Introduction to Singularity

Le Yan

Goals

- Understand
  - The targeted use cases of Singularity
  - How Singularity works
- Learn
  - How to build Singularity images on local computers
  - How to run Singularity containers on HPC clusters

Pain Points for HPC Users

- Dependencies of an application are
  - Not available on the host OS
    - For example, GLIBC version too low
  - Complex and difficult to resolve/install
- Reproducibility is not always guaranteed
- Difficult to share workflows, pipelines and environments with colleagues

Pain Points for HPC Users

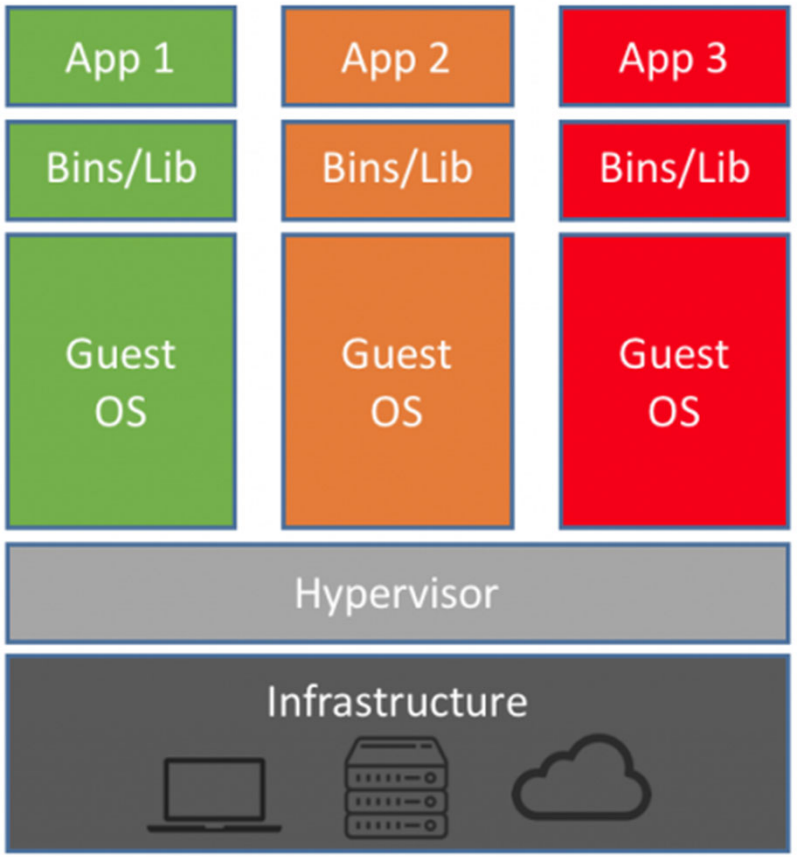
- Dependencies of an application are
  - Not available on the host OS

The purpose of Singularity is to eliminate or ease these difficulties.

- Difficult to share workflows, pipelines and environments with colleagues

Virtualization

- Virtualization is “the act of creating a virtual (rather than actual) version of something” (Wikipedia)
- So that multiple applications (that have different dependencies) can share the hardware resources on one physical computer

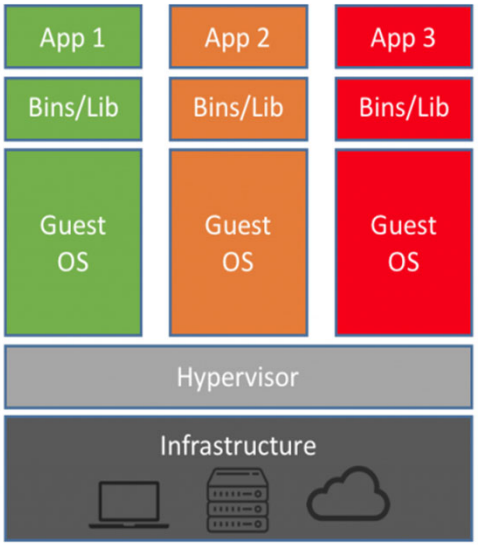


https://blog.netapp.com/blogs/containers-vs-vms/

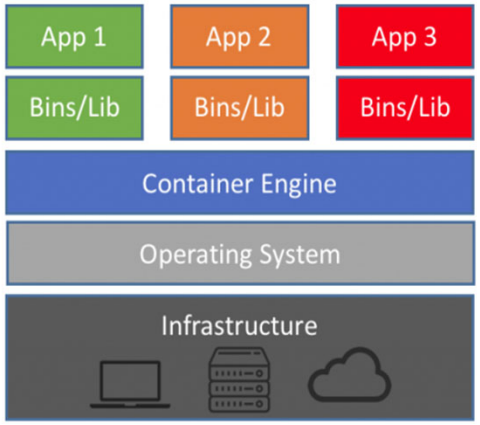
https://en.wikipedia.org/wiki/Virtualization

Virtual Machines vs. Containers

Virtual machines	Containers
Very flexible, e.g. one can run a Windows guest OS on Linux or vice versa	Less flexible, On Linux systems only
Heavyweight, need to install all files of a guest OS	Very lightweight, will use the kernel of the host OS



Machine Virtualization



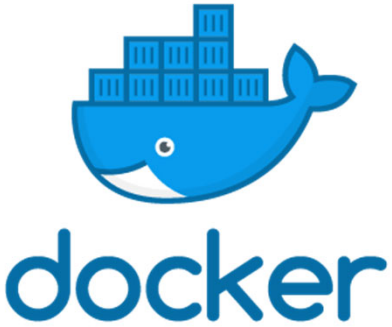
Containers

https://blog.netapp.com/blogs/containers-vs-vms/

What is Singularity

- Singularity is an open-source container software
- Allows users to **pack an application/workflow/pipeline and its dependencies into a single image (file)**
- "Container for HPC"
  - Assumes that the user does not have root privileges on the host OS
  - There are a few others, e.g. Charliecloud, Shifter

Containers: Docker vs. Singularity



Docker	Singularity
Assumes that the user has root privileges in the production environment	Assumes that the user does not have root privileges in the production environment
Designed for system services	Designed for HPC use cases

Singularity Vocabulary

- Singularity – the software
  - As in “Singularity 3.5”
- Image – a compressed, read-only file
  - As in “build a Tensorflow 2.6 image”
- Container
  - The technology
    - As in “containers vs virtual machines”
  - An instance of an image
    - As in “process my data in a Singularity container of Tensorflow”

Why Singularity: HPC Users' Perspective

Pain points using HPC
Dependencies of an application are not available on the host OS, e.g. GLIBC version too low
Dependencies of an application are complex and difficult to resolve/install
Reproducibility is not guaranteed
Difficult to share workflows, pipelines and environments

Why Singularity: HPC Users' Perspective

Pain points using HPC	With Singularity
Dependencies of an application are not available on the host OS, e.g. GLIBC version too low	Build an image with an different OS
Dependencies of an application are complex and difficult to resolve/install	Get an image/recipe (from the developers or other users)
Reproducibility is not guaranteed	Share an image/recipe
Difficult to share workflows, pipelines and environments	Share an image/recipe

Demo 1
First encounter

Singularity Basics: Command Line

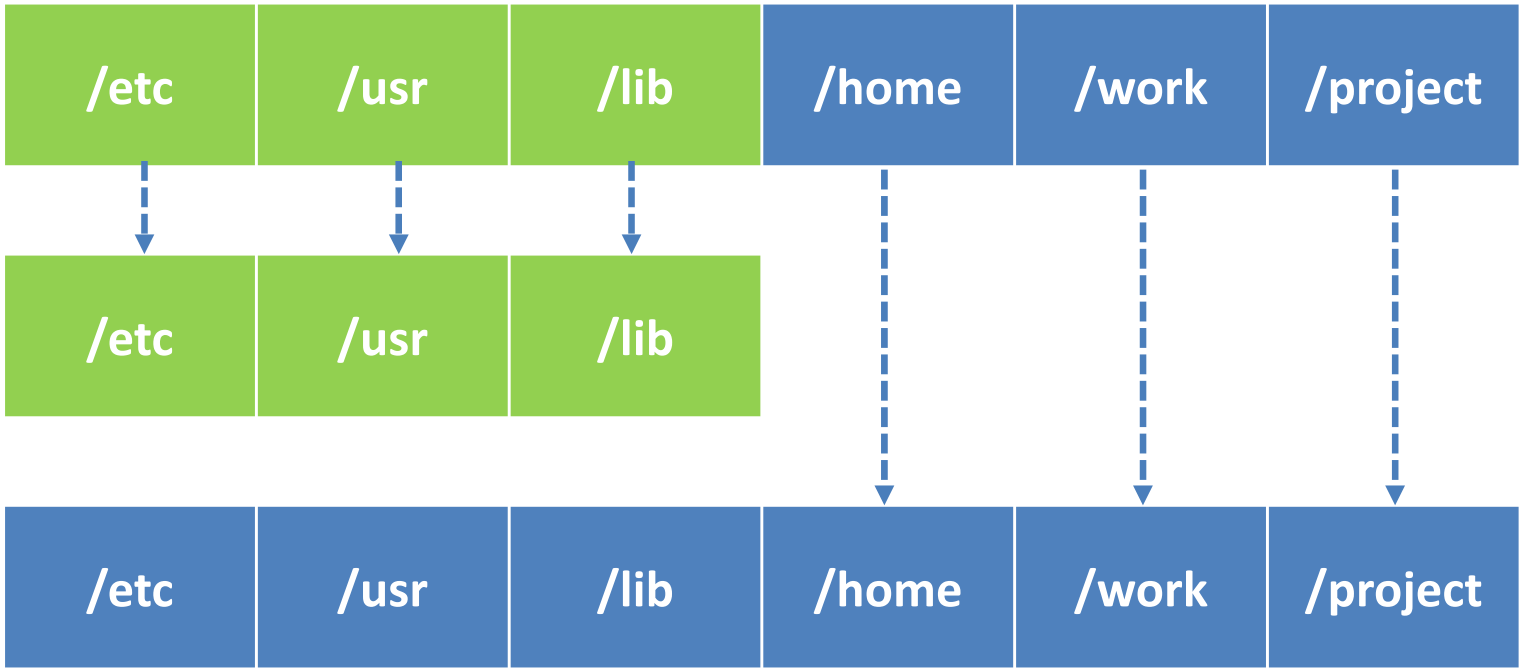
- Native command line interface
  - Syntax: `singularity <command> <options> <arguments>`
- To get help information for a specific command:
  - `singularity <command> --help`

Singularity Basics: Overlay File System

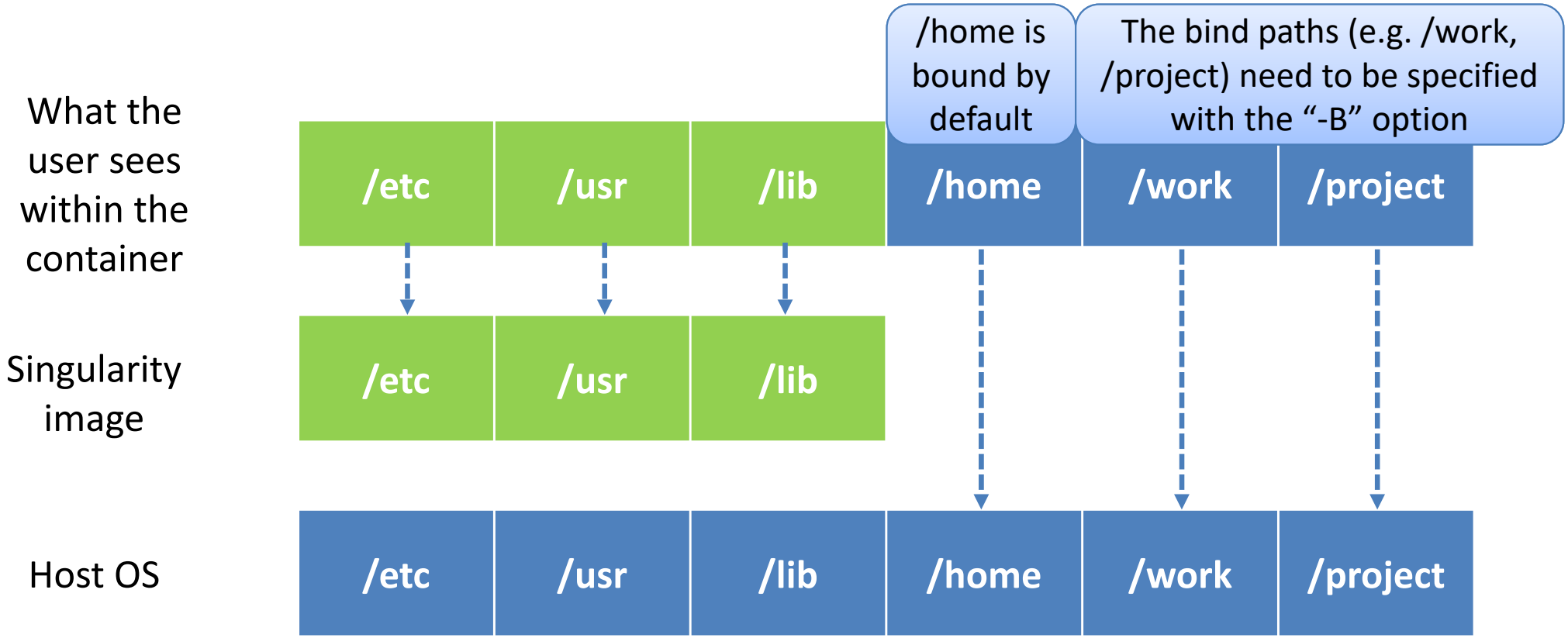
What the user sees within the container

Singularity image

Host OS



Singularity Basics: Overlay File System



Singularity Basics: Privilege Escalation

- If you do not have root privileges outside the container, you do not have them inside the container either.
- Need to build images on your local computer (where you have root privileges)

Singularity Workflow

- Step 1: Install Singularity on a local Linux machine (or a Linux VM on a Windows machine)
  - Root privilege is needed
- Step 2: Build Singularity images on the local machine
  - Root privilege is needed
- Step 3: Upload images onto the HPC cluster
  - Root privilege is NOT needed
- Step 4: Run containers on the HPC cluster
  - Root privilege is NOT needed

Installing Singularity

- On Linux
  - Install binary (recommended)
    - Use either `apt-get` or `rpm/yum`
  - Install from source
    - https://github.com/sylabs/singularity
- On Windows or Mac
  - Install a Linux VM first

Building Singularity Images (1)

- Use the "`build`" command to build Singularity images
- Need root privileges
- Syntax:
  - `singularity build [build options…] <image file path> <BUILD TARGET>`

Build an Ubuntu 22 image:

```
sudo singularity build ubuntu22.sif docker://ubuntu:22.04
```

Building Singularity Images (2)

- The "`BUILD TARGET`" defines the method how an image is built
  - A URI to a base OS/container image
    - Docker Hub images begins with **docker://**
    - Singularity Hub images begins with **shub://**
  - Path to a Singularity sandbox (see next slide)
  - Path to a Singularity recipe (definition file)
    - More on this later

Building Singularity Images (3)

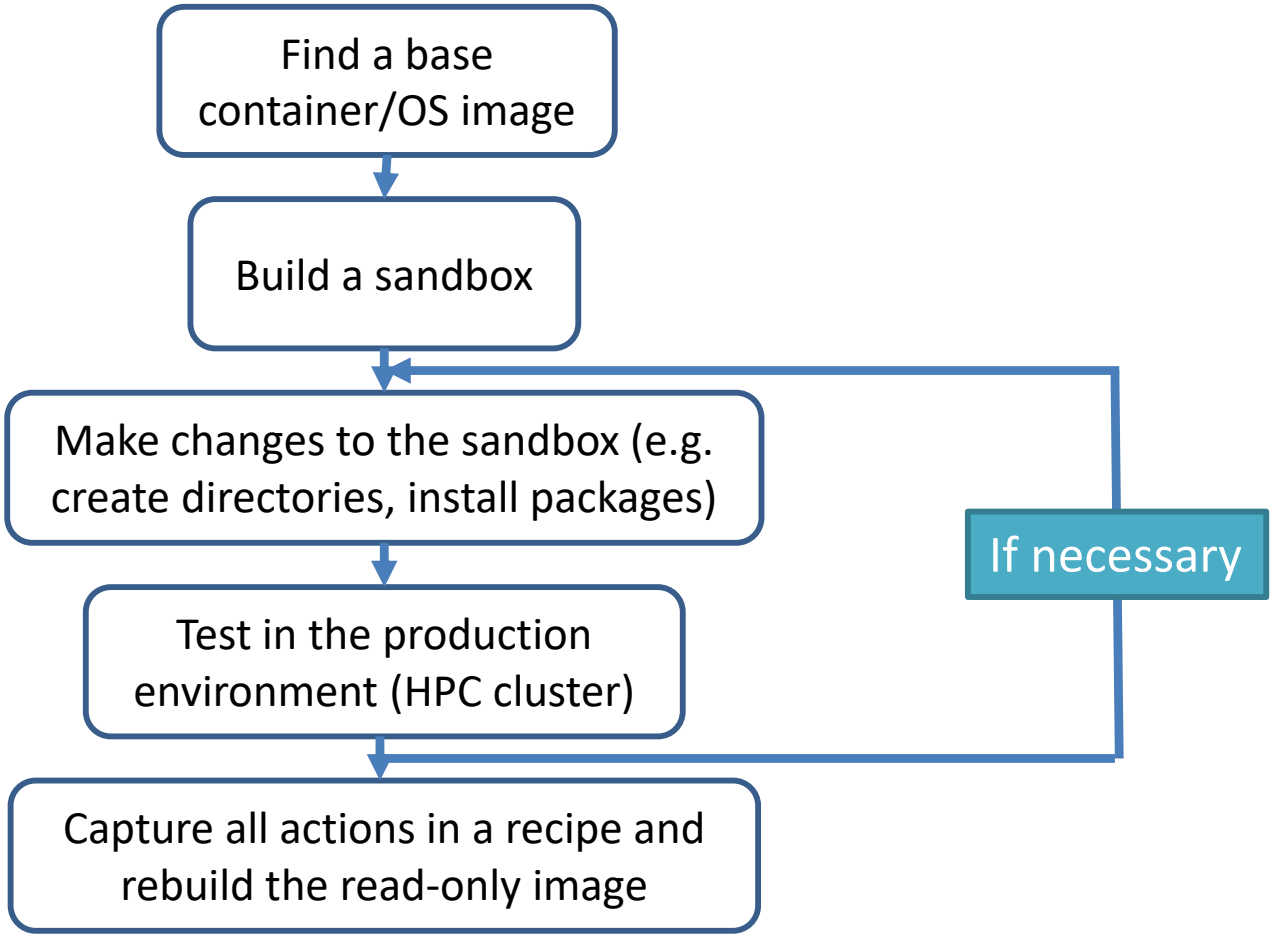
- By default, a compressed, read-only image will be built
- The "`--sandbox`" option tells Singularity to build a sandbox to which changes can be made
- To make changes to the sandbox, use the `singularity shell` command with the "`--writable`" option
  - Otherwise any change made will be wiped when the session ends
  - Then you can
    - Manage files and directories
    - Install packages/dependencies

Build an Ubuntu 22 image as a sandbox:

```
sudo singularity build --sandbox ubuntu22 docker://ubuntu:22.04
```

Demo 2
Build Singularity Images

Building Workflow



Singularity Definition Files (Recipes)

- Capture all the interactive building steps

```
BootStrap: docker
From: ubuntu:latest

%labels
    Author lyan1@lsu.edu

%post
apt update
apt-get install -y python3 vim

# Create bind points for HPC environment
mkdir /project /work

%environment
export LC_ALL=C

%runscript
echo "Hello, world!"
```

Header: describes the base container image

Label: metadata for the container

Post: commands executed within the container after the base OS has been installed at build time.

Environment: define environment variables

Runscript: commands that will be run when the container is run by “singularity run”

Base OS/Container Images (1)

- Repositories:
  - Docker hub: https://hub.docker.com
  - Singularity hub: https://singularity-hub.org
  - NVIDIA GPU Cloud: https://ngc.nvidia.com
  - QUAY: https://quay.io
  - Distribution repo
    - YUM/RHEL
    - Debian/Ubuntu
- See examples from "`singularity build --help`"

Base OS/Container Images (2)

- Pay attention to the OS version
  - Singularity uses the kernel of the host OS
  - Do not deviate too much from the host OS kernel
    - Otherwise you will get error messages like “FATAL: kernel too old/new”

Inspecting Singularity Images

- Use the "`inspect`" command to query
  - How an image is built
  - What the runscript is
  - What environment variables are set
- Syntax: `singularity inspect [options] <container image>`
  - The options are self-explanatory: "--labels", "--runscript", "--deffile", "--environment" etc.

Demo 3
Build Singularity containers from recipes

Singularity on HPC Clusters

- Singularity is installed on all compute nodes on all HPC clusters
  - No Singularity on the head nodes
- You need to
  - Send an email to sys-help@loni.org and ask to be added to the "singularity" user group (one time)
  - The image file needs to be owned by the "singularity" user group
    - Use the "chgrp" command
    - Incorrect group ownership will generate an error: "FATAL: failed to retrieve group information for cvmfs: group: unknown group cvmfs"
- You will **NOT** be able to build Singularity images on the HPC clusters

Running Singularity on HPC Clusters

- Syntax
  - `Singularity <command> [options] <container image>`
- Commands
  - `shell`: run an interactive bash shell
  - `run`: launch the runscript
  - `exec`: execute a command

Frequently Used Options

- "`-B`" or "`--bind`": directory binding
  - To bind a directory, it needs to be present both within and without the container
  - The home directory is bound automatically
  - Can be called multiple times
- "`--nv`": enable NVIDIA GPU support

Running Singularity As Batch Jobs

- Singularity can run in a job script just like any other application

```
#!/bin/bash
#PBS -A loni_loniadmin1
#PBS -q checkpt
#PBS -l nodes=1:ppn=20
#PBS -l walltime=24:00:00
#PBS -N TF_benchmark

cd $PBS_O_WORKDIR

SIMG=/home/admin/singularity/tensorflow-2.2-gpu-dockerhub.simg

singularity exec -B /project --nv $SIMG \
  python3 benchmarks/scripts/tf_cnn_benchmarks/tf_cnn_benchmarks.py \
  --num_gpus=2 -batch_size=32 -model=resnet50 \
  --variable_update=parameter_server
```

Demo 4
Run Singularity containers on clusters

Singularity Workflow

- 1. Install Singularity on local computer – **need root**
- 2. Build a Singularity image – **need root**
  - A. Build a sandbox from an existing base image
  - B. Make changes to the sandbox
  - C. Test the image on the production environment (HPC clusters)
    - Go back to step 2B if necessary
  - D. Capture all actions in a recipe and build a read-only image from it
    - Alternative: build the read-only image from the sandbox (harder to share with others)
- 3. Run on the HPC cluster
  - Need to be added to the “singularity” user group
  - The image needs to be owned by the “singularity” group

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Services Provided by HPC

- Prebuilt Singularity images
  - Located under `/home/admin/singularity` on all clusters
- User documentation
  - https://www.hpc.lsu.edu/docs/singularity.php
- Recipes
  - https://github.com/lsuhpchelp/singularity
- Troubleshooting and consulting

Questions?