Tutorial: Fundamentals of Containers

**Singularity** and **Charliecloud**

on **ACES**

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Outline

- Overview of Containers
- Overview of Charliecloud
- Overview of Singularity
- Getting Started
- Working with Images
- Container Recipes
Learning Resources

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

- A lightweight, fully-unprivileged container solution

Presented by Charliecloud

Small Software Delivering Big Flexibility to HPC

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
  - module load charliecloud
- Charliecloud images can be large on disk. Be aware of your storage quota. (/scratch > /home)
- 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.
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
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](http://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.
Authentication via CIlogin

Log-in using your ACCESS CI credentials.

Select the Identity Provider appropriate for your account.
Get a Shell on ACES

Click on “Clusters” menu → _aces Shell Access
Success!

Welcome to the ACES login node.
Set Up Your Charliecloud Environment

On the login node:

```
module load charliecloud
module list
```

Note. *light green highlight* means please perform this exercise in your ACES shell terminal.
Your First Charliecloud 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 Charliecloud 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
```

Launch a bash shell, investigate linux, and stop the container.

```
ch-run almalinux:8 bash
cat /etc/redhat-release
exit
```
Set Up Your Singularity Environment

Get to a compute node (from the login node)

```
srun --time=90 --mem=4G --pty bash -i
```

The compute node should be similar to the login node

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

Set your singularity cache directory

```
export SINGULARITY_CACHEDIR=$TMPDIR
```

Connect to the internet

```
module load WebProxy
```
Your First Singularity Container

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

```
singularity shell --help
```

Fetch that same image (again) and launch a shell from it (again)

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

Don’t forget to return to the login node

```
exit
```
Congratulations!

Welcome to containers
Working with Images
Charliecloud 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

Create a space on the login node for yourself

```
mkdir /tmp/$USER
```

Convert our image in the cache to a directory image. *(note the order of the arguments)*

```
ch-convert almalinux:8 /tmp/$USER/almalinux/
```

What did we make?

```
ls /tmp/$USER/almalinux/
```
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/almalinux/ bash
mkdir /my_dir
exit
```

Are the changes still there?

```
ch-run /tmp/$USER/almalinux/ bash
ls /
exit
```
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`. 
Set Up Your Environment

Create a workspace in your **scratch** directory.

```bash
cd $SCRATCH
mkdir c_tutorial
cd c_tutorial
pwd
```
Convert to Squashfs Exercise

Make sure you are still in your `c_tutorial` directory in `$SCRATCH`
```
pwd
```

Then convert *(note the order of the arguments)*
```
ch-convert /tmp/$USER/almalinux/ almalinux.sqfs
```

Are your changes still there?
```
ch-run almalinux.sqfs /bin/bash
ls
exit
```
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.
Set Up Your Singularity Environment

Get to a compute node (from the login node)
```
srun --time=90 --mem=4G --pty bash -i
```

Set your singularity cache directory
```
export SINGULARITY_CACHEDIR=$TMPDIR
```

Connect to the internet
```
module load WebProxy
```

Return to your scratch area
```
cd $SCRATCH/c_tutorial
```
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 /
```
Are Directory Images All Compatible?

Let's try an experiment. Still on your compute node,

```
module load charliecloud
ch-run $TMPDIR/almalinux bash
ls /
```

**Directory images are universal.**
They can come from a variety of sources, for example: [https://github.com/alpinelinux/docker-alpine/](https://github.com/alpinelinux/docker-alpine/)
this github repo contains a Linux package in a directory format that's designed for containers.
Navigate to your tmp space

```
cd $TMPDIR
```

Fetch the distro’s tarball:

```
wget -O alpine.tar.xz 'https://github.com/alpinelinux/docker-alpine/blob/v3.18/x86_64/alpine-minirootfs-3.18.6-x86_64.tar.gz?raw=true'
```

or

```
cp /scratch/training/containers/alpine.tar.xz .
```
Container from Tarball Exercise (2/3)

Oh no! the tarball is a tar bomb (too many files)
```
tar tf alpine.tar.xz | head -10
```

Unpack it in a new subdirectory.
```
mkdir alpine
cd alpine
tar xf ../alpine.tar.xz
ls
cd ..
```
Container from Tarball Exercise (3/3)

Now we can run a shell in the container!

```
ch-run ./alpine -- /bin/sh
cat /etc/alpine-release
exit
```

```
singularity shell ./alpine
cat /etc/alpine-release
exit
```

(alpine doesn’t have bash)
(singularity knew what to do, charliecloud needed a hint)
Container Recipes
Container Recipes

- Modifying containers by hand is bad in practice. The information about what steps were taken is lost.
- Better to write down those steps in a recipe file.
- Docker uses a recipe file named Dockerfile.
- Chariecloud supports Dockerfiles.
- Singularity uses a different recipe file called a Definition file.
Target Recipe

1. Start with the almalinux:8 image

2. Install Python 3.
   
   ```
   yum -y install python39 *(do not attempt)*
   ```

3. Add a “hello.py” python script (and make it executable).
   
   ```
   #!/usr/bin/python3
   print("Hello World!")
   ```
   
   ```
   chmod 755 hello.py
   ```

   And we shall name the image “hello”.

Elements of a Dockerfile

1. **FROM**: We are extending the almalinux:8 base image.

2. **RUN**: Install the python39 RPM package

3. **COPY**: Copy the file hello.py from outside the image into the root directory of the image.

4. **RUN**: Make that file executable.
Charliecloud Recipe

Take a moment to set up this workspace in $SCRATCH:

c_tutorial/
  hello.src.docker/
    hello.py

Dockerfile

```bash
FROM almalinux:8
RUN yum -y install python36
COPY ./hello.py /
RUN chmod 755 /hello.py
```

```python
#!/usr/bin/python3
print("Hello World!")
```
Build from Dockerfile

Make sure you have charliecloud loaded, then build the image:

```sh
cd $SCRATCH/c_tutorial #if necessary
cd hello.src.docker
ch-image build -t hello -f Dockerfile .
ch-image list
```

ch-image build arguments:
- `(-t hello)` Build an image named (a.k.a. tagged) “hello”.
- `(-f Dockerfile)` Use the Recipe named “Dockerfile”.
- `(.)` Use the current directory as the context directory.
Testing the Recipe Image

Convert from image cache to flat image

\texttt{ch-convert hello hello.sqfs}

run the container and launch hello from python

\texttt{ch-run hello.sqfs -- /hello.py}

run the container and check for python

\texttt{ch-run hello.sqfs -- python3 --version}

Does python3 exist on the local node?

\texttt{python3 --version}
Elements of a Definition File

1. **BOOTSTRAP**: Base image comes from Docker Hub.

2. **FROM**: Base image is almalinux:8

3. **%files**:  
   Copy the file hello.py from outside the image into the root directory of the image.

4. **%post**:  
   a. Install the python39 RPM  
   b. Make `/hello.py` executable.

```
Bootstrap: docker  
From: almalinux:8  
%files  
   hello.py  
%post  
   yum -y install python39  
   chmod 755 /hello.py
```
Singularity Recipe

Take a moment to set up this workspace in $SCRATCH:

```
c_tutorial/
    hello.src.def/
        hello.py
```

**Definition**

```bash
# Bootstrap: docker
From: almalinux:8
%files
    hello.py
%post
    yum -y install python36
    chmod 755 /hello.py
```

```python
#!/usr/bin/python3
print("Hello World!")
```
Build from Definition file

Make sure you are on the compute node, then build the image:

```bash
cd $SCRATCH/c_tutorial #if necessary
cd hello.src.def
singularity build --fakeroot hello.sif Definition
```

singularity build arguments:
- (``--fakeroot``) Needed for `yum` install permission.
- (``Definition``) Use the Recipe named “Definition”.
- (``hello.sif``) save the result in an SIF image.
Testing the Recipe Image

Singularity exec is used for running non-shell containers.

```bash
singularity exec --help
```

run the container and launch hello from python

```bash
singularity exec hello.sif /hello.py
```

run the container and check for python

```bash
singularity exec hello.sif python3 --version
```

Does python3 exist on the local node?

```bash
python3 --version
```
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https://hprc.tamu.edu

HPRC Helpdesk:
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Help us help you. Please include details in your request for support, such as, Cluster (ACES, Faster, Grace, ViDaL), NetID (UserID), Job information (Job id(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.