Container Support in Pegasus 4.8.x

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Containers

- Lightweight and a reproducible way to run application on heterogeneous nodes.

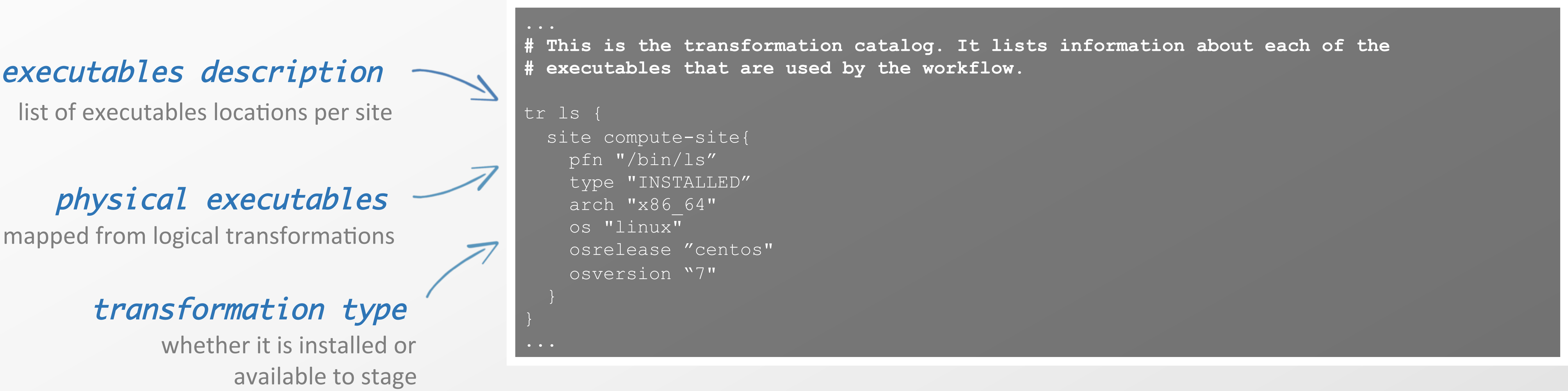
- Separates the application from the node OS.

- Popular Container Technologies
  - Docker
    - Popular in the enterprise world.
    - By default, application launched in container run as root
      - A concern when running on shared infrastructure
  - Singularity
    - Popular in HPC environments.
    - Is run in user space.

Why use Containers for your workflow?

Traditional way of referring user executable in Pegasus

- Jobs in the input abstract workflow (DAX) refer to logical transformations.
- Users define mapping of logical transformation to actual executable in a Transformation Catalog



executables description

list of executables locations per site

physical executables

mapped from logical transformations

transformation type

whether it is installed or
available to stage

```
...
# This is the transformation catalog. It lists information about each of the
# executables that are used by the workflow.

tr ls {
  site compute-site{
    pfn "/bin/ls”
    type "INSTALLED”
    arch "x86_64"
    os "linux"
    osrelease ”centos"
    osversion “7"
  }
}
...
```

Executable staging works if executable is statically linked , OR

if libraries are installed on the nodes for dynamically linked executables

Why use Containers for your workflow?

Traditional way of referring user executable in Pegasus

- Pegasus matches the attributes of an executable defined in Transformation Catalog against the attributes specified for site in Site Catalog.

- This approach works fine if your site is made of homogenous nodes

- However, problems occur when

  ① you run on a site with hetrogeneous nodes and your job lands on a node where OS is incompatible with your executable

  ② Application is a mis-match to the compute node environment

  - Install libraries in your shared space and make sure environment refers to those libraries
  - Need cooperation from Site Admins. On OSG , you can install things in CVMFS
  - TensorFlow requires specific python libraries and versions. Some libraries maybe easy to install on latest Ubuntu, but not on EL7

Pegasus Container Support

- Introduced in Pegasus Release 4.8
  - Support for both Docker and Singularity

- Users can now refer to containers in the Transformation Catalog with their executables preinstalled.

- Users can refer to a container they want to use. However, they can let Pegasus stage their executable to the node.
  - Useful if you want to use a site recommended/standard container image.
  - Users are using generic image with executable staging.

Specifying Containers in Transformation Catalog

container

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

type

Can be either docker or singularity

image

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

```
...
tr pegasus::keg{

  site isi {
    pfn "/usr/bin/pegasus-keg
    arch "x86"
    os "linux"
    osrelease ”centos"
    osversion “7"

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

    #optional attribute to specify the container to use
    container "centos-pegasus"
  }
}

cont centos-pegasus{
     type "docker”

     image "docker:///centos:7"

     # optional site attribute to tell pegasus which site tar file
     # exists. useful for handling file URL's correctly
     image_site "optional site"

     # 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"
}
...
```

Data Management for Containers

- Users can refer to container images as
  - Docker or Singularity Hub 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/Singularity Hub repeatedly for large workflows
- Pegasus worker package is not required to be pre-installed in the container
  - If a matching worker package is not installed, the required worker package is installed at runtime when container starts

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 launches user application
- Shut down the container (applicable for Docker)
- Ship out the output data generated by the application
- Cleanup the job directory

- Traditional shared-fs approach does not support containers.

Directories Mounted

- Only the job directory where PegasusLite places the inputs is mounted in the container
  - Docker – Mounted as /scratch
  - Singularity – Mounted as /srv

- PegasusLite ensures that user application is launched in the directory mounted
  - Consistent with the Pegasus model of ensuring that user job is launched in directory where it's input data exists.

User Running in the Container

- Singularity containers always run in user space.

- Docker
  - Pegasus before launching the user application
    - Creates the user in the container that is the same as the user under which the job is launched by the Local Resource Manager on the remote node
  - Why do we do this?
    - By default, Docker runs user application as root
    - Not recommended for HPC environment
    - Creates problems with staging the outputs created in the container

Reference

- Documentation
  - https://pegasus.isi.edu/documentation/containers.php

- Example
  - https://github.com/pegasus-isi/montage-workflow-v2/
  - Script example-dss-containers.sh will run the montage workflow jobs in a container pulled from the singularity hub

Pegasus est. 2001

Automate, recover, and debug scientific computations.

Thank You

Questions?

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