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

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ACES
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High Performance Research Computing
DIVISION OF RESEARCH

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ACCESS
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Outline

- Overview of Containers
- Overview of Charliecloud
- Getting Started
- Scientific Container Image Sources
- Working with Images
- Working with Containers
- Scientific Use Cases on ACES
    - Tensorflow
    - LAMMPS
    - Clara Parabricks

Learning Resources

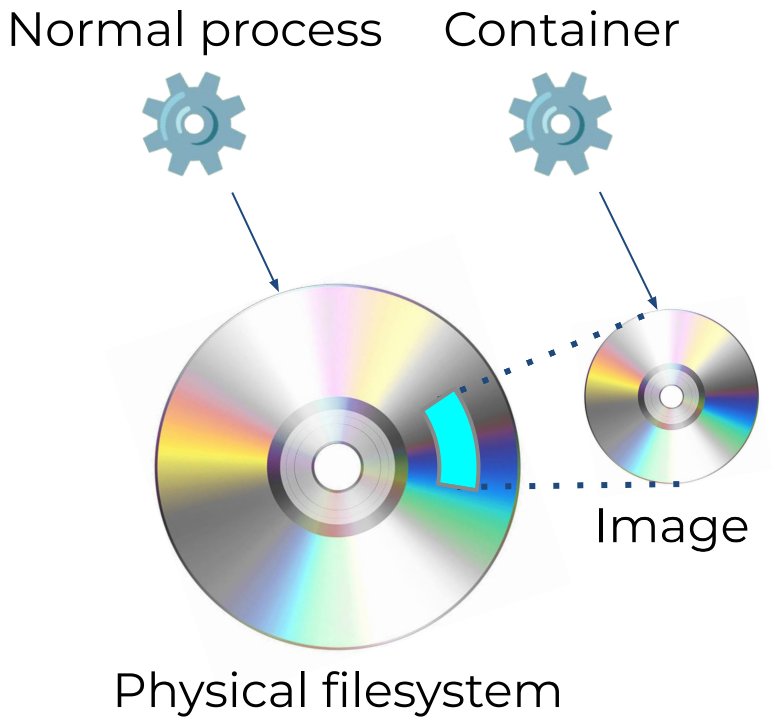
- Slides on the course web page
  https://hprc.tamu.edu/training/aces_containers.html
- HPRC Knowledge Base
  https://hprc.tamu.edu/kb/Software/CharlieCloud/
- HPRC on YouTube
  https://www.youtube.com/c/TexasAMHPRC
- Charliecloud Documentation
  https://hpc.github.io/charliecloud/
- ACCESS Links
  https://support.access-ci.org/ci-links

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



Normal process

Container

Image

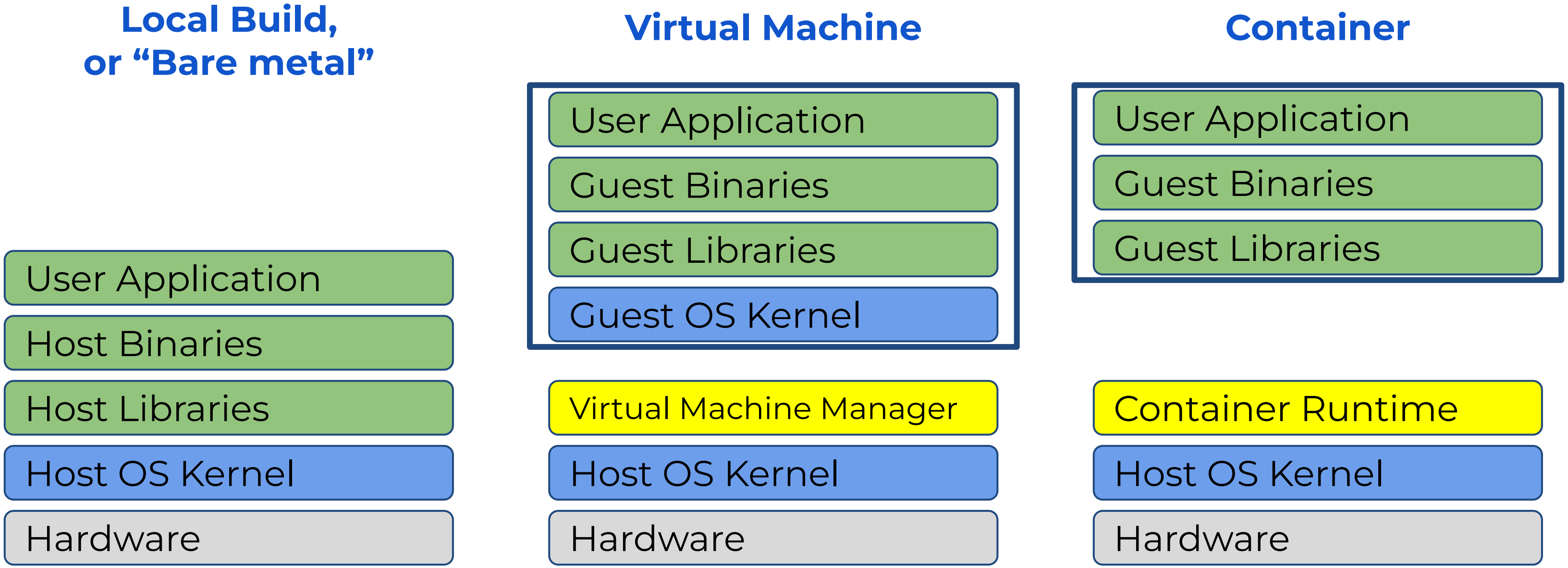
Physical filesystem

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



Local Build,
or “Bare metal”

User Application
Host Binaries
Host Libraries
Host OS Kernel
Hardware

Virtual Machine

User Application
Guest Binaries
Guest Libraries
Guest OS Kernel
Virtual Machine Manager
Host OS Kernel
Hardware

Container

User Application
Guest Binaries
Guest Libraries
Container Runtime
Host OS Kernel
Hardware

Popular Container Runtimes

Instant deployment to users on different devices!

LXC 2008

Docker 2013

Singularity 2015

Shifter 2016

Charliecloud 2017

Podman 2018

Overview of Charliecloud

Charliecloud

- A lightweight, fully-unprivileged container solution

Presented by

Los Alamos NATIONAL LABORATORY

Charliecloud Features

- Charliecloud is a container runtime and an image builder
- Charliecloud can read and convert Docker images
- Filesystem inside container is isolated
- User inside container is isolated
- Works with high-performance cluster technologies

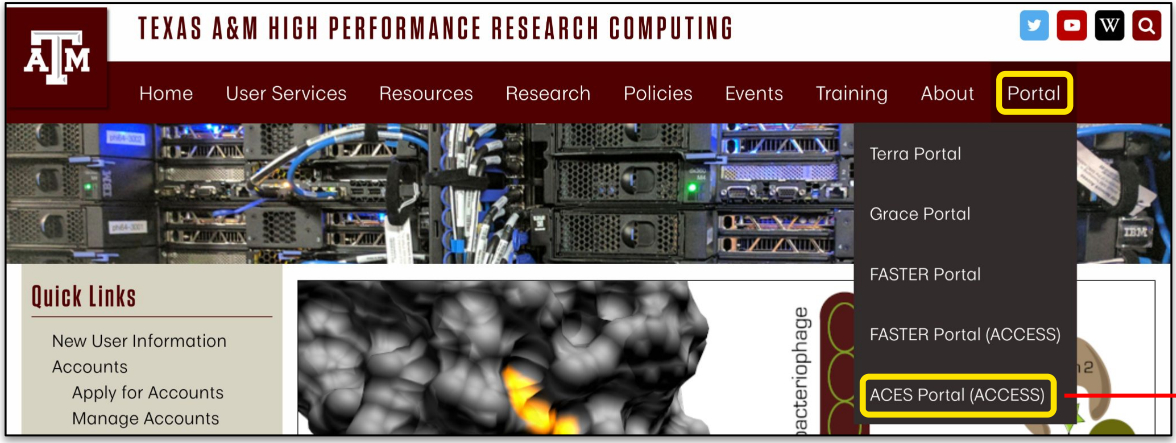
Read more in the Charliecloud manual on github
https://hpc.github.io/charliecloud/

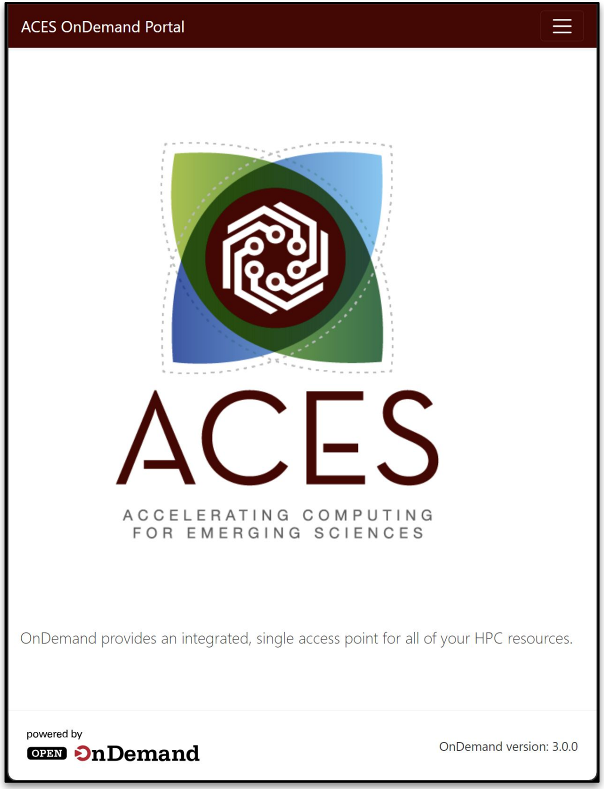
Charliecloud on ACES

- Charliecloud is available from our module system
  - execute `module load charliecloud`
- Charliecloud images can be large on disk. Be aware of your storage quota.
- Some container activities may be too cpu-intense for the *shared* login node. Be courteous to others and use a compute node for large image operations.
- 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


TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING


ACES OnDemand Portal

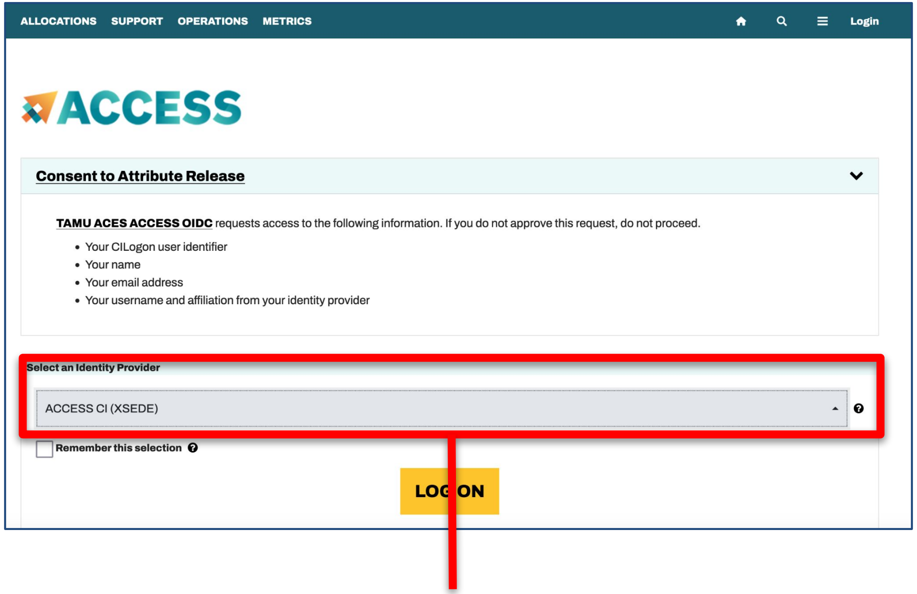
OnDemand provides an integrated, single access point for all of your HPC resources.

OnDemand version: 3.0.0

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)



Consent to Attribute Release

TAMU ACES ACCESS OIDC requests access to the following information. If you do not approve this request, do not proceed.

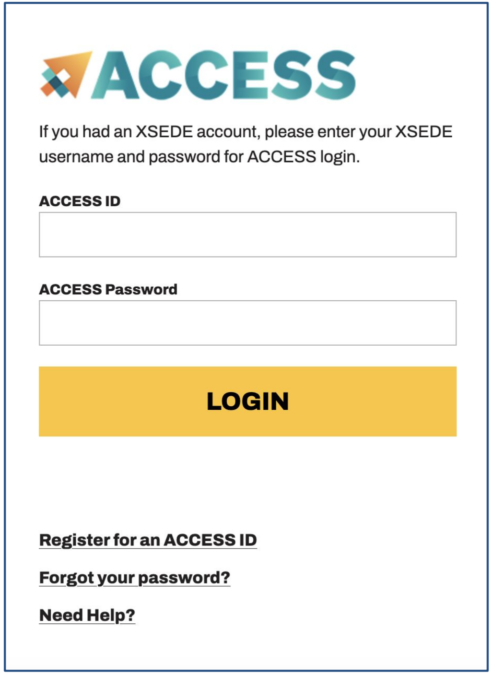
- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

Select an Identity Provider

ACCESS CI (XSEDE)

☐ **Remember this selection**

Select the Identity Provider appropriate for your account.



If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login.

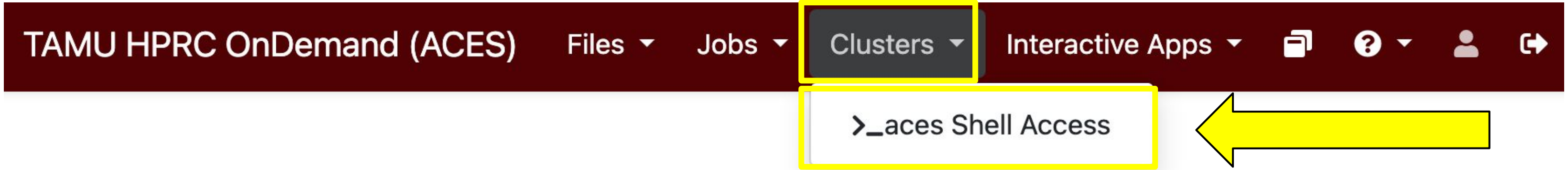
ACCESS ID

ACCESS Password

Log-in using your ACCESS or institutional credentials.

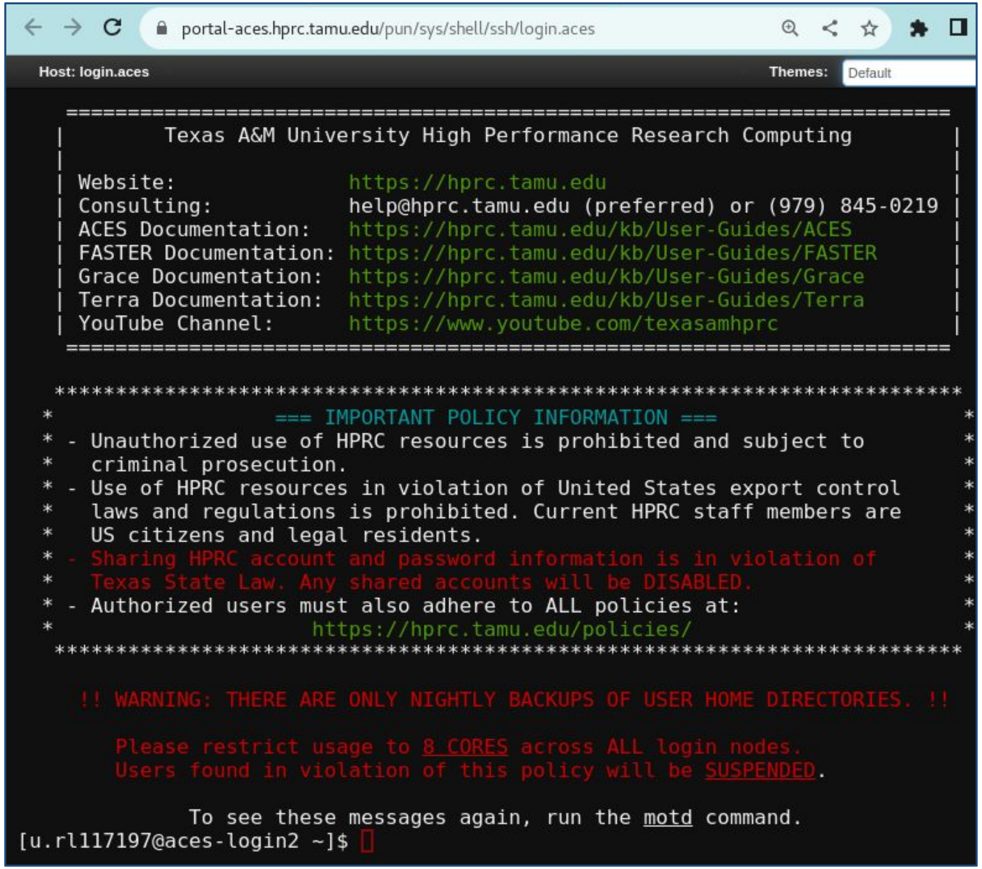
Get a Shell on ACES

Click on “Clusters” menu → _aces Shell Access



Success!

Welcome to the ACES login node.



```
    ========================================================================
   |        Texas A&M University High Performance Research Computing        |
   |                                                                        |
   | Website:                     https://hprc.tamu.edu                     |
   | Consulting:                  help@hprc.tamu.edu (preferred) or (979) 845-0219 |
   | ACES Documentation:          https://hprc.tamu.edu/kb/User-Guides/ACES |
   | FASTER Documentation:        https://hprc.tamu.edu/kb/User-Guides/FASTER |
   | Grace Documentation:         https://hprc.tamu.edu/kb/User-Guides/Grace |
   | Terra Documentation:         https://hprc.tamu.edu/kb/User-Guides/Terra |
   | YouTube Channel:             https://www.youtube.com/texasamhprc       |
    ========================================================================

  **************************************************************************
  *                  === IMPORTANT POLICY INFORMATION ===                  *
  * - Unauthorized use of HPRC resources is prohibited and subject to      *
  *   criminal prosecution.                                                *
  * - Use of HPRC resources in violation of United States export control   *
  *   laws and regulations is prohibited. Current HPRC staff members are   *
  *   US citizens and legal residents.                                     *
  * - Sharing HPRC account and password information is in violation of     *
  *   Texas State Law. Any shared accounts will be DISABLED.               *
  * - Authorized users must also adhere to ALL policies at:                *
  *                  https://hprc.tamu.edu/policies/                       *
  **************************************************************************

    !! WARNING: THERE ARE ONLY NIGHTLY BACKUPS OF USER HOME DIRECTORIES. !!

       Please restrict usage to 8 CORES across ALL login nodes.
       Users found in violation of this policy will be SUSPENDED.

              To see these messages again, run the motd command.
[u.rl117197@aces-login2 ~]$ 
```

Set Up Your Environment

```
cd $SCRATCH
mkdir ch_tutorial
cd ch_tutorial
pwd

export TRAINING=/scratch/training/charliecloud
ls $TRAINING

module load charliecloud
module list
```

Your First Image

The charliecloud image tool helps you build and organize your images.

```
ch-image --help
```

Let’s fetch a small, basic linux distro: Almalinux.

```
ch-image pull almalinux:8
ch-image list
```

The image is in your personal temporary local image repository.

```
echo $CH_IMAGE_STORAGE
ls $CH_IMAGE_STORAGE/img/
```

Your First Container

The ACES login node has Red Hat Enterprise linux installed.

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

The charliecloud-run tool launches containers out of existing images.

```
ch-run --help
```

Let's launch a bash shell, investigate, and stop the container.

```
ch-run almalinux:8 bash
cat /etc/redhat-release
exit
```

Congratulations!

Welcome to containers

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

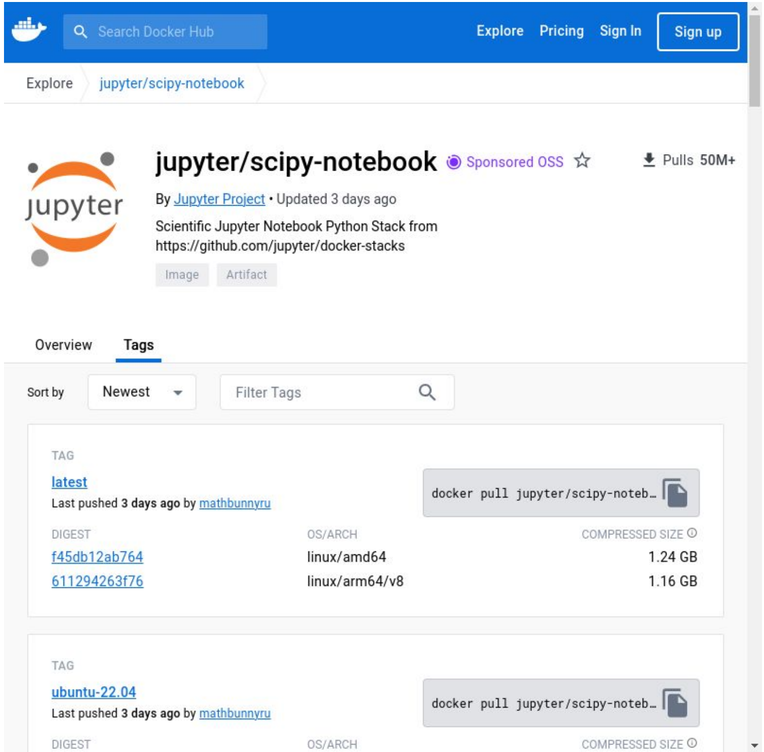
See
https://hprc.tamu.edu/kb/Software/Singularity/Examples/#popular-repositories

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`



jupyter/scipy-notebook Sponsored OSS

Pulls 50M+

By Jupyter Project • Updated 3 days ago

Scientific Jupyter Notebook Python Stack from https://github.com/jupyter/docker-stacks

TAG

latest

Last pushed **3 days ago** by mathbunnyru

`docker pull jupyter/scipy-noteb…`

DIGEST	OS/ARCH	COMPRESSED SIZE
f45db12ab764	linux/amd64	1.24 GB
611294263f76	linux/arm64/v8	1.16 GB

TAG

ubuntu-22.04

Last pushed **3 days ago** by mathbunnyru

`docker pull jupyter/scipy-noteb…`

DIGEST OS/ARCH COMPRESSED SIZE

Docker Hub Pull Exercise

The `<source>` argument for an image pull looks like

- `<url>/<group>/<name>[:<tag>]`
- No url is needed for this exercise because Docker Hub is the default repository for Charliecloud

Therefore the pull command based the previous slide is:

```
ch-image pull jupyter/scipy-notebook:latest
```

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

Backup copy at
`/scratch/training/charliecloud/jupyter-scipy-notebook-2023.sqfs`

Clara Parabricks for GPU from NVIDIA

Performance Comparison

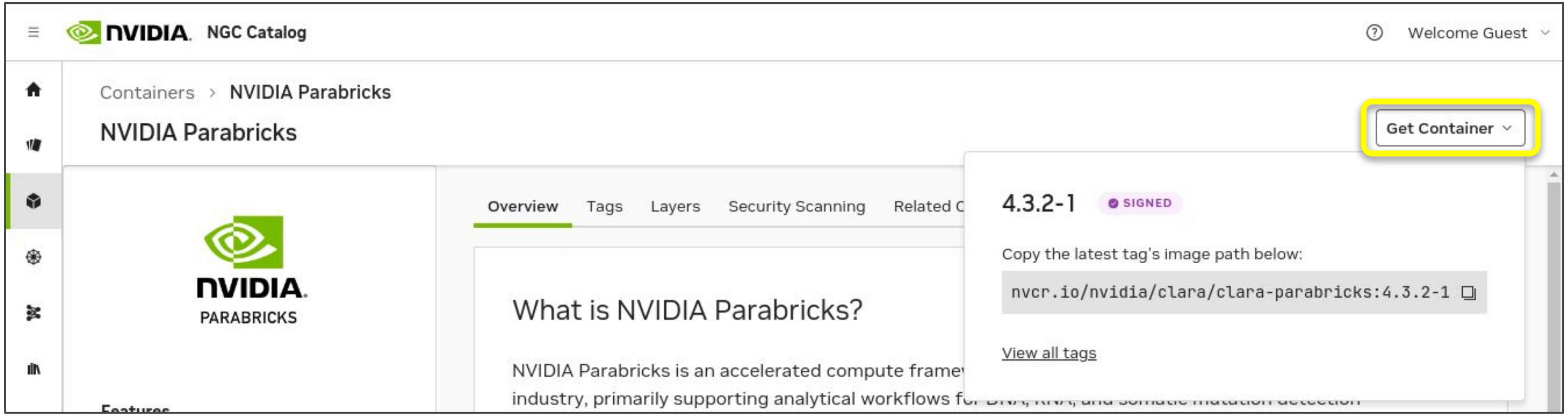
Germline End-To-End Secondary Analysis

Data was generated using publicly available data (https://precision.fda.gov/challenges/truth) for NA12878, deprecating the data to 30X coverage. For the 22-minute runtime, DGX A100 with 320G memory was used. The native GATK4.1 numbers were generated using 32 vCPU (3.1 GHz Intel Xeon® Platinum 8175M) using 320Gb RAM.

NVIDIA Product Sheet:
https://resources.nvidia.com/en-us-genomics-ug-ep/healthcare-genomics-?lx=M-s96I&ncid=em-nurt-521116&mkt_tok=MTU2LU9GTi03NDIAAAGG5gQCuzMHKWvhCg5ODJ9NTi9KCxm57Lxjd5DcahRJvhUUc-q_yTLDcNVB3HBmOyWbGWigpg4yq1h3SK9QNOLnbLU6cm8VhMCHmup4BGcunnUvwRCy#cid=ix09_em-nurt_en-us

NVIDIA Repository Example

Navigate to catalog.ngc.nvidia.com and search “Clara Parabricks”.



What is NVIDIA Parabricks?

NVIDIA Parabricks is an accelerated compute frame

industry, primarily supporting analytical workflows fo

Copy the latest tag's image path below:

```
nvcr.io/nvidia/clara/clara-parabricks:4.3.2-1
```

Private repositories need a url in addition to the image name.

`<url>…/<group>/<name>[:<tag>]`

Click the “Get Container” button on the Tags tab and copy the path.

Working with Images

Image Formats

- Charliecloud container images come in two main formats:
  1. Directory
  2. Single file. HPRC supports the squashfs filesystem format for single file images. (more about that on a later slide)
- The `ch-convert` tool copies images into different formats

```
ch-convert --help
```

Directory Image Format

- The image name should end in `/`.
- Directory images are writable.
- Directory read/write operation are slow, so put directory images on the high-speed `/tmp` filesystem.
- Images in `$CH_IMAGE_STORAGE` are also directory images, but you refer to them by name without the trailing slash.

Convert to Directory Exercise

Convert our image in the cache to a directory image.

```
mkdir /tmp/$USER
ch-convert jupyter/scipy-notebook:latest /tmp/$USER/jupyter/
```

What did we make?

```
ls /tmp/$USER/jupyter/
```

Note: `/tmp` is a local disk that's specific to this login node.

Editing Images Exercise

Directory images can be modified by adding the

```
--write
```

flag to `ch-run`. Any changes you make will be saved.

```
ch-run --write /tmp/$USER/jupyter/ bash
mkdir /scratch
exit
```

Are the changes still there?

```
ch-run /tmp/$USER/jupyter/ bash
ls
```

Squashfs Image Format

- Squashfs is an open-source file format for filesystem images
- The whole filesystem becomes one single file
- The image name should end in `.sqfs`
- Squashfs images are read-only.
- Squashfs read operations are fast, so put squashfs images on the network filesystem `/scratch`.

Convert to Squashfs Exercise

Make sure you are still in your `ch_tutorial` directory in `$SCRATCH`

```
pwd
```

Then convert

```
ch-convert /tmp/$USER/jupyter/ jupyter.sqfs
```

Are your changes still there?

```
ch-run jupyter.sqfs /bin/bash
ls
exit
```

Working with Containers

Mounting your Scratch Space

- The option `-b` is used to mount the `/scratch` filesystem outside the container over the empty `/scratch` directory inside the container.
- The option `-c` is used to set the starting working directory in the container.

```
ch-run -b /scratch -c $SCRATCH jupyter.sqfs bash
pwd
ls
exit
```

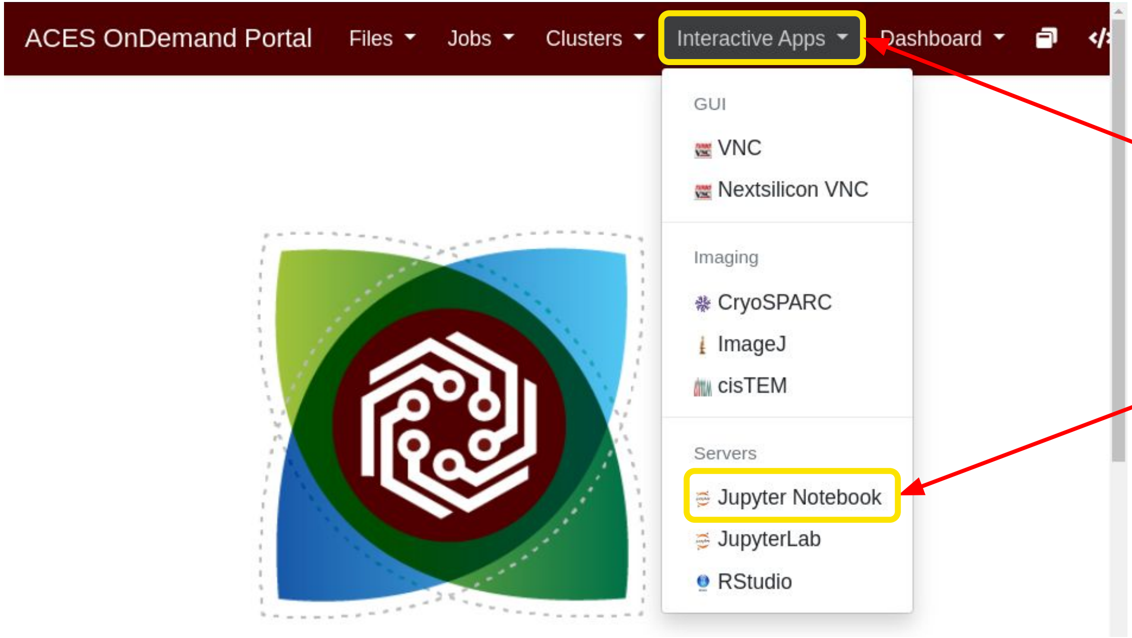
Working with Variables

Some containers come with environment variables that are needed in order for the application to function properly. The `--set-env` option is used to turn those on.

```
ch-run --set-env jupyter.sqfs python
>>> import numpy
>>> print(numpy)
>>> exit()
```

Python with Numpy was installed in a Conda environment. It requires the `PYTHONPATH` variable to function.

Interactive Graphical Computing

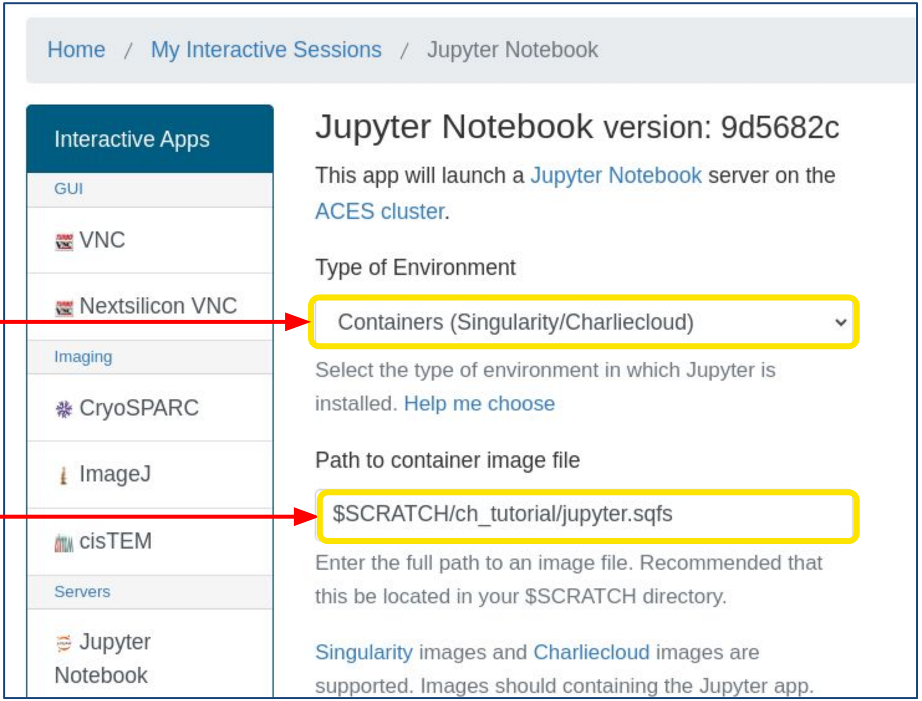


click
click

Containerized Jupyter Notebook

Choose *Containers*

Enter `$SCRATCH/ch_tutorial/jupyter.sqfs` or wherever your file actually is



Home / My Interactive Sessions / Jupyter Notebook

Jupyter Notebook version: 9d5682c

This app will launch a Jupyter Notebook server on the ACES cluster.

Type of Environment

Containers (Singularity/Charliecloud)

Select the type of environment in which Jupyter is installed. Help me choose

Path to container image file

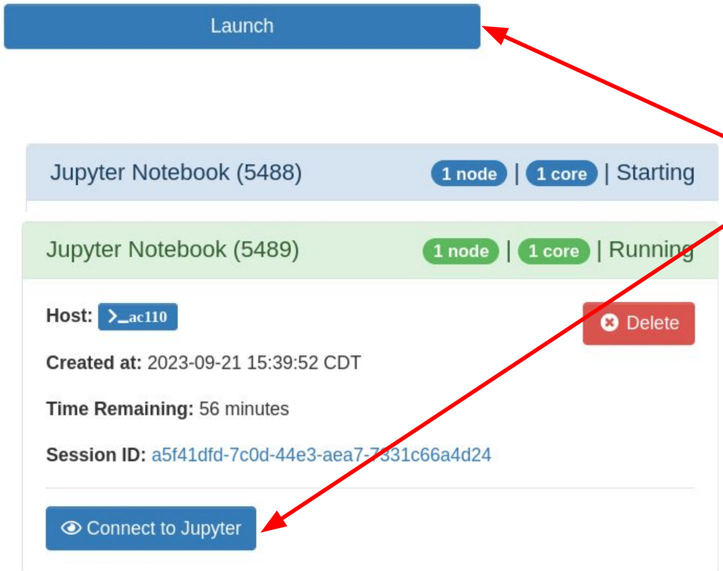
$SCRATCH/ch_tutorial/jupyter.sqfs

Enter the full path to an image file. Recommended that this be located in your $SCRATCH directory.

Singularity images and Charliecloud images are supported. Images should containing the Jupyter app.

Backup copy at `/scratch/training/charliecloud/jupyter-scipy-notebook-2023.sqfs`

…Continued



Jupyter Notebook (5488) 1 node | 1 core | Starting

Jupyter Notebook (5489) 1 node | 1 core | Running

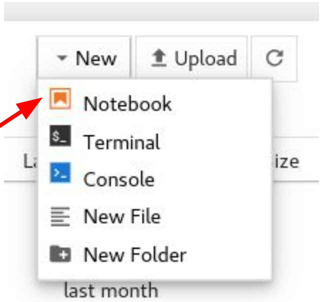
Host: >_ac110

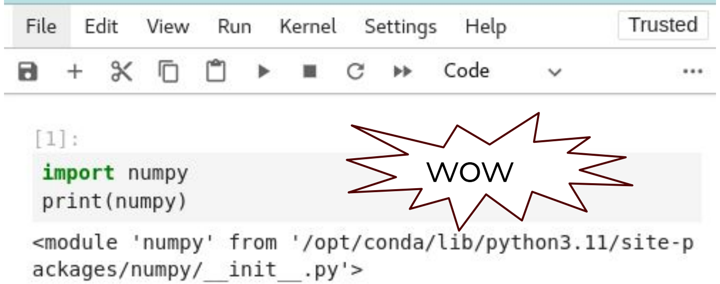
Created at: 2023-09-21 15:39:52 CDT

Time Remaining: 56 minutes

Session ID: a5f41dfd-7c0d-44e3-aea7-7331c66a4d24

click
…wait
click
…wait
click



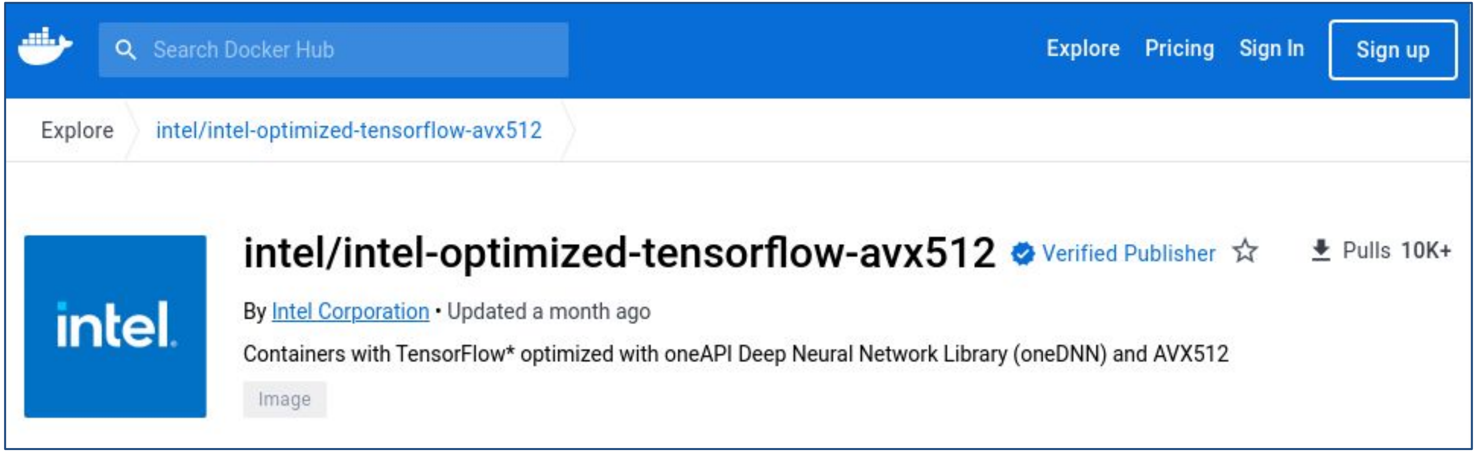


```
[1]: import numpy
     print(numpy)

<module 'numpy' from '/opt/conda/lib/python3.11/site-p
ackages/numpy/__init__.py'>
```

Containerized Scientific Applications

Machine Learning with TensorFlow



intel/intel-optimized-tensorflow-avx512

By Intel Corporation • Updated a month ago

Containers with TensorFlow* optimized with oneAPI Deep Neural Network Library (oneDNN) and AVX512

Pull this intel-optimized image and convert it to Squashfs

```
ch-image pull intel/intel-optimized-tensorflow-avx512
ch-convert intel/intel-optimized-tensorflow-avx512 intel-tensorflow.sqfs
```

TensorFlow in Container

Run the container and import TensorFlow:

```
ch-run intel-tensorflow.sqfs python
Python 3.10.6 …
>>> import tensorflow as tf
…
>>> print(“TensorFlow version:”, tf.__version__)
TensorFlow version: 2.13.0
>>> exit()
```

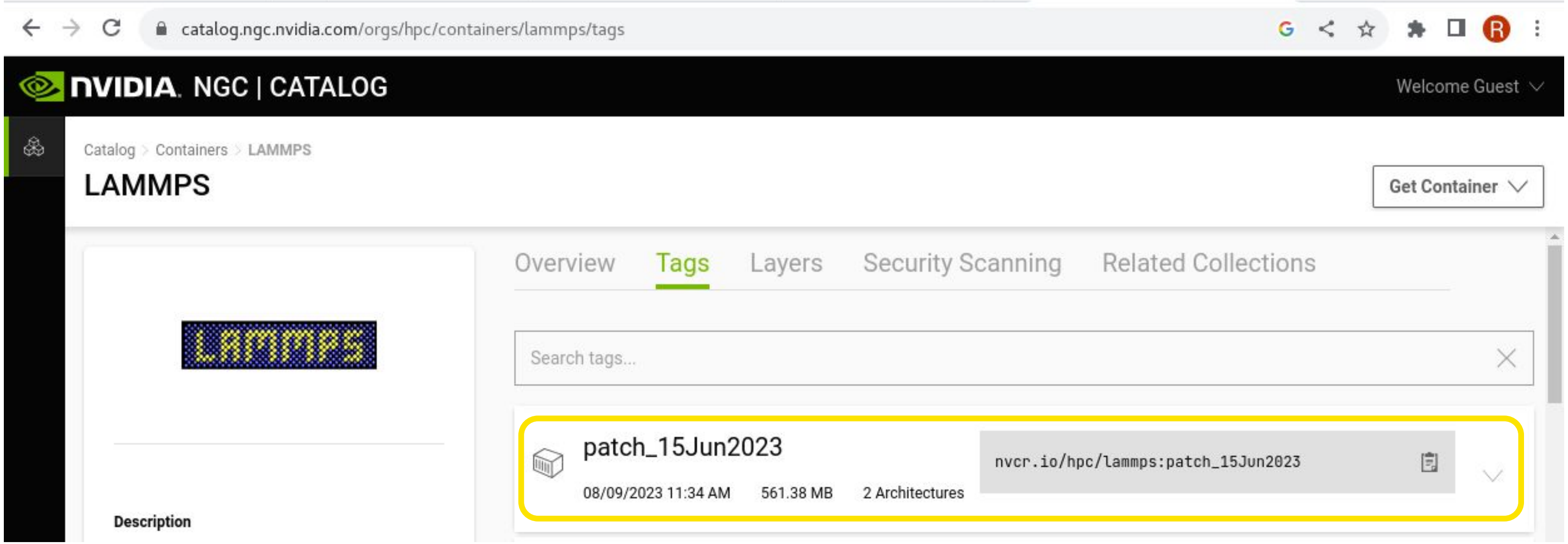
Backup copy at
`/scratch/training/charliecloud/intel-tensorflow.sqfs`

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



catalog.ngc.nvidia.com/orgs/hpc/containers/lammps/tags

patch_15Jun2023

08/09/2023 11:34 AM   561.38 MB   2 Architectures

`nvcr.io/hpc/lammps:patch_15Jun2023`

Using GPUs with Charliecloud

- Need to “inject” two things into the container
  1. nvidia libraries and executables
  2. the nvidia runscript
- Tools needed to do the injection
  a. NVIDIA `nvidia-container-cli` tool
  b. charliecloud `ch-fromhost` tool

- On ACES:
  - nvidia-container-cli is provided as a module
  - *Compute nodes* with GPUs have the nvidia libraries
  - We have a copy of the runscript in `$TRAINING`

Get to a Compute Node

Return to login node if necessary

```
exit
```

(All on one line):

```
srun --partition=gpu --gres=gpu:h100:1
   --reservation=charliecloud -n 16 --pty bash
```

Does the compute node have GPUs?

```
nvidia-smi
```

Set Up Your Environment

Set up your environment again; yes it’s necessary

```
export TRAINING=/scratch/training/charliecloud
cd $SCRATCH/ch_tutorial
module load charliecloud nvidia-container-cli WebProxy
```

Build a GPU-ready image

(on compute node):

```
ch-image pull nvcr.io/hpc/lammps:patch_15Jun2023
ch-convert nvcr.io/hpc/lammps:patch_15Jun2023 $TMPDIR/lammps
ch-fromhost --nvidia $TMPDIR/lammps
ch-fromhost -d / -p $TRAINING/runscript $TMPDIR/lammps
ch-convert $TMPDIR/lammps lammps.sqfs
```

Note: `$TMPDIR` is a location in `/tmp` that's specific to compute nodes.

LAMMPS in Container

We can now test the container:

```
ch-run --set-env lammps.sqfs -- /runscript mpirun lmp -h
```

Notes: `mpirun` is used to execute LAMMPS to work around a problem with `srun`. `lmp` is the LAMMPS executable

Backup copy at
`/scratch/training/charliecloud/lammps_nv_patch_15Jun2023.sqfs`

LAMMPS on GPUs

Now that we know the container works, we can run a benchmarking example provided by LAMMPS:

```
cp $TRAINING/in.lj.txt .
cp $TRAINING/benchmark.sh .
```

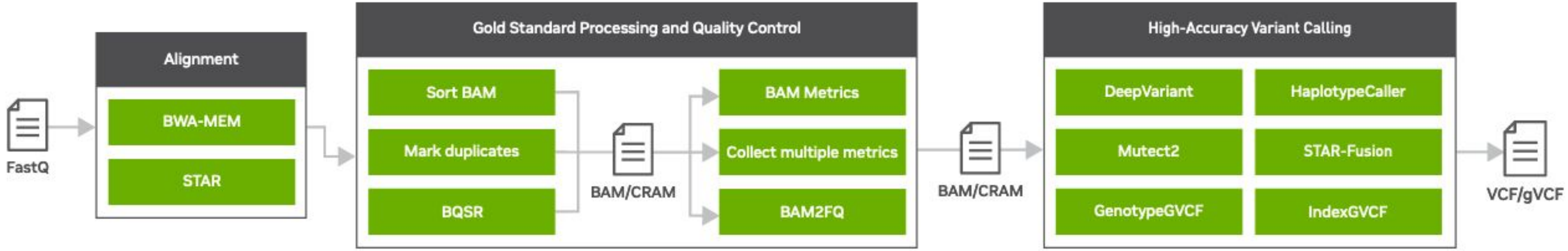
(all on one line)

```
ch-run --set-env -b "$PWD:/host_pwd" -c /host_pwd
lammps.sqfs -- /runscript bash benchmark.sh
```

Backup copy at
`/scratch/training/charliecloud/lammps_nv_patch_15Jun2023.sqfs`

Genomic Analyses with NVIDIA's Clara Parabricks

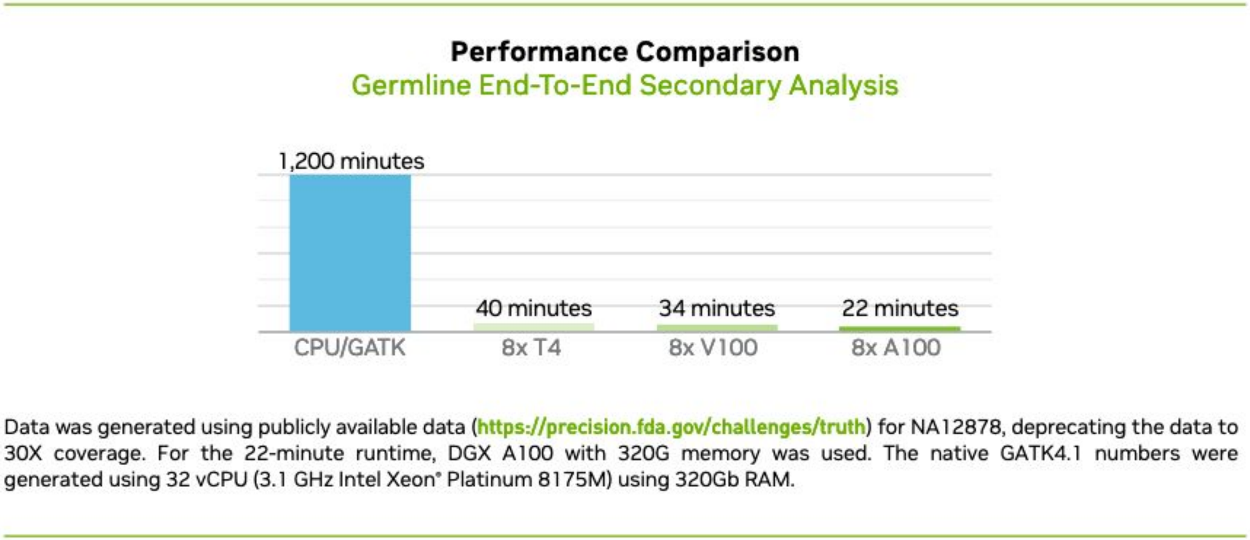
- GPU-accelerated version of common bioinformatics pipeline
- Works with both RNA-seq and WGS data
- NVIDIA provides images that containers easily integrate with Charliecloud
- Today's exercise will focus on completing the first portion of the pipeline



Parabricks

NVIDIA

Genomic Analyses with NVIDIA's Clara Parabricks



Performance Comparison

Germline End-To-End Secondary Analysis

Data was generated using publicly available data (https://precision.fda.gov/challenges/truth) for NA12878, deprecating the data to 30X coverage. For the 22-minute runtime, DGX A100 with 320G memory was used. The native GATK4.1 numbers were generated using 32 vCPU (3.1 GHz Intel Xeon® Platinum 8175M) using 320Gb RAM.

Parabricks

NVIDIA.

Get to a Compute Node (reminder)

Reminder: if you aren’t on a compute node,
(all on one line)

```
srun --mem=240G --time=01:00:00 --gres=gpu:h100:1
    --partition=gpu --cpus-per-task=48
    --reservation=charliecloud --pty bash -i
```

Followed by:

```
module load charliecloud nvidia-container-cli WebProxy
```

Genomic Analyses Example Files

Make a subdirectory

```
cd $SCRATCH/ch_tutorial
mkdir ch_parabricks
cd ch_parabricks
```

Copy the example material

```
cp $TRAINING/sample* .
cp $TRAINING/Homo* .
ls
```

Build a GPU-ready Clara Parabricks Image

Pull the parabricks image from NVIDIA using Charliecloud:
(all on one line)

```
ch-image pull
nvcr.io/nvidia/clara/clara-parabricks:4.1.1-1
parabricks-4.1.1-1
```

Build the GPU-ready image

```
ch-convert parabricks-4.1.1-1 $TMPDIR/parabricks4.1
ch-fromhost --nvidia $TMPDIR/parabricks4.1
ch-convert $TMPDIR/parabricks4.1 parabricks4.1.sqfs
```

NVIDIA's Clara Parabricks in Container

- Now we are ready to run Parabricks!

(all on one line)

```
ch-run -b "$PWD:/mnt/1" -c "mnt/1" parabricks4.1.sqfs
        pbrun fq2bam -- --ref Homo_sapiens_assembly38.fasta
        --in-fq sample_1.fastq.gz sample_2.fastq.gz --out-bam test.bam
```

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