Custom Execution Environments with Containers in Pegasus-enabled Scientific Workflows


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https://pegasus.isi.edu
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
**Outline**

**Motivation**  Reproducibility for Workflows

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

**Pegasus**  Introduction  Container Support

**Experiments**  Setup  Results
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

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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https://pegasus.isi.edu
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. NSF funded project since 2001, with close collaboration with HTCondor team.
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 filesystem
  ▪ 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
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
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.

• Egress Traffic on the Submit Node
  • Submit host is data staging site for the non shared filesystem setup.
  • High because of transfer of associated data transfers of containers per job.
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 I/O Requests using Singularity with NFS symlinking
  • Singularity images are read directly
  • And are much smaller in size
Case Study: LIGO PyCBC Workflows

• PyCBC
  • Python based software package for 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.