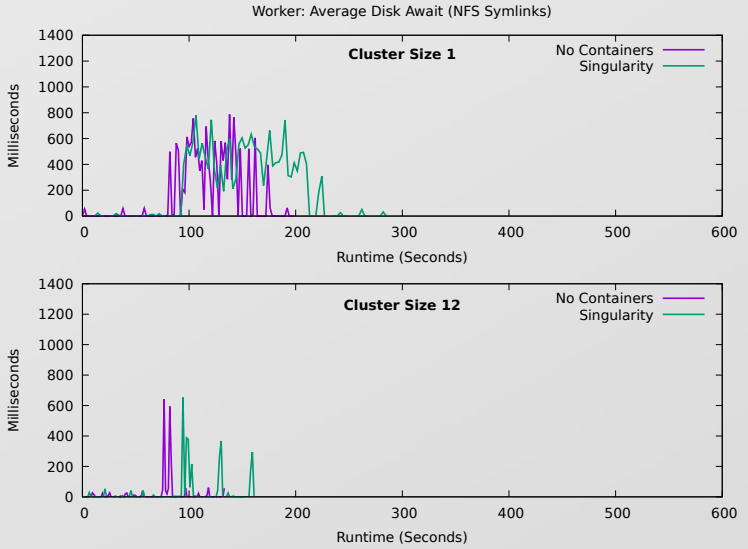
Results:

- Average Service time I/O Requests using Docker with NFS symlinking
  - Negligible effect in case of NO containers
  - Using Docker, leads to significant increase even when symlinking.
  - Docker image still needs to be un-tarred on local node and loaded to local registry.



Average service time of I/O requests on worker 4 using Docker containers with NFS symlinking

- Average Service time I/O Requests using Singularity with NFS symlinking
  - Singularity images are read directly
  - And are much smaller in size



Average service time of I/O requests on worker 4 using Singularity containers with NFS symlinking

Case Study: LIGO PyCBC Workflows

- PyCBC
  - Python based software package fpr exploring astrophysical sources of gravitational waves
  - Used in discoveries of gravitational waves from binary black holes and binary neutron stars.
- Complex Runtime Environment
  - Call functions from both Python libraries (third party and PyCBC both) and also compiled code from shared object libraries
  - Requires build and runtime environments are compatible (compatible versions of glibc, gcc, python)
  - For LIGO managed clusters can be solved using virtualenv and standard software installation
  - However does not work for OSG and XSEDE
  - Tried building bundled executables using PyInstaller. Not completely static and requires dynamically linked glibc
- Containers via Pegasus
  - Deployment of containers managed by Pegasus
  - Mount CVMFS inside the container for access to existing data on the site

Pegasus Container Support: Experiences

- Direct Access to Singularity Images via CVMFS
  - On OSG, singularity images distributed using CVMFS available on all nodes
  - Pegasus opted to pull image once to data staging site and pull to the compute node at runtime.
  - Disadvantage of not being able to use out of band caching and distribution made available by CVMFS
  - We updated Pegasus to enable bypass of container staging, and symlink directly against images on CVMFS
- Moved Data Staging inside of the container
  - Earlier the data staging happened outside of the container on the HOST OS.
  - Allowed us to rely on infrastructure provided tools on the HOST OS.
  - However, left user no control to using their own choice of transfer tools.
  - In Pegasus 4.9.1 moved data staging to occur inside the container
- Loading multiple Docker image tar files.
  - Adverse affect on local disk performance if multiple jobs try loading an image on the same node in a short period of time.

Questions?

Pegasus est. 2001

Automate, recover, and debug scientific computations.

Get Started

Pegasus Website
https://pegasus.isi.edu

Users Mailing List
pegasus-users@isi.edu

Support
pegasus-support@isi.edu

Pegasus Online Office Hours
https://pegasus.isi.edu/blog/online-pegasus-office-hours/

Bi-monthly basis on second Friday of the month, where we address user questions and also apprise the community of new developments