Using Containers on HPC resources

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Overview

Welcome!

In this workshop, we will go over using containers on HPC resources, like UCLA's Hoffman2

- We will go over basic container concepts
- Also, some basic examples of using containers on HPC resources
- Look more more advance container building in a future workshop!!

Any suggestions for upcoming workshops, email me at cpeterson@oarc.ucla.edu

Files for this Presentation

This presentation can be found on github under `container_04_18_2022` folder

https://github.com/ucla/hpc_workshops

The `slides` folder has this slides.

- PDF format: `ContainerWS.pdf`
- html format: `html` directory
  - `ContainerWS.html`

Note: This presentation was build with Quarto/Rstudio.

- Quarto file: `ContainerWS.qmd`

What are Containers?

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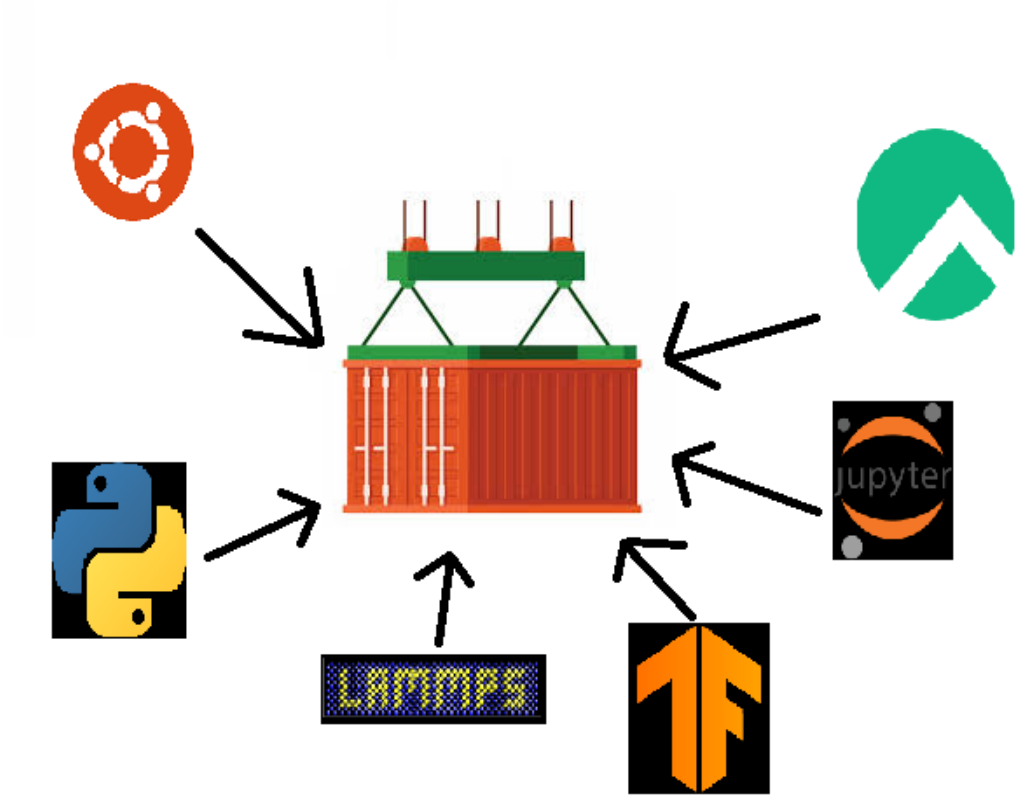
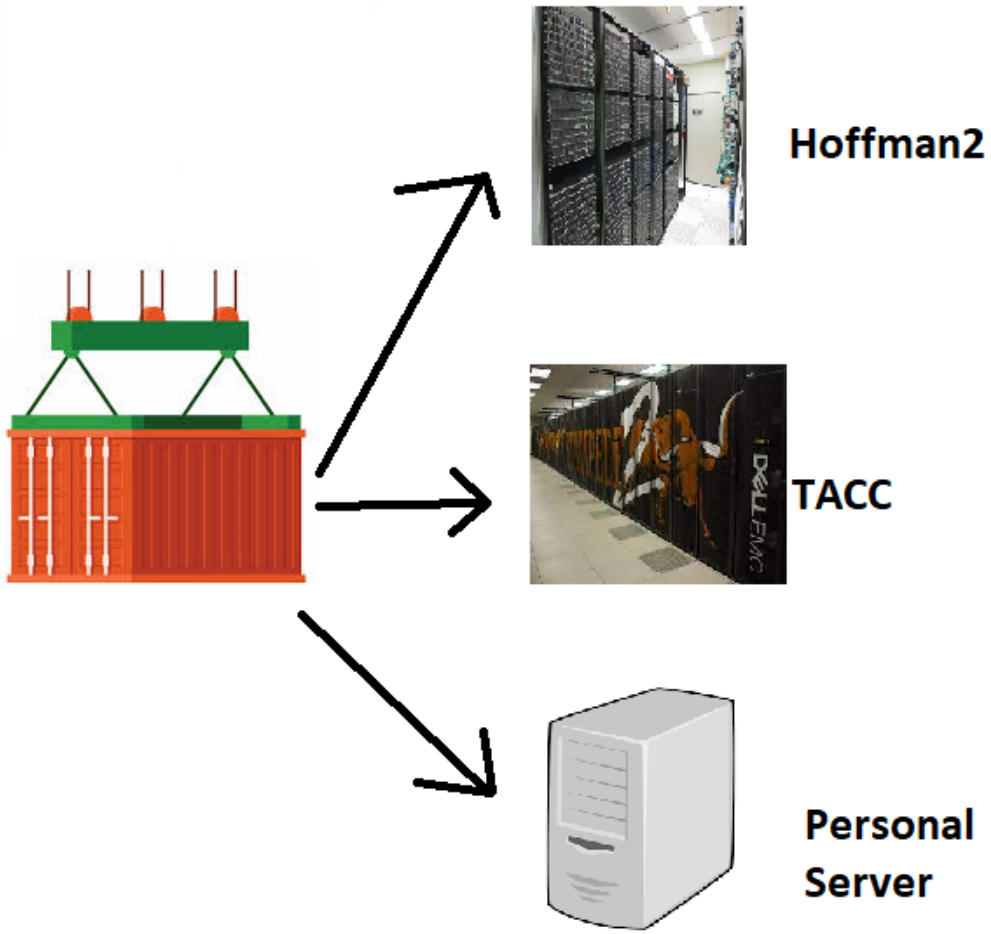


What are Containers?

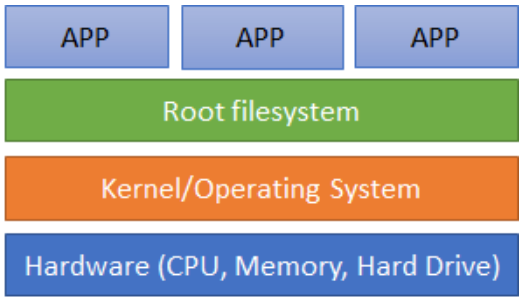


Virtualization

To understand how Containers work, we will have a brief overview on virtualization

Bare computer setup

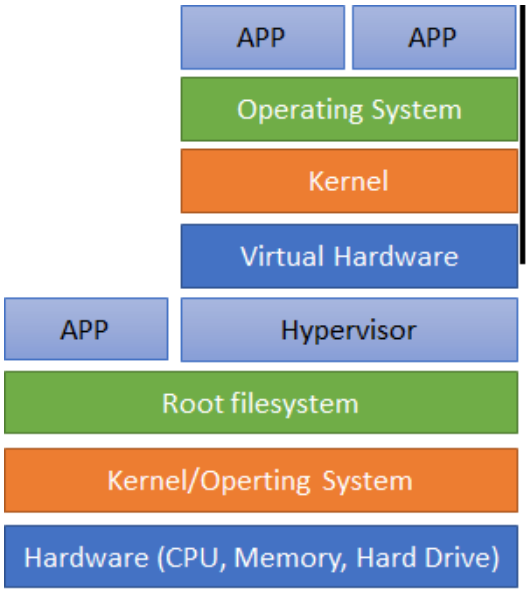
- Typical setup in which your software applications run directly on the OS from the **physical** hardware
- Many HPC users run their applications in this fashion



Virtualization

Virtual Machine setup

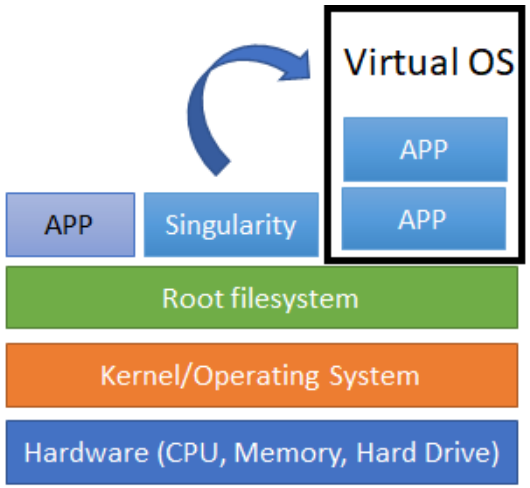
- Applications running inside of a VM are running on a computely different set of (virtual) resources
  - Example: VirtualBox, VMWare, AWS EC2
- A “Machine” within a “Machine”



Virtualization

Container Setup

- Applications running inside of a container are running with the **SAME** kernal and physical resources as the host OS
- A “OS” within a “OS”



Why use Conatiners?

- Bring your own OS
- Portability
- Reproducibility
- Design your own environment
- Version control

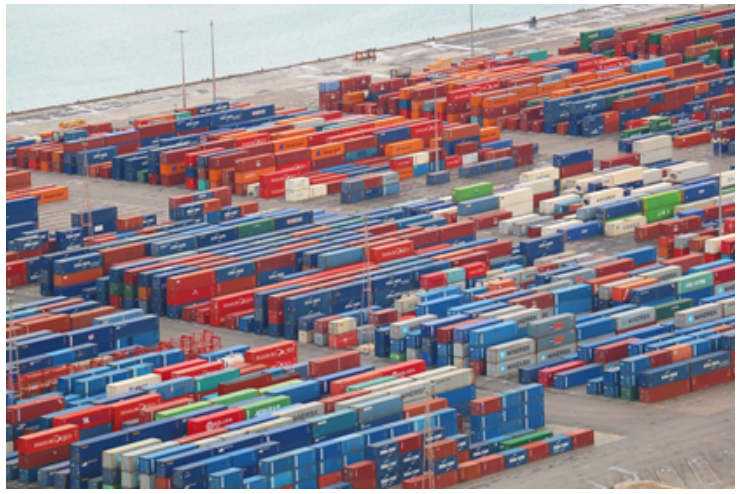
Problems installing software

- Researchers typically have to spends lots of time installing software in their personal (HOME) directories, load modules, every time software is used
- Then start all over when using software on a different HPC resource

HPC resources (like Hoffman2) are **SHARED** resources

- Researchers are running software on the same computing resource
- No ‘sudo’ and limited yum/apt-get commands available

Container Advantages

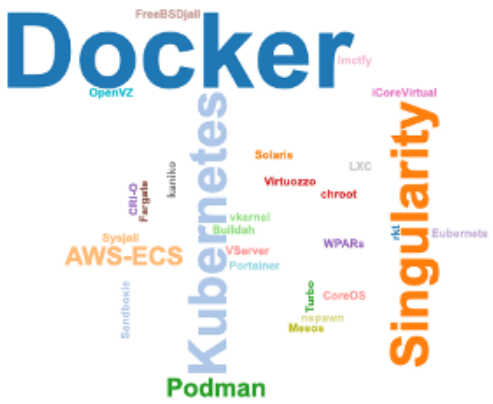


- Install your application once
  - Use on any HPC resource
- A ‘virtual’ OS
  - users can have complete OS admin control

- Great to easily install software with apt/yum
- Great if you software requires MANY dependencies that would be complex installing on Hoffman2.

- Easily share containers!!
  - containers as a .SIF file
  - save to a Cloud Container Registry
    - DockerHub, GitHub packages, Nvidia NGC

Software for Containers



Docker

- One of the most popular containerize software
- Many popular cloud container registries to store Docker containers
  - DockerHub, GitHub Packages, Nvidia NGC
- MPI over multiple servers not well supported
- Most likely NOT available on many HPC systems (not on Hoffman2)

Podman

- Similar syntax as with Docker
- Doesn’t have a root daemon process
- On some HPC resources (not on Hoffman2, yet)

Apptainer

- Formerly Singularity
- Designed and developed for HPC systems
- Mostly likely installed on HPC systems (installed on Hoffman2)
- Supports Infiniband, GPUs, MPI, and other devices on the Host
- Can run Docker containers

Security considerations

- Built with shared user system environments in mind
- NO daemon run by root
- NO privilege escalation. Cannot gain control over host/Hoffman2
- All permission restrictions outside of the a container

Apptainer workflow

Create

Transfer

Run

Apptainer workflow (Create)

Create

Transfer

Run

- Build a container by installing Appainer on your computer (where you have root/sudo access) to create a container
- Use a pre-built container
  - Search Container Registries for container
  - DockerHub, GitHub packages, Nvidia NGC

Apptainer workflow (Transfer)

Create

Transfer

Run

Bring your container to Hoffman2

- Copy your container to Hoffman2

```
scp test.sif H2USERNAME@hoffman2.idre.ucla.
```

- Pull a container from online Container Register

```
apptainer pull docker://ubuntu:20.04
```

- Use a container pre-built on Hoffman2

```
#Pre-built container location on Hoffman2
ls $H2_CONTAINER_LOC
```

Apptainer workflow (Run)

Create

Transfer

Run

Run Apptainer on your container

Can run in an interactive (qrsh) session

```
qrsh -l h_data=5G
module load apptainer/1.0.0
apptainer exec mypython.sif python3 test.py
```

Or run as a Batch (qsub) job

```
cat << EOF >> myjob.job
module load apptainer/1.0.0
apptainer exec mypython.sif python3 test.py
EOF

qsub -l h_data=5G myjob.job
```

Apptainer container run like any other application

Just add an apptainer command to any command you

Common Usage

On Hoffman2, to use apptainer, all you need to do is load the module

```
1 module load apptainer/1.0.0
```

- Only module you need to load!
  - Expect MPI module if running parallel

Common Apptainer commands:

- Getting a container from somewhere

```
1 apptainer pull [options]
2 apptainer pull docker://ubuntu:20.04
```

- Build a container

```
1 apptainer build [options]
2 apptainer build myapp.sif myapp.def
```

Common Usage

Common Apptainer commands:

- Run a command within a container

```
apptainer exec [options] container.sif
apptainer exec mypython.sif python3 test.py
# Runs the command `python3 test.py` inside the container
```

- Start an interactive session inside your container

```
apptainer shell [options] container.sif
apptainer shell mypython.sif
```

NOTE: Apptainer will NOT run on Hoffman2 login nodes.

MAJOR TAKEWAY

You will run the same commands as you normally do, just add the `apptainer shell/exec container.sif` line in front of your command

So....

```
python3 test.py
R CMD BATCH test.R
```

Turns into to

```
apptainer exec myPython.sif python3 test.py
apptainer exec myR.sif R CMD BATCH test.R
```

Examples

- Example 1: Simple container jobs
- Example 2: Using GPUs
- Example 3: Using MPI
- Example 4: Simple custom build container

Workshop material

```
git clone https://github.com/ucla/hpc_workshops
cd hpc_workshops/containerWS-04202022
```

Example 1: TensorFlow

This example will use Tensorflow

A great library for develop Machine Learning models

- Go to `EX1` directory
- Look at `tf-example.py`
  - Simple example to train MNIST dataset

To run this job, we will run

```
python3 tf-example.py
```

Need tensorflow!!!

- Instead of installing it yourself, let is find a container

Visit DockerHub

Example 1: TensorFlow (interactive)

Running on Hoffman2

- Start an interactive session

```
qrsh -l h_data=10G
```

- load the apptainer module

```
module load apptainer/1.0.0
```

- pull the TensorFlow container from DockerHub

```
apptainer pull docker://tensorflow/tensorflow:2.7.1
```

- We see a SIF file named, tensorflow_2.7.1.sif
- Start an interactive shell **INSIDE** the container

```
apptainer shell tensorflow_2.7.1.sif
python3 tf-example.py
```

Example 1: TensorFlow (batch)

Run a command inside the container

```
qrsh -l h_data=10G
module load apptainer/1.0.0
apptainer pull docker://tensorflow/tensorflow:2.7.1
apptainer exec tensorflow_2.7.1.sif python3 tf-example.py
```

Alternatively, you can submit this as a batch job

- Example job script: `tf-example.job`

```
qsub tf-example.job
```

NOTE:

- See that we didn't need to load any python module!
- We didn't need to install any TF packages ourselves!!

Example 2: GPU containers (PyTorch)

This example uses PyTorch with GPU support for faster speed.

PyTorch is another great Machine Learning framework.

Look under EX2

- File: `pytorch_gpu.py`

This example will optimize a polynomial to a sine function

Let us go to Nvidia GPU Cloud (NGC)

- Containers built by Nvidia
- Optimized for GPU jobs

Example 2: GPU job

First, you will need a GPU compute node

```
qrsh -l h_data=10G,gpu
```

Download PyTorch from Nvidia NGC

```
module load apptainer/1.0.0
apptainer pull docker://nvcr.io/nvidia/pytorch:22.03-py3
```

Run apptainer with the `--nv` option. This option will find the GPU drivers from Host compute node

- See if container can find the GPUs

```
apptainer shell pytorch_22.03-py3

apptainer exec --nv tensorflow_2.7.1.sif python3 tf-example.py
```

Alternatively, you can submit this as a batch job

```
qsub pytorch_gpu.job
```

Example 3: Parallel MPI containers

One of my fav Computational Chemistry application is NWChem

This example will run a parallel MPI container

- Many applications use MPI to run over many CPUs.

On Hoffman2, we have already built a NWChem container with MPI

- `$H2_CONTAINER_LOC/h2_nwchem:7.0.2.sif`

Run the Parallel NWChem job

```
1 qsub nwchem-MPI.job
```

Example 3: Parallel MPI containers

NOTE: Typically, you will run MPI application by following the format

```
module load intel/2022.1.1
mpirun myapp.x
```

Inside the container, you have mpirun before the `apptainer` command

```
module load intel/2022.1.1
module load apptainer/1.0.0
mpirun apptainer exec myapp.sif myapp.x
```

For running MPI inside the container, you **MUST** have MPI on the Host (outside of the container).

In this case, `intel/2022.1.1` will have IntelMPI

Example 4: Building container

I coded a chemistry app located on github

- https://github.com/charliecpeterson/QUILL

We need:

- Python with the PySCF package
- Eigen3

Instead of installing these dependencies on H2 (or looking for modules), lets build a container!!

Build using three methods

- Writable sandbox
- Using a definition file (.def)
- Using Docker (Dockerfile)

Example 4

For this example, you will need Apptainer and/or Docker installed on a machine that you have admin/sudo access.

In order to build or modify containers, you must have admin access

- So you cannot do this on Hoffman2

You may use `wscontainers.ova` VM to use with VirtualBox. Both Apptainer and Docker pre-installed.

- Username & password : wscontainer

You can find how to install this software on your own from the `install.md` file

Example 4: Method 1 - Writable Sandbox

This example will create a container by installing software inside of a container interactively

- Create a writable container, starting from base ubuntu image. We will call is container, `quill.sif`

```
sudo apptainer build --sandbox quill_SB docker://ubuntu:20.04
```

- Go inside the writable container (Modifications will be saved)

```
sudo apptainer shell --writable quill_SB
```

Example 4: Method 1 - Writable Sandbox

- Install QUILL

```
apt-get update
DEBIAN_FRONTEND=noninteractive apt-get install -y --no-install-recommends \
       git python3 python3-dev python3-pip \
       libeigen3-dev ca-certificates cmake make gcc g++
rm -rf /var/lib/apt/lists/*

pip3 install pyscf
ln -s /usr/bin/python3 /usr/bin/python
mkdir -pv /apps
cd /apps
git clone https://github.com/charliecpeterson/QUILL
cd QUILL
mkdir build ; cd build
cmake ..
exit
```

Move final container to Hoffman2

```
#Convert Sanbox to SIF
sudo apptainer build QUILL.sif QUILL_SB
scp -r QUILL.sif H2USERNAME@hoffman2.idre.ucla.edu
```

Example 4: Method 2: Definition file

Install QUILL with a Definition file

Look at `quill.def`

This file has all steps needed to build the QUILL container.

```
1 sudo apptainer build quill.sif quill.def
```

The `quill.sif` container is created

Move container to Hoffman2

```
1 scp QUILL.sif H2USERNAME@hoffman2.idre.ucla.edu
```

Example 4: Method 3: Docker

You can use Docker to create containers for apptainer

The `Dockerfile-quill` file is used by Docker to create the container

```
sudo docker build . -t quill:1.0 -f Dockerfile-quill
```

See built docker container

```
sudo docker image list
```

Save docker image to apptainer container

```
sudo docker save quill:1.0 > quill.tar
apptainer build QUILL.sif docker-archive://quill.tar
scp QUILL.sif H2USERNAME@hoffman2.idre.ucla.edu
```

Alternatively, you can `docker push` your container to DockerHub, GitHub, etc and run `docker pull` on

Example 4: Running Container

Once the container is on Hoffman2, submit job.

```
1 qsub quill.job
```

More information on using Definition files

- https://apptainer.org/docs/user/1.0/definition_files.html

More information on using Dockerfiles

- https://docs.docker.com/engine/reference/builder/

Things to Think About

Size of container

- Try to keep the size of your container small and minimal
  - Only have the things necessary for your applications to run
- Large containers will need more **memory** and will take more take to start up
- Currently, the non-setid version of Appatiner will convert all .sif files to sandbox before running - Large containers can increase the conversion time.
- Good idea to build a sandbox container before running appainer to save time

```
appatiner build --sandbox test-sandbox/ test.sif
```

More Things to Think About

- Share .sif files with your friends!
  - Save your (Docker) containers to DockerHub or GitHub Packages
- Find examples of Dockerfiles and Apptainer def files on my GitHub
  - https://github.com/charliecpeterson/containers

- Experiment creating your containers with writable sandboxs, then create Def/Dockerfile to with all your commands so to rebuild/modify containers later
- Look out for a follow-up workshop
  - Container Building

Thank you!

Questions? Comments?

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