REPRODUCIBLE PIPELINES IN HPC WITH APPTAINER

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Outline

1. Introduction to Apptainer container
2. Use a pre-built Apptainer container
3. Make a custom Apptainer container
4. Q&A

Objectives

- Learn what containers are
- Understand when to use Apptainer containers on HPC
- Know how to use Apptainer container on HPC systems
- Able to build custom Apptainer container

Note

- The slides can be found in Github: https://github.com/ualberta-rcg/Apptainer_Container_On_HPC

- There are also some useful links below:
- Apptainer home
- **Apptainer Documentation**
- Apptainer on GitHub

- Singularity Hub
- **Docker Hub**

- Please reach out if you have any questions about the documentation or would like to see any additions.

1. Introduction to Apptainer Container

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HPC Software Pain Points

- Difficult to be installed in HPC system by a user:
  - Dependencies are not available in the host system (e.g. HPC cluster GLIBC version is too low)
  - Software installation needs admin power such as “yum install”, “apt-get”
  - Cannot use Conda in many HPC clusters (e.g. National systems such as Cedar)

- Difficult to share tools and/or workflows with others

- Reproducibility is not guaranteed (e.g. new software stack installed in the system).

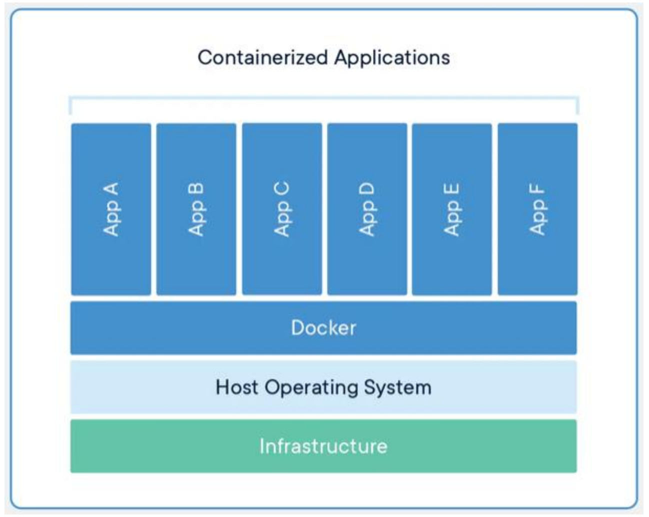
How can these pain points be addressed?

Apptainer containers! (Previously called Singularity)

- Designed for HPC
- It assumes you don't have root access when using it (*not building it)
- Easy to share and reproduce
- Independent of the host environment

What is a container?

- Package of code, dependencies, and libraries necessary to run software in (nearly) any computing environment
- Provides virtualization at the operating system level
- Two main types of containers you may have heard of: Docker and Apptainer (singularity)
- Containers are stored as image files
  - Apptainer = .sif (Singularity Image Format)
  - Dockerfile = no extension



Source: https://www.docker.com/resources/what-container/

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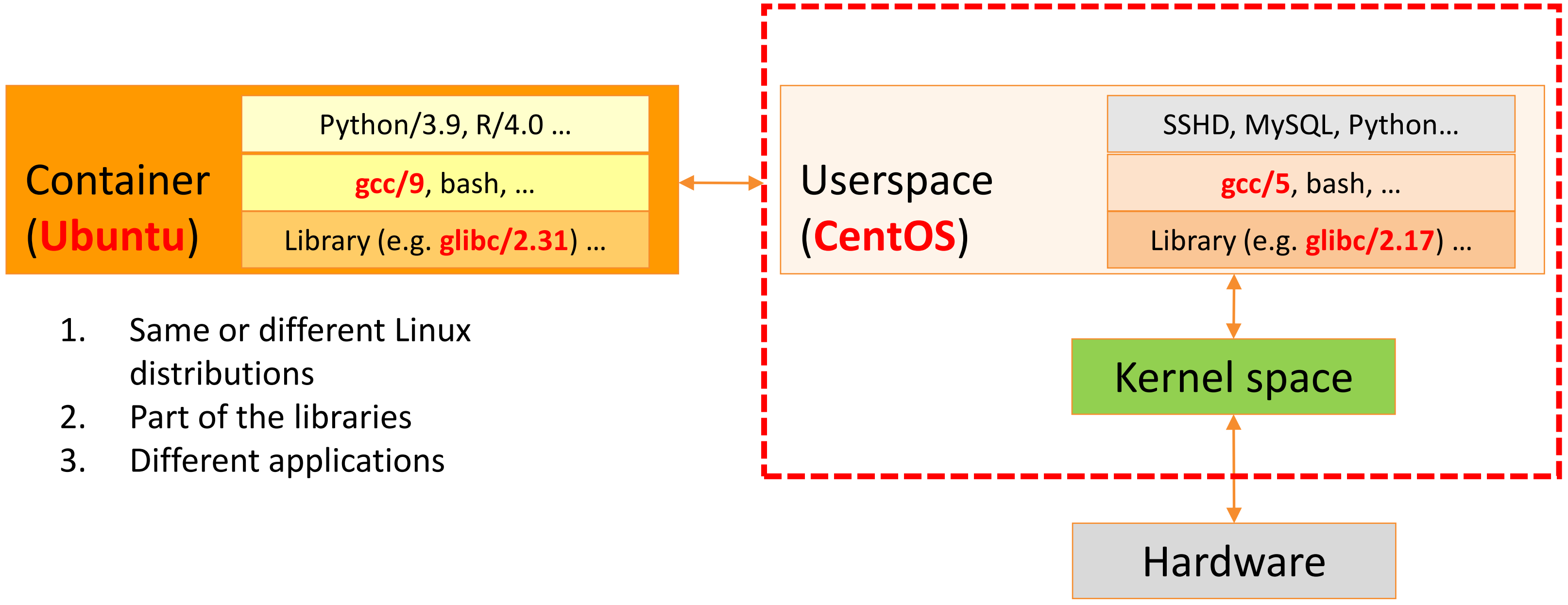
What is a container?



1. Same or different Linux distributions
2. Part of the libraries
3. Different applications

Note: Singularity rebranded as "Apptainer"

https://apptainer.org/

Singularity joined Linux Foundation November 2021.

Sockeye and Cedar have singularity 3.3-3.8 for now.

Singularity is using "Apptainer" since version 3.9, and we will eventually use "Apptainer" as the executable instead of singularity.

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Question?

2. Use pre-built container

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Get an account and login

- Open the doc:

  https://tinyurl.com/263de9k6

- **Login:**

```
ssh user00@winter2025-uofa.c3.ca
Password:thething-747
```

Pull down the container image from dockerhub

- Pull down a docker image, examples:

```
mkdir apptainer
cd apptainer
salloc --time=4:00:00 --account=def-sponsor00 --cpus-per-task=1 --mem=2G
module load apptainer
apptainer pull docker://python:3.11
```

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Repository space of pre-built container

- Find pre-built container images:
  - **Docker Hub:** https://hub.docker.com/
  - Singularity Hub: https://singularityhub.github.io/singularityhub-docs/
    Read-only and not maintained
  - NVIDIA GPU Cloud (NGC) Catalog for AI, HPC, and Visualization: https://docs.nvidia.com/ngc/ngc-catalog-user-guide/index.html

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Note: run the following in another window

- Start a new SSH session

- Run the following command

```
module load apptainer
cd apptainer
salloc --time=4:00:00 --account=def-sponsor00 --cpus-per-task=1 --mem=2G
apptainer build --sandbox --fakeroot python_3.11.sandbox docker://python:3.11
```

Pull down a different version

- Check the tag in dockerhub and specify the version by “:”

```
module load apptainer
apptainer pull docker://python:3.8
```

Use the container

- Two ways of running the program in a container:

```
apptainer shell python_3.11.sif
python –version
exit
```

```
apptainer exec python_3.11.sif python --version
```

SIF is not editable

-
  ```
  # Outside the container:
  ls -l /usr/local/bin
  mkdir /usr/local/bin/test

  # Inside the container:
  apptainer exec python_3.11.sif ls -l /usr/local/bin
  apptainer exec python_3.11.sif mkdir /usr/local/bin/test
  ```

Use the input/output in the host

- Read input in the host

```
echo -e "import sys\nprint(sys.version)" > $HOME/test.py
python $HOME/test.py
apptainer exec python_3.11.sif python $HOME/test.py
```

File system of Apptainer

- Compare the root directory in the host with Apptainer container

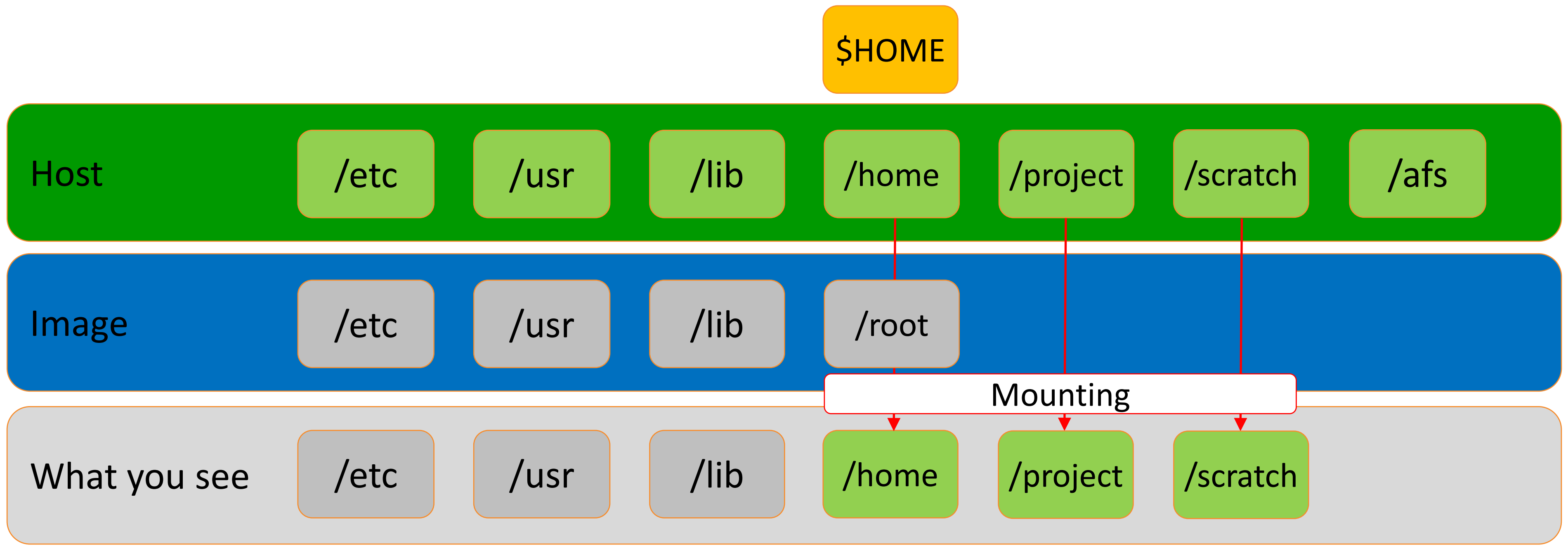
In host:

```
ls -l /
ls -ld /afs
ls -l /usr/local/bin
ls -l $HOME
```

In container

```
apptainer exec $HOME/python_3.11.sif ls -l /
apptainer exec $HOME/python_3.11.sif ls -ld /afs
apptainer exec $HOME/python_3.11.sif ls -l /usr/local/bin
apptainer exec $HOME/python_3.11.sif ls -l $HOME
```

File system of Apptainer



FYI. Please check whether your sandbox is generated in the other window you just opened.

IMPORTANT: clean the cache often

- Check the cache space

```
cd $HOME
ls -la
cd .apptainer
du -h

apptainer cache clean
du -h
```

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Practice: fill the following job script

- How to run apptainer in a batch job

```
#!/bin/bash
#SBATCH --account=def-sponsor00
#SBATCH --time=0-0:05:00
#SBATCH --cpus-per-task=1
#SBATCH --ntasks=1
#SBATCH --nodes=1
#SBATCH --mem=2G
#SBATCH -o test.out
#SBATCH -e test.err


<fill the command here>
```

Question?

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3. Make a custom container

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Run this command first

- Open your second ssh window with sandbox created:

```
APPTAINER_BIND= apptainer shell --writable --fakeroot -c -e python_3.11.sandbox/
```

- Install the dependencies

```
apt-get update && apt-get install gdal-bin libgdal-dev
```

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Why do we want to make a custom container

- I want to install a tool/package/module

- I want to change the environment (i.e. activate a virtual environment automatically)

- I want to use Conda, which is not supported by the Alliance cluster

- I want to build my pipeline into the container and share it with others

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Install a python package

- Install the python package by pip:

```
cd $HOME/apptainer
apptainer shell python_3.11.sif
cp /etc/ssl/certs/ca-certificates.crt ~/my-ca-bundle.crt
export REQUESTS_CA_BUNDLE=~/my-ca-bundle.crt
pip install emoji
```

- Test the package

```
python
import emoji
print(emoji.emojize("Python is fun :snake:"))
quit()
```

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Install a python package

- You may encounter errors:

```
pip install GDAL==3.6
```

Install a python package

- Try with sandbox

- Install the dependencies

```
APPTAINER_BIND= apptainer shell --writable --fakeroot -c -e python_3.11.sandbox/
apt-get update && apt-get install gdal-bin libgdal-dev                # already run
pip install GDAL==3.6
python -c "from osgeo import gdal"
```

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Where are those packages installed

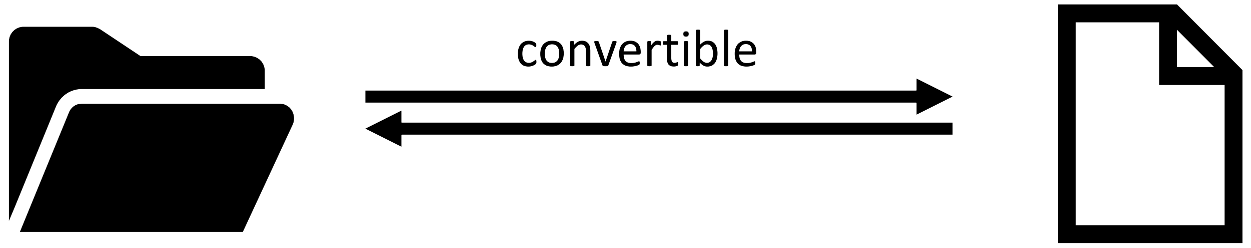
- Install packages in sandbox

```
pip show GDAL
pip show emoji
pip install emoji
pip show emoji
exit
```

Sandbox vs SIF

Sandbox

Singularity Image File (SIF)



Sandbox:

- A directory
- Editable
- Not easy to share

Singularity Image File (SIF):

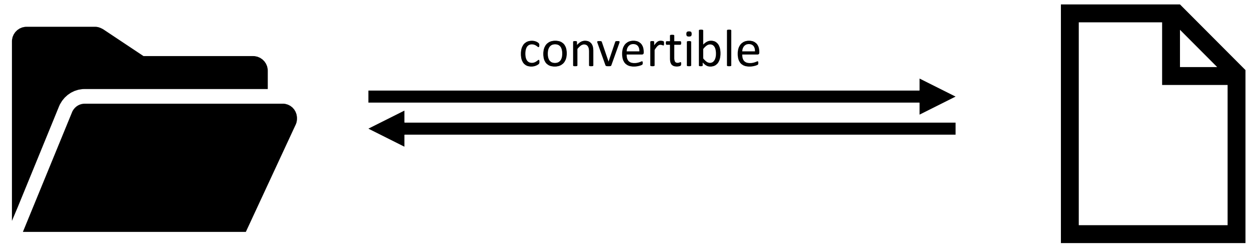
- A single file
- NOT editable
- Easy to share

```
apptainer build <output> <input>
```

Question

Sandbox

Singularity Image File (SIF)



- A directory
- Editable
- Not easy to share

- A single file
- NOT editable
- Easy to share

Can I delete sandbox after getting .sif?

Definition file (.def)

```
Bootstrap: docker
From: python:3.11
Stage: build

%environment

%post
    export DEBIAN_FRONTEND=noninteractive
    apt-get update && apt-get -y install gdal-bin libgdal-dev
    pip install GDAL==3.6

%runscript

%startscript

%test

%labels
    UofA Bootcamp
    Date 2024-01-30

%help
    This is a container for training
```

```
cp ~/projects/def-sponsor00/example.def .
apptainer build example.sif example.def
```

Install Conda inside the container

- Test the package

```
APPTAINER_BIND= apptainer shell --writable --fakeroot -c -e python_3.11.sandbox/
mkdir /conda
cd /conda
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh -O miniconda.sh
bash miniconda.sh -b -u -p miniconda3
rm miniconda.sh
source miniconda3/bin/activate
conda create -n test
conda activate test
conda install bioconda::bwa
echo 'source /conda/miniconda3/bin/activate test' >> /environment
```

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Best practice & tips

- Add --nv when running GPU jobs

```
apptainer exec --nv container.sif python model.py
```

- For MPI jobs, install the same version of openMPI inside the container

- You can change your home and working directory when needed

```
apptainer exec --home /scratch/user00/new_home --workdir /scratch/user00/workdir container.sif python model.py
```

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Question?

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Thank you!

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