Tutorial: Introduction to Containers for Scientific Container-Native Workflows: **Singularity** on **ACES**

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ACES
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High Performance Research Computing
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Outline

- Overview of Containers
- Overview of Singularity
- Getting Started
- Container Image Sources
- Working with Images
- Working with Containers
- Containerized Scientific Applications on ACES
  - PyTorch
  - LAMMPS

Learning Resources

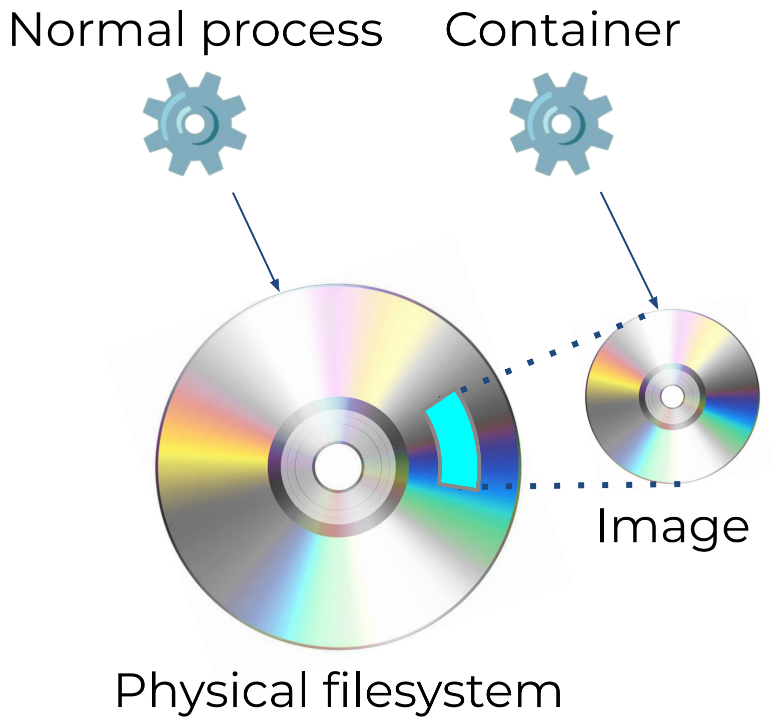
- Slides on the course web page
  https://hprc.tamu.edu/training/aces_containers_scientific.html
  highly recommended for working along)
- HPRC's Knowledge Base
  https://hprc.tamu.edu/kb/Software/Singularity/
- HPRC on YouTube
  https://www.youtube.com/c/TexasAMHPRC
- ACCESS Links
  https://support.access-ci.org/ci-links

Overview of Containers

What Are Containers?

- A container is a process (⚙️) that has its own **view** of local resources:
  - Filesystem
  - User IDs
  - Network

  etc.
- Example: this container (⚙️on the right) sees the **image** instead of the physical filesystem

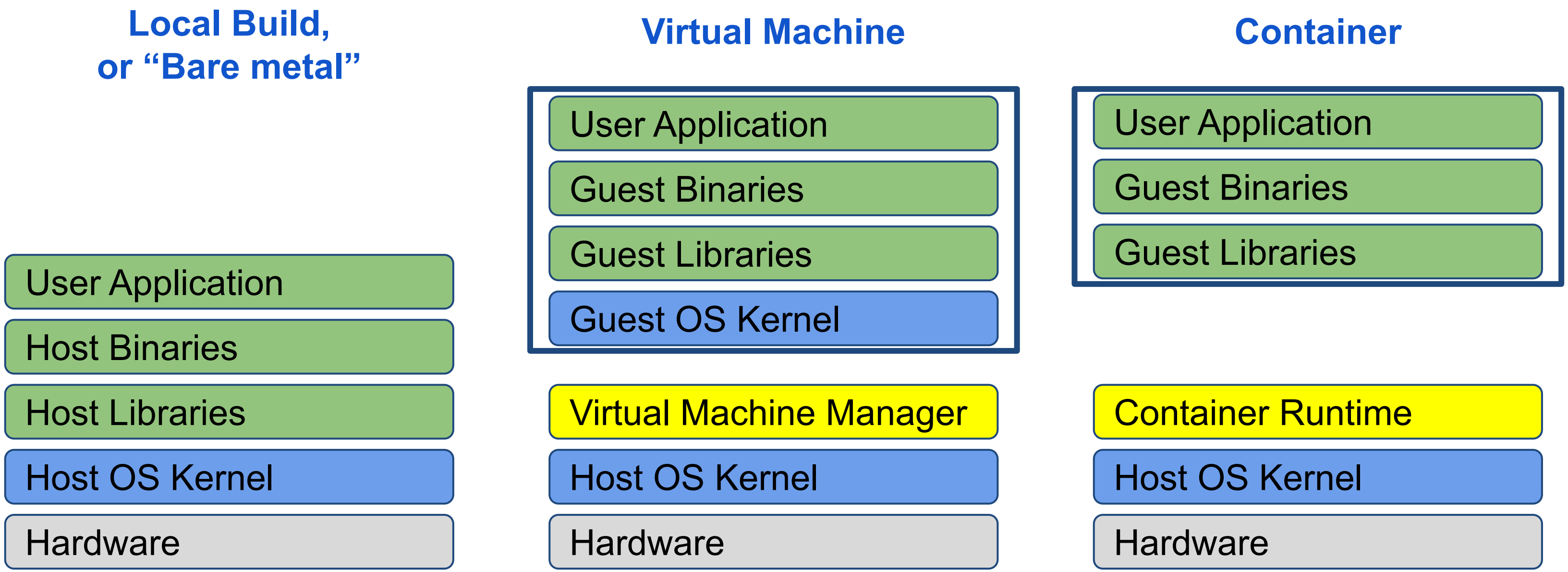


Why Use Containers?

- **Shareability**:
    - Share your container image file by uploading to a public repository
    - Use images shared by others
- **Portability**:
    - Use images on any computer with the same architecture (x84-64)
- **Reproducibility**:
    - Container users are largely unaffected by changes to the cluster environments

What Goes In Container Images?

- Unlike in VMs, the OS Kernel is not duplicated
- Container images are smaller than VM images



Popular Container Runtimes

Instant deployment to users on different devices!

LXC
2008

Docker
2013

Singularity
2015

Shifter 2016

Charliecloud
2017

Podman
2018

Overview of Singularity

Singularity

- An easy-to-use, high-performance container solution

Deploying Secure Container

Solutions from Edge to Exascale

Presented by

Sylabs

Singularity is Apptainer

Sylabs

THE LINUX FOUNDATION

Singularity Features

- Singularity is a container runtime and an image builder
- Singularity can read and convert Docker images
- Filesystem inside container is isolated
- User inside container is the same as the user outside
- Works with high-performance cluster technologies

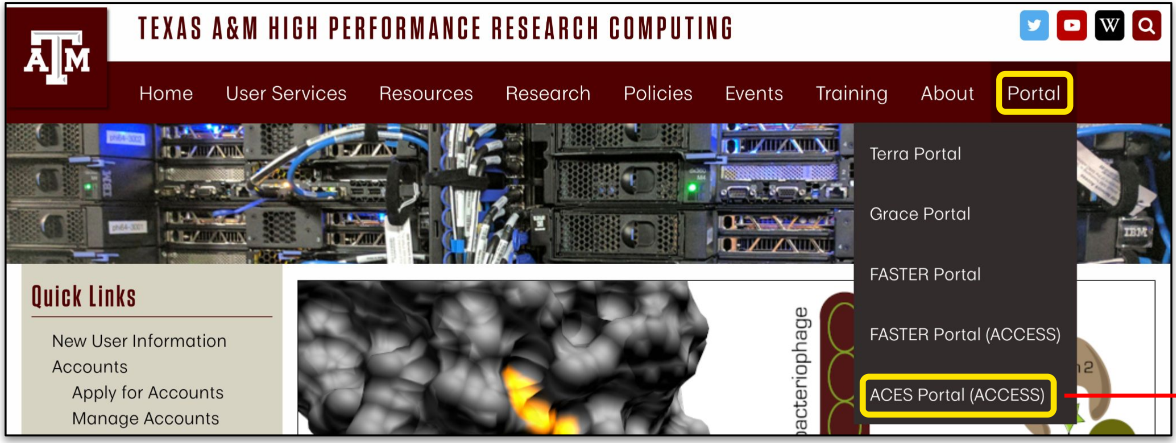
Read more in the Apptainer manual
https://apptainer.org/user-docs/3.8/

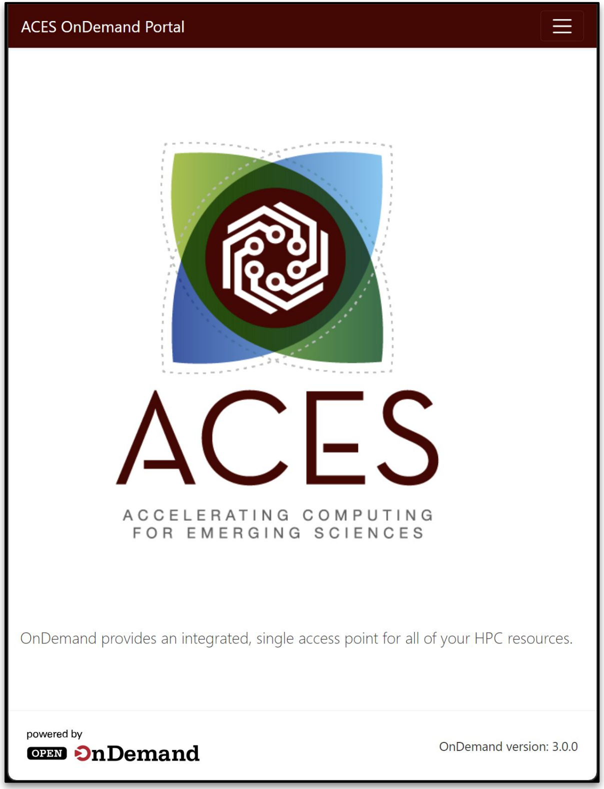
Singularity on ACES

- Singularity is available on Compute nodes
    - Singularity activities are too cpu-intensive for login nodes.
- Singularity images can be large on disk. Be aware of your storage quota. (`/scratch` > `/home`)
- Some container activities may be too I/O-intense for the shared network filesystem. Be courteous to others and use a local filesystem for large image operations.

Getting Started

ACES Portal

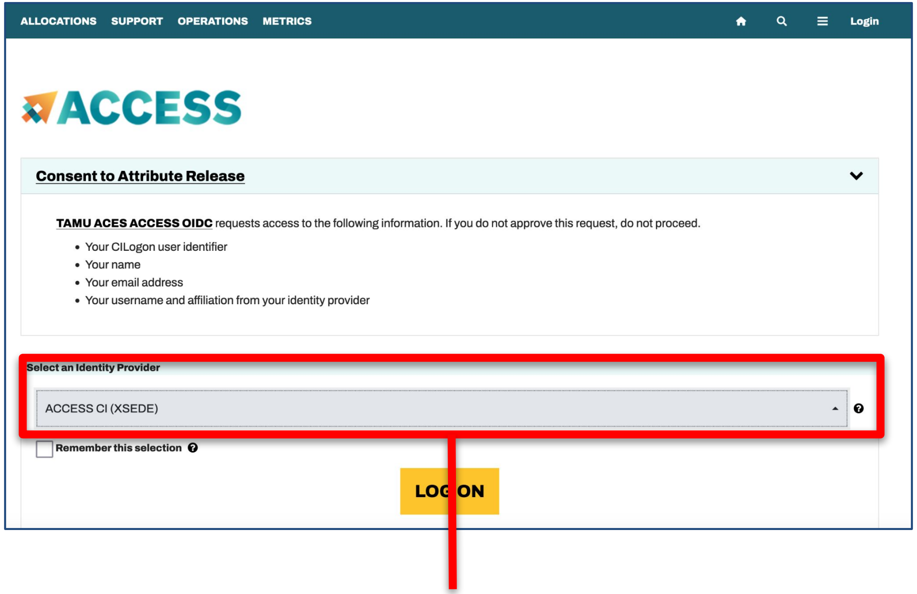




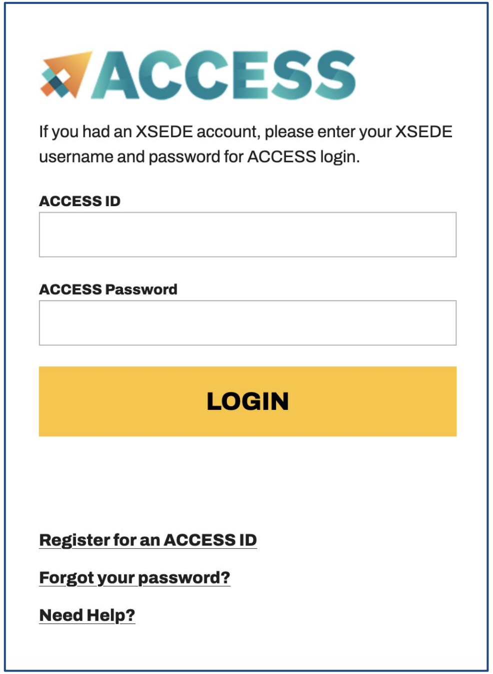
ACES Portal portal-aces.hprc.tamu.edu
is the web-based user interface for the ACES cluster

Open OnDemand (OOD) is an advanced web-based graphical interface framework for HPC users

Accessing ACES via the Portal (ACCESS)



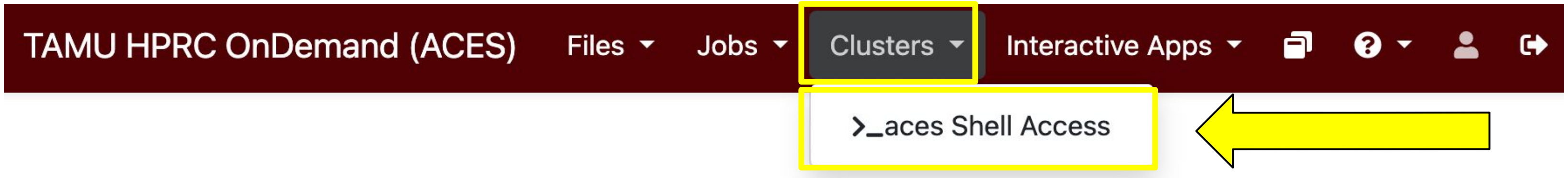
Select the Identity Provider appropriate for your account.



Log-in using your ACCESS or institutional credentials.

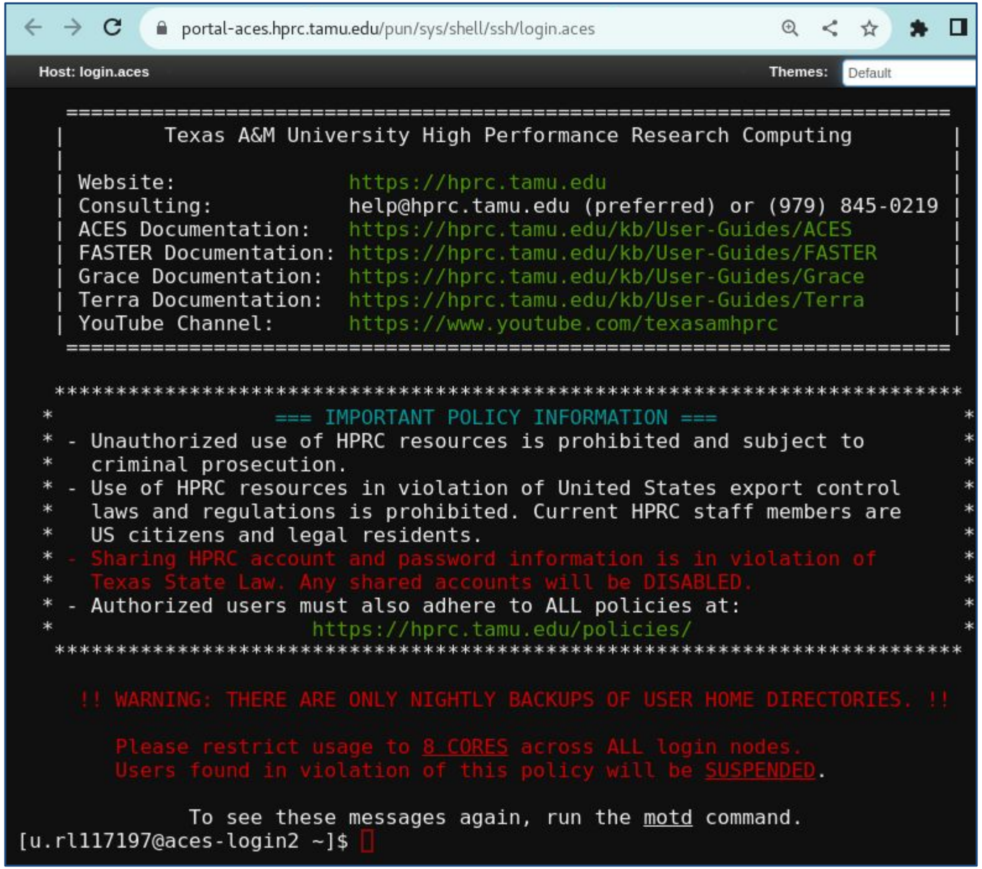
Get a Shell on ACES

Click on “Clusters” menu → _aces Shell Access



Success!

Welcome to the ACES login node.



Set Up Your Tutorial Environment

```
cd $SCRATCH
mkdir s_tutorial
cd s_tutorial
pwd

export TRAINING=/scratch/training/singularity
ls $TRAINING
```

Set Up Your Singularity Environment

Get to a compute node from the login node

```
srun --time=120 --mem=4G --pty bash -i
```

following along live? add:
`--reservation=containers`

Return to your tutorial directory (if necessary)

```
cd $SCRATCH/s_tutorial
```

Set your singularity cache directory for temporary files

```
export SINGULARITY_CACHEDIR=$TMPDIR
```

Connect to the internet for fetching images

```
module load WebProxy
```

Your First Singularity Container

Singularity can fetch an image *and* launch a shell in one line.

```
singularity shell --help
```

Fetch an image and launch a shell from it

```
singularity shell docker://almalinux:8
cat /etc/redhat-release
exit
```

The ACES compute nodes also have Red Hat linux installed.

```
cat /etc/redhat-release
```


Congratulations!
Welcome to containers
WWW.FUNIMADA.COM

Container Image Sources

Popular Repositories

The most common repository is:

- Docker Hub

Others repositories include:

- Singularity Hub
- Singularity Library
- NVIDIA GPU Cloud
- Quay.io
- BioContainers

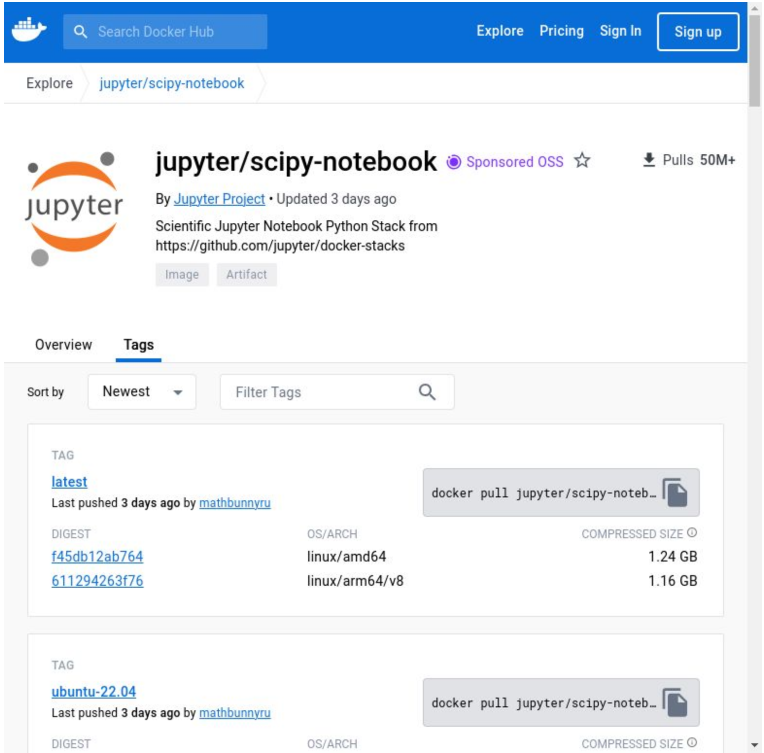
See
https://hprc.tamu.edu/kb/Software/Singularity/Examples/#popular-repositories

Docker Hub Example

Docker Hub repositories are named in the form `<group>/<name>` similar to GitHub.

Each image within a repository has a `<tag>` that describes how and when it was built.

This example is `jupyter/scipy-notebook:latest`



Singularity Pull

Singularity can fetch images from repositories and also convert them to the singularity file format at the same time.

```
singularity pull [target-filename] <source>
```

Where `<source>` refers to something on the internet. The syntax depends on where the source is located.

and `[target-filename]` includes the file extension.

Singularity Pull Example

The `<source>` argument for Docker images looks like

```
docker://<group>/<name>[:<tag>]
```

Therefore the pull command for the Jupyter example is,

```
singularity pull docker://jupyter/scipy-notebook:latest
```

(Download now or copy from `$TRAINING`; we will need this later)

The default filename will be `scipy-notebook_latest.sif`

Working with Images

Singularity Image Formats

- Singularity container images come in two main formats:
  1. Directory
  2. Single file. Singularity uses the `SIF` format for single file images. This is the default.
- The `singularity build` tool can convert images in both formats.

```
singularity build --help
```

- The `--sandbox` option is used to create directory-format images.

Singularity Image Exercise

Singularity pull can fetch an image and write to either file format.
(note the order of the arguments)

```
singularity pull almalinux.sif docker://almalinux:8
```

Singularity can convert an image to the directory file format.
Use the --sandbox argument to specify the directory type.
(note the order of the arguments)

```
singularity build --sandbox $TMPDIR/almalinux almalinux.sif
```

Singularity Write Exercise

Directory images are writable. Simply add the `--writeable` flag to your container command.

```
singularity shell --writable $TMPDIR/almalinux
mkdir /my_dir
exit
```

Are the changes still there?

```
singularity shell $TMPDIR/almalinux
ls /
```

Singularity Read-only Exercise

`SIF` files are safe for network file system `/scratch`.

```
singularity build --fakeroot my_almalinux.sif $TMPDIR/almalinux
```

Are the changes still there?

```
singularity shell my_almalinux.sif
ls /
exit
```

What about the `--writeable` flag?

```
singularity shell --writable my_almalinux.sif
no.
```

Working with Containers

Launching Processes

Singularity has three methods for launching processes:

- **Interactive**: singularity `shell`
- **Batch processing**: singularity `exec`
- **Container-as-executable**: singularity `run`

Singularity Run Exercise

Singularity run will execute the default runscript, if one was defined. You may also execute the container directly.

```
singularity pull docker://hello-world
singularity run hello-world_latest.sif
Hello from Docker!
./hello-world_latest.sif
Hello from Docker!
```

Docker hello-world is a minimal image. This is all it can do.

Singularity Exec Exercise

Singularity Exec lets you access executables and other commands in a container. This is appropriate for batch jobs.

ACES nodes have Python 3.

```
python3 --version
Python 3.6.8
```

Our singularity image has a different Python 3.

```
singularity exec scipy-notebook_latest.sif python3 --version
Python 3.11.6
```

Working with Files

- Filesystem inside a container is isolated from the real, physical filesystem.
- To access your files, ensure the directory is *mounted*.
- By default, Singularity will mount `$HOME` and `$PWD` if it can.
- To specify additional directories, use the `SINGULARITY_BINDPATH` environment variable or the `--bind` command line option.

Working with Files Exercise

Recommended that you mount `/scratch` to get access to your data storage, and `/tmp` to get access to the local disk on the node.

```
singularity shell --bind "/scratch,/tmp" <image>
mkdir $TMPDIR/my_dir; exit
ls $TMPDIR
```

Notice that your variables like `$TMPDIR` get passed into the container by default.

(singularity on ACES already binds these directories by default)

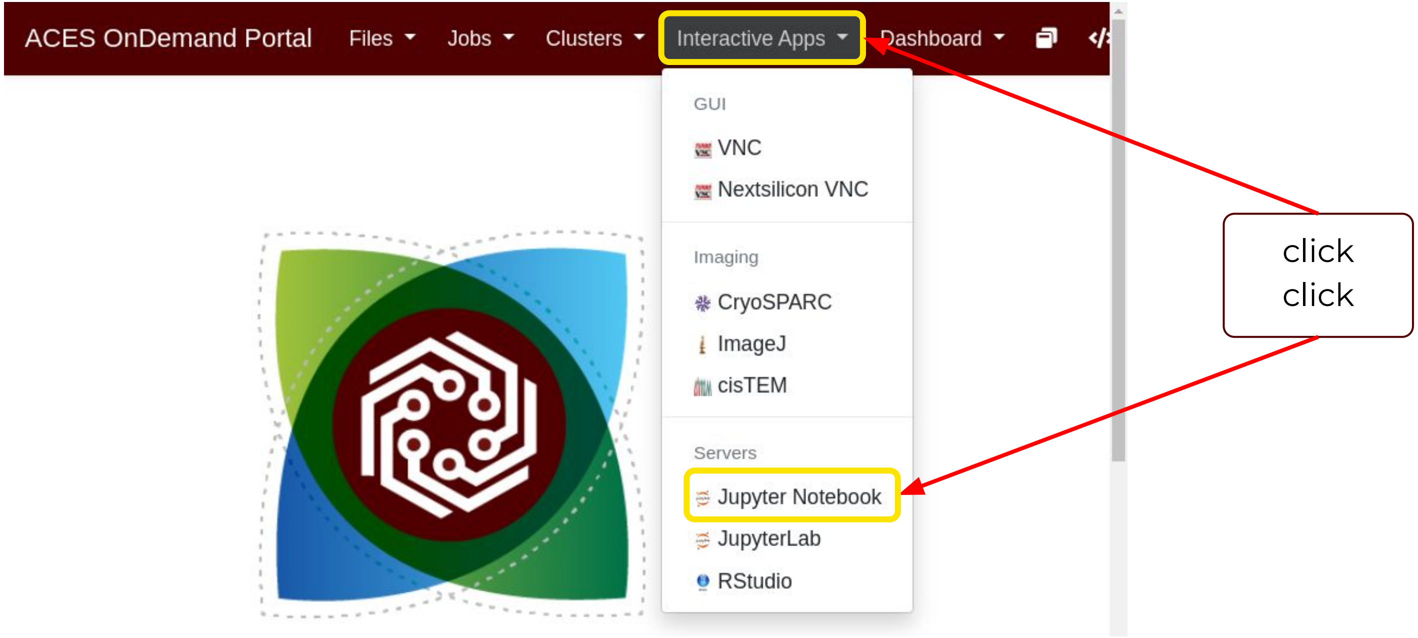
Singularity Batch Example

```
#!/bin/bash

## JOB SPECIFICATIONS
#SBATCH --job-name=sing_test          #Set the job name to "sing_test"
#SBATCH --time=00:10:00               #Set the wall clock limit to 1hr and 30min
#SBATCH --ntasks=4                    #Request 4 task
#SBATCH --mem=2560M                   #Request 2560MB (2.5GB) per node
#SBATCH --output=sing_test.%j         #Send stdout/err to "sing_test.[jobID]"

export SINGULARITY_BINDPATH="/scratch,/tmp"

# execute the default runscript defined in the container
singularity run hello-world_latest.sif

# execute a command within container
# specify the full path if the command is not in PATH
singularity exec scipy-notebook_latest.sif python3 hello.py
```

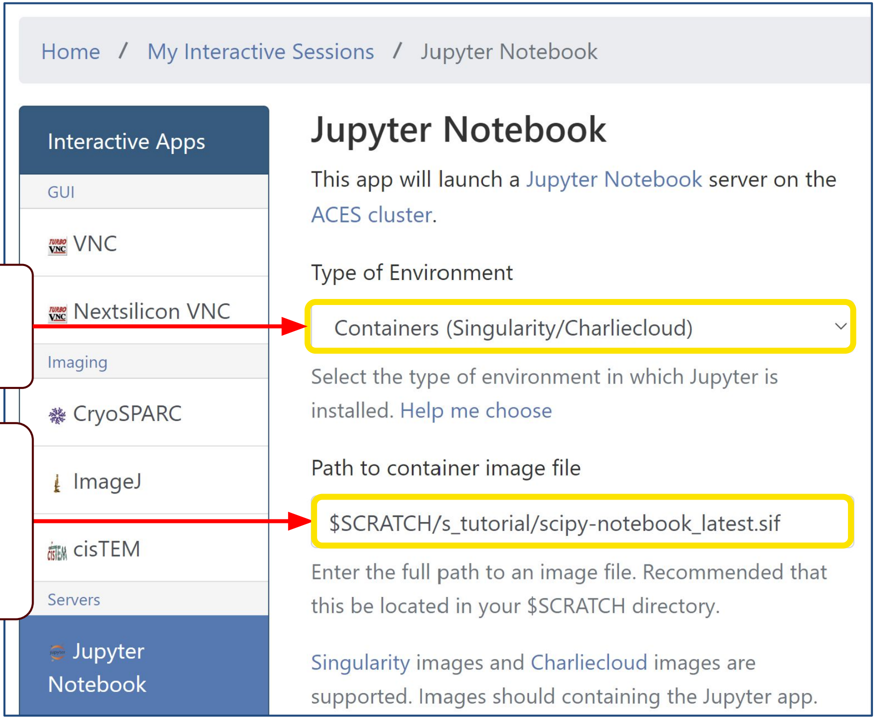
ONE VARIABLE

2 CONTAINERS

Interactive Graphical Computing



Containerized Jupyter Notebook



Choose *Containers*

Enter

`$SCRATCH/s_tutorial/scipy-notebook_latest.sif`

or wherever your file actually is (see Slide 27)

Backup copy at
`/scratch/training/singularity/scipy-notebook_2023.sif`

...Continued

Launch
Jupyter Notebook (5488) 1 node | 1 core | Starting
Jupyter Notebook (5489) 1 node | 1 core | Running
Host: ac110
Delete
Created at: 2023-09-21 15:39:52 CDT
Time Remaining: 56 minutes
Session ID: a5f41dfd-7c0d-44e3-aea7-7331c66a4d24
Connect to Jupyter
click
...wait
click
...wait
click
New
Upload
Notebook
Terminal
Console
New File
New Folder
last month
File Edit View Run Kernel Settings Help
Trusted
Code
[1]:
import numpy
print(numpy)
<module 'numpy' from '/opt/conda/lib/python3.11/site-packages/numpy/__init__.py'>
WOW

Containerized Scientific Applications

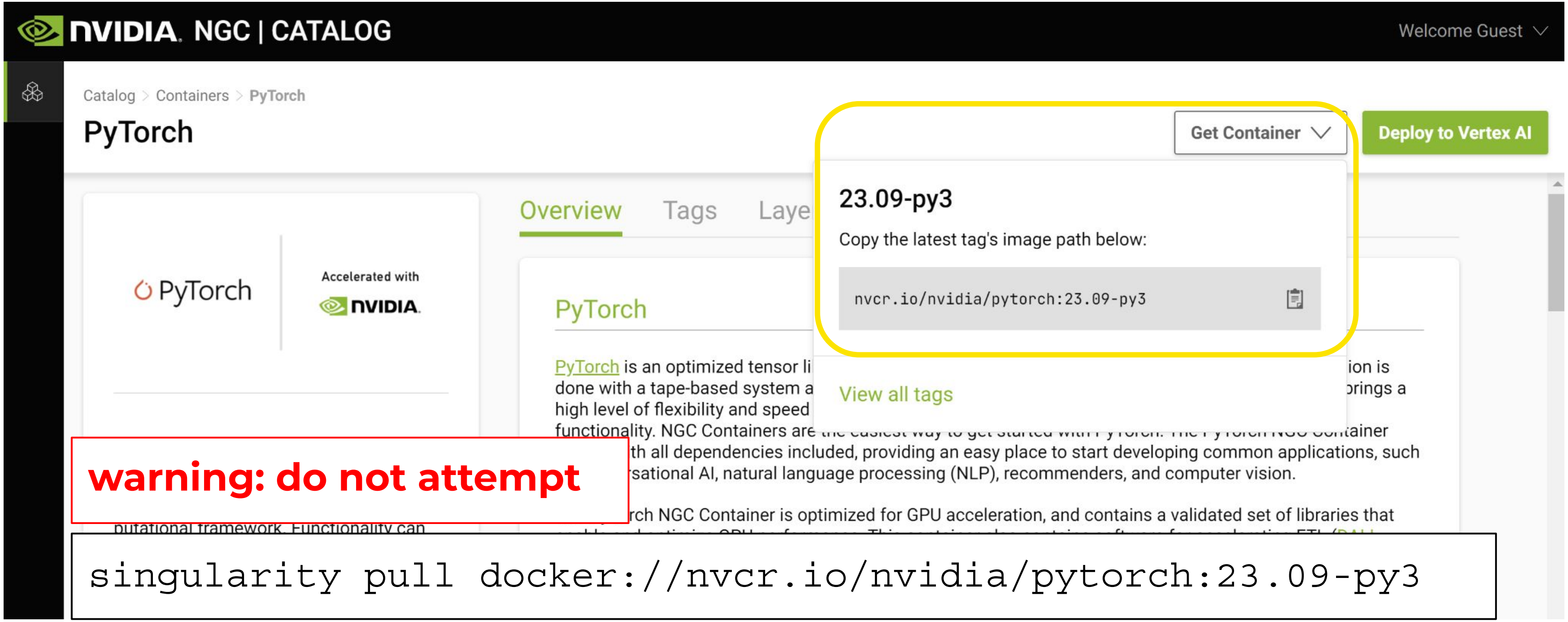
Singularity with GPU

- Containers should be built with CUDA version compatible with local GPUs (CUDA ≧ 11)
- Just add the `--nv` flag to your singularity command

Many repositories on Docker Hub have GPU-ready images. Search for images with “gpu” in tags

The nvidia cloud also provides GPU-ready images. See:
https://hprc.tamu.edu/wiki/SW:Singularity:Examples#NVIDIA_GPU_Cloud

NVIDIA Container Registry Example



warning: do not attempt

```
singularity pull docker://nvcr.io/nvidia/pytorch:23.09-py3
```

PyTorch GPU Exercise

Image file: `pytorch_23.09-py3.sif`

from `docker://nvcr.io/nvidia/pytorch:23.09-py3`

Located at `/scratch/training/singularity/`

From the login node: (all on one line)

```
srun --mem=4G --time=60
--gres=gpu:1 --partition=gpu --pty bash -i
```

following along live? add: `--reservation=containers`

From the compute node: (all on one line)

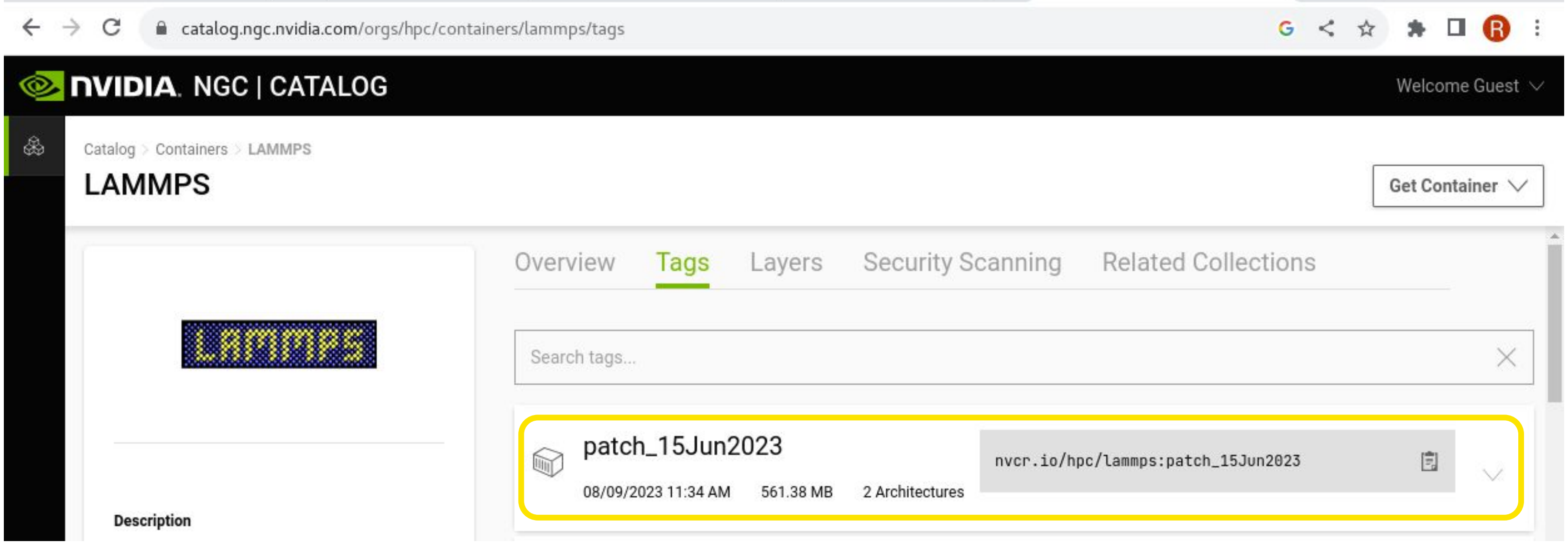
```
singularity exec --nv pytorch_23.09-py3.sif
python3 -c "import torch;
print(torch.cuda.device_count())"
```

LAMMPS Molecular Dynamics on GPUs

- LAMMPS is a classical MD code
- https://www.lammps.org/ has a cool animated logo.
- NVIDIA provides GPU-ready container images for lammps. https://catalog.ngc.nvidia.com/orgs/hpc/containers/lammps

LAMMPS on H100 GPUs

- *This* specific build works with H100 GPUs



LAMMPS on GPUs

Image file: `lammps-nv-patch_15Jun2023.sif`

from `docker://nvcr.io/hpc/lammps:patch_15Jun2023`

Located at `/scratch/training/singularity/`

From the login node: (all on one line)

```
srun --mem=4G --time=60
--gres=gpu:1 --partition=gpu --pty bash -i
```

following along live? add:
`--reservation=containers`

From the compute node:

```
cd /scratch/training/singularity
```

(all on one line):

```
singularity run --nv lammps-nv-patch_15Jun2023.sif
bash benchmark.sh
```

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    - 2019129 - FASTER - Fostering Accelerated Scientific Transformations, Education, and Research
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- ACCESS CCEP pilot program, Tier-II

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Help us help you. Please include details in your request for support, such as, Cluster (ACES, FASTER, Grace, Launch), NetID (UserID), Job information (JobID(s), Location of your jobfile, input/output files, Application, Module(s) loaded, Error messages, etc), and Steps you have taken, so we can reproduce the problem.