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. Applications of Apptainer container
5. 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

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).

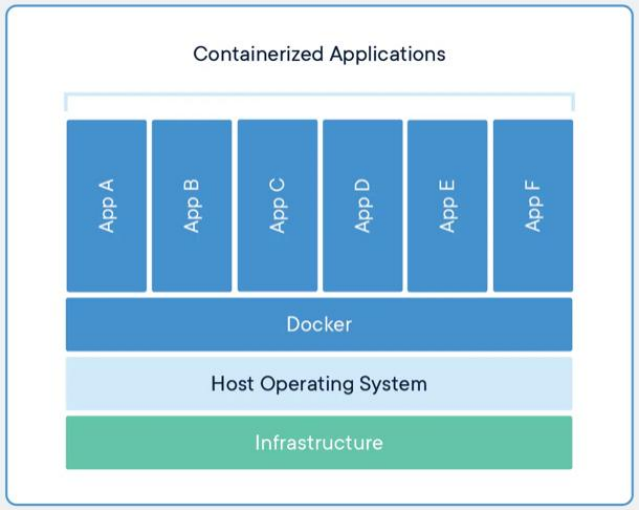
How can these pain points be addressed?

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

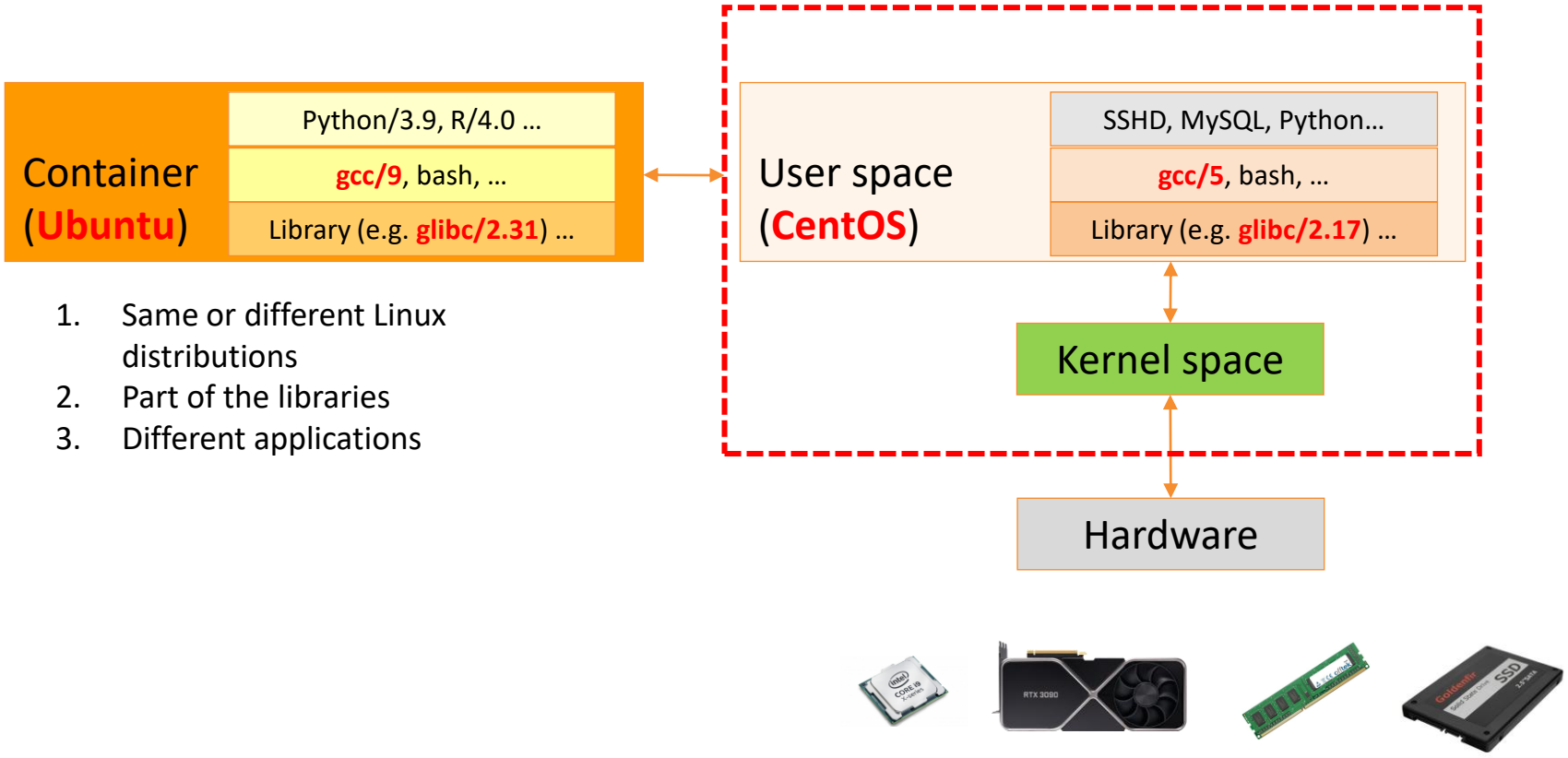
What is a container?

- 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/

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.

Question?

2. Use pre-built container

Get an account and login

- Open the doc:

  https://tinyurl.com/DRS-Apptainer

- **Login:**

```
ssh user00@fall2025-uofa.c3.ca
Password: eltoroloco-abc123
```

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:3.11.13
```

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

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_3.11.13.sif
python --version
exit
```

```
apptainer exec python_3.11.13.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_3.11.13.sif ls -l /usr/local/bin
  apptainer exec python_3.11.13.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_3.11.13.sif python $HOME/test.py
```

File system of Apptainer

- Compare the root directory in the host with Apptainer container

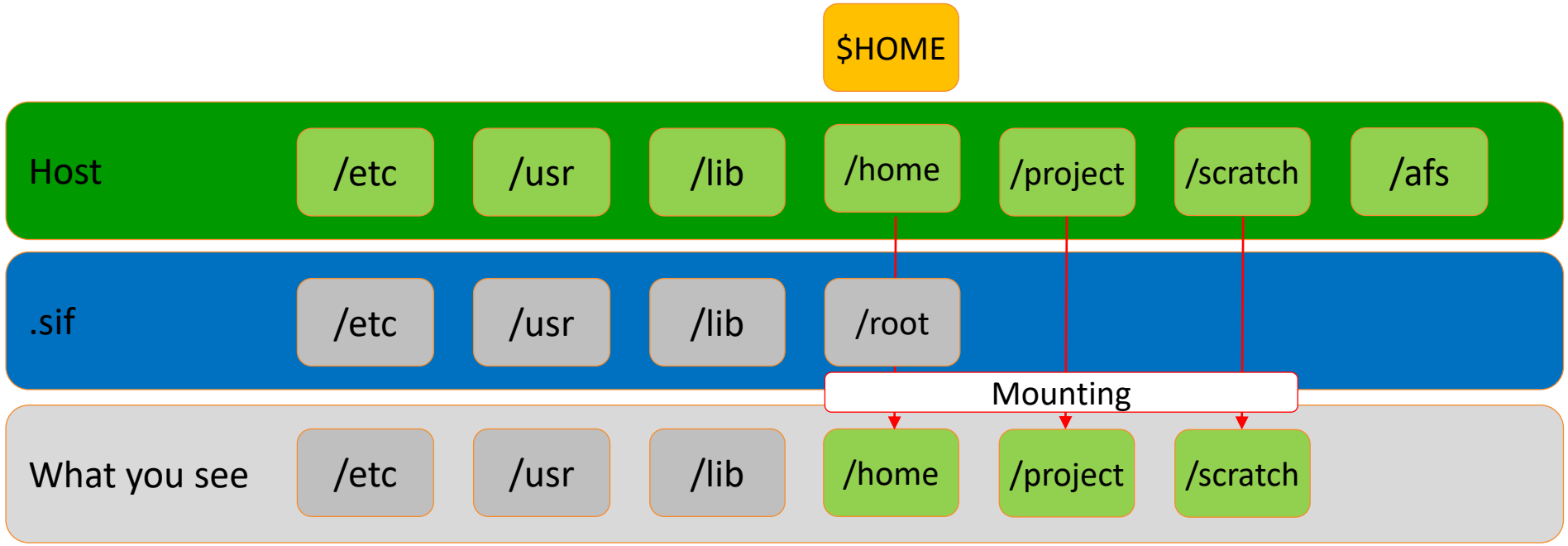
  In host:

```
ls -l /
ls -ld /afs
ls -l $HOME
echo $HOME
```

- In container

```
apptainer exec python_3.11.13.sif ls -l /
apptainer exec python_3.11.13.sif ls -ld /afs
apptainer exec python_3.11.13.sif ls -l $HOME
apptainer exec python_3.11.13.sif echo $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
```

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

<command>
```

- Two ways of running the program in a container:

```
apptainer shell python_3.11.13.sif
python --version
exit
```

```
apptainer exec python_3.11.13.sif python --version
```

Question?

3. Make a custom container

Note: run the following in another window

- Start a new SSH session

```
# Sandbox
```

- 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_3.11.13.sandbox docker://python:3.11.13
```

Run this command first

- Open your second ssh window with sandbox created:

```
# Sandbox
APPTAINER_BIND= apptainer shell --writable --fakeroot -c -e python_3.11.13.sandbox/
```

- Install the dependencies

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

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

Install a python package

- Install the python package by pip:

```
# SIF
cd $HOME/apptainer
apptainer shell python_3.11.13.sif
cp /etc/ssl/certs/ca-certificates.crt ~/my-ca-bundle.crt
export REQUESTS_CA_BUNDLE=~/my-ca-bundle.crt
pip install emoji
```

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

Install a python package

- You may encounter errors:

```
#SIF
pip install GDAL==3.6
```

Install a python package

- Try with sandbox

- Install the dependencies

```
# Sandbox
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 emoji
pip install GDAL==3.6
python -c "from osgeo import gdal"
```

Where are those packages installed

- Install packages in sandbox

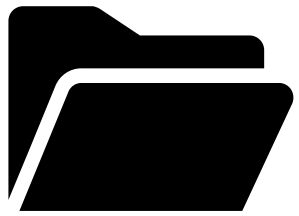
```
#  Sandbox
pip show GDAL
pip show emoji
exit
```

Convert Sandbox To .sif

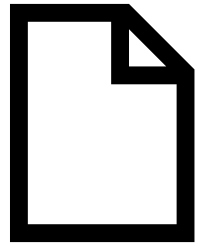
```
#  Sandbox
apptainer build python_new01.sif python_3.11.13.sandbox
exit
```

Sandbox ⇔ SIF

Sandbox



convertible



Singularity Image File (SIF)

- A directory
- Editable
- Not easy to share

- A single file
- NOT editable
- Easy to share

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

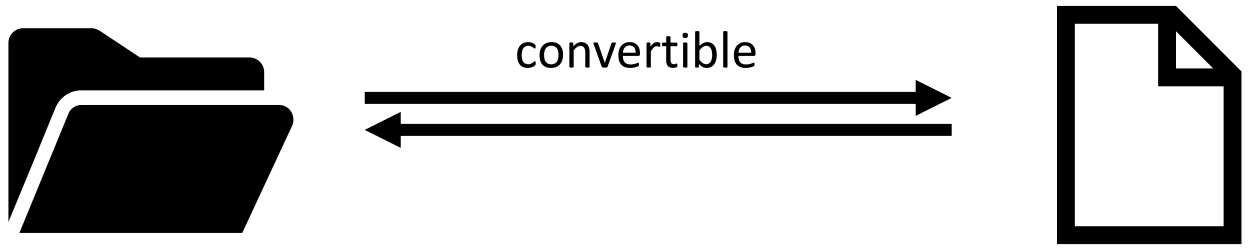
Question?

4. Applications of Apptainer Container

Sandbox ⇔ SIF

Sandbox

Singularity Image File (SIF)



- A directory
- Editable
- Not easy to share

- A single file
- NOT editable
- Easy to share

Question:
Should I delete Sandbox after generating .sif?

.sif ⇔ sandbox

```
cd $HOME/apptainer
ls -l
```

```
python_3.11.13.sandbox
python_3.11.13.sif
python_new01.sif
```

```
# if you don’t have these files/folders, please do:
mkdir /apptainer
cp -r /project/apptainer/day1/* apptainer/
```

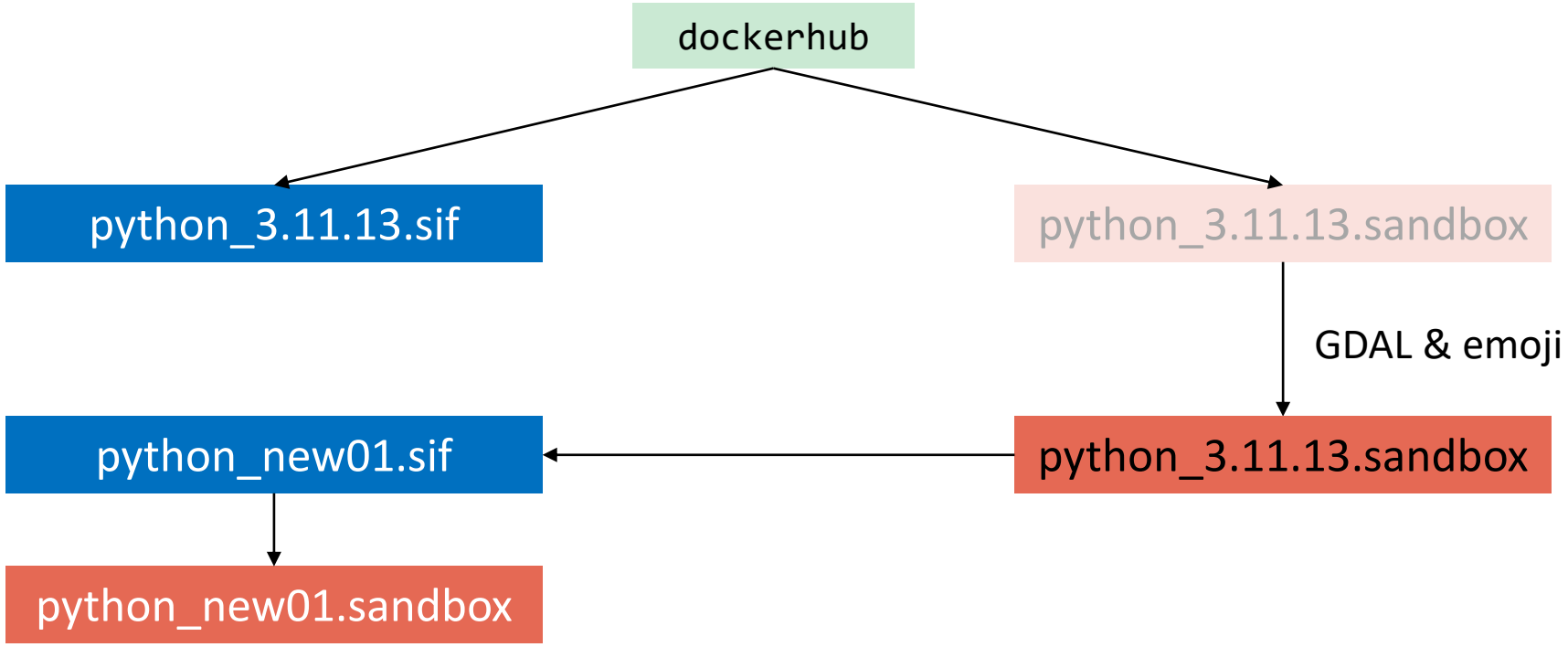
.sif ⇔ sandbox

```
apptainer build python_new01.sandbox python_new01.sif
```

```
Question: what’s the difference between python_new01.sandbox and python_3.11.13.sandbox ?

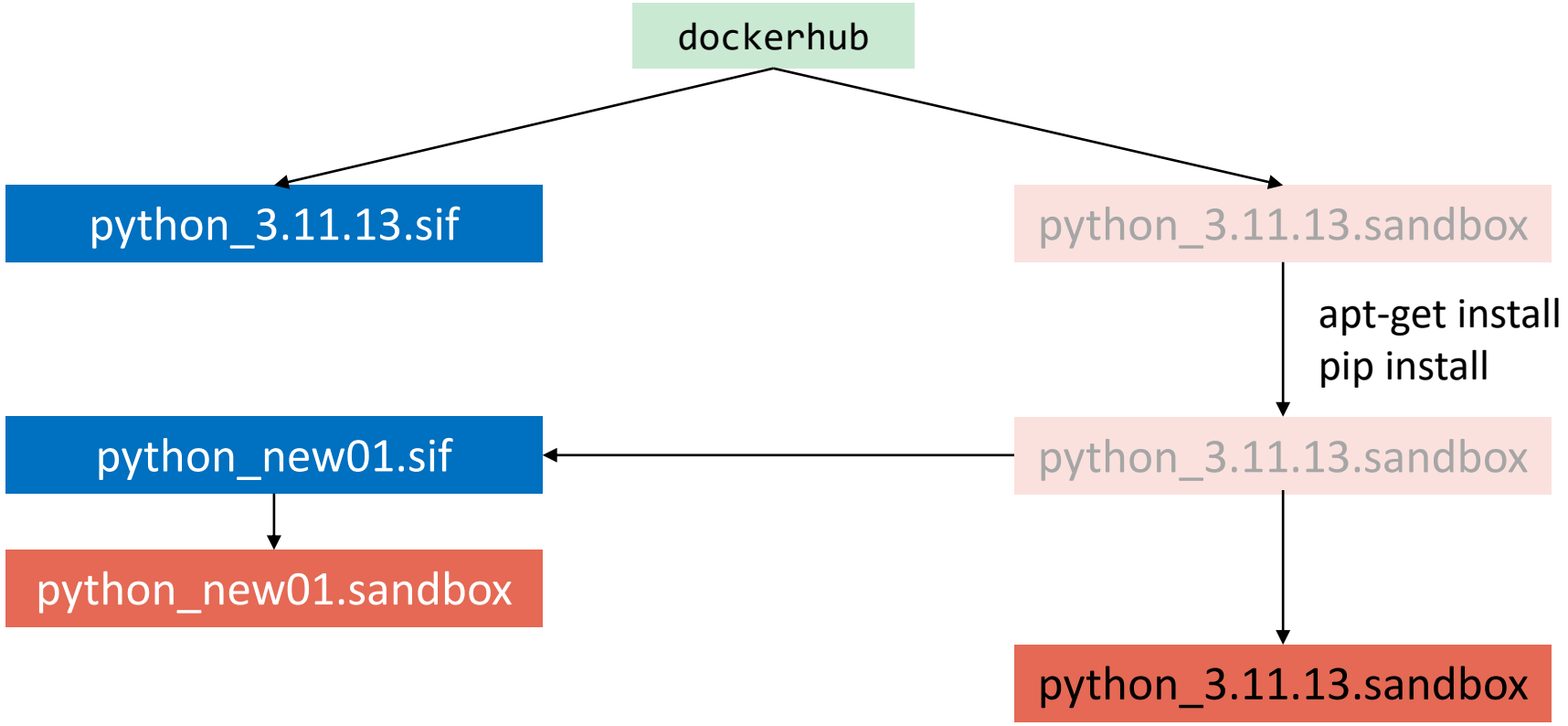
A) python version
B) Whether emoji is installed
C) Whether GDAL is installed
D) No difference
```

.sif ⇔ sandbox




```
salloc --time=4:00:00 --account=def-sponsor00 --cpus-per-task=1 --mem=2G
module load apptainer
APPTAINER_BIND= apptainer shell --writable --fakeroot -c -e python_3.11.13.sandbox/
mkdir /conda
```

.sif ⇔ sandbox




```
exit
rm -rf python_new01.*
```

Install Conda inside the container

```
APPTAINER_BIND= apptainer shell --writable --fakeroot -c -e python_3.11.13.sandbox/
mkdir /conda        # already run
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
cat /environment
exit
apptainer exec python_3.11.13.sandbox bwa
```

Definition file (.def)

```
Bootstrap: docker
From: python:3.11.13
Stage: build
%environment
          export LC_ALL=C
          source /usr/local/miniconda3/bin/activate test
%post
          apt update && apt install -y wget
          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 /usr/local/miniconda3
          rm miniconda.sh
          export PATH="/usr/local/miniconda3/bin":$PATH
          eval "$(/usr/local/miniconda3/bin/conda shell.bash hook)"
          conda create -y -n test
          conda activate test
          conda install -n test -y bioconda::bwa
          rm -rf /conda
%runscript

%startscript

%test

%labels

%help
```

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```
cp ~/projects/def-sponsor00/conda.def .
apptainer build example.1.sif conda.def
```

Definition file (.def)

```
Bootstrap: localimage
From: /home/user070/apptainer/example.1.sif
Stage: build

%environment

%post
    conda install -n test -y bioconda::samtools

%runscript

%startscript

%test

%labels
    UofA Bootcamp
    Date 2025-10-07

%help
    This is a container for training
```

```
cp ~/projects/def-sponsor00/samtools.def .
apptainer build samtools.sif samtools.def
apptainer exec samtools.sif samtools --help
```

Jupyter Notebook with Apptainer

```
cp /project/def-sponsor00/apptainer/jupyter.sh .
sbatch jupyter.sh
```

```
Practice: What Apptainer function should I use to get datascience-notebook.sif from dockerhub?

A) apptainer shell
B) apptainer pull
C) apptainer exec
D) apptainer push
```

File System – Mount Host Directory

```
mkdir hello
echo 'hello world' > hello/hello_world.txt

apptainer exec python_3.11.13.sif cat /hello/hello_world.txt
apptainer exec -B $PWD/hello:/hello python_3.11.13.sif cat /hello/hello_world.txt
apptainer exec -B $PWD/hello:/usr/world python_3.11.13.sif cat /usr/world/hello_world.txt
```

File System – Reset tmp and var_tmp

```
mkdir tmp
yes "abcdef" | head -n 5000000 > big.txt

apptainer exec python_3.11.13.sif timeout --signal=KILL 1s sort --buffer-size=256K $PWD/big.txt > /dev/null || true

apptainer exec -W $HOME/apptainer/tmp -c -B $PWD python_3.11.13.sif timeout --signal=KILL 1s sort --buffer-size=256K $PWD/big.txt > /dev/null || true


# For heavy I/O
mkdir $SLURM_TMPDIR/outputs
apptainer exec -W $SLURM_TMPDIR/outputs -c -B $PWD python_3.11.13.sif timeout --signal=KILL 1s sort --buffer-size=256K $PWD/big.txt > /dev/null || true
```

Running MPI Job with Apptainer

```
Bootstrap: docker
From: mfisherman/openmpi:4.1.5
Stage: build
%environment

%files
          hello_mpi.c           /usr/local/bin/hello_mpi.c

%post
          mpicc -o /usr/local/bin/hello_mpi /usr/local/bin/hello_mpi.c
```

```
cd $HOME/apptainer
mkdir MPI
cd MPI
cp /project/def-sponsor00/apptainer/MPI/hello_mpi.* .
module load apptainer
apptainer build --fakeroot --ignore-fakeroot-command openmpi.sif hello_mpi.def          # you can skip
this step as the .sif is already built

# Why do we use openmpi/4.1.5?

sbatch hello_mpi.sh
```

Use GPU

- Add --nv when running GPU jobs

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

Question?

Thank you!

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