Containers for HPC

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Introduction

What is a Container?

An answer:

An encapsulated software environment that runs using a separate linux kernel

What does this mean?

- You can package the software and data you think is important together
  - Reproducibility, portability, scalability, consistency
- This package runs using a container runtime
  - Various runtimes exist on/for different systems
- The package uses the host machine’s linux kernel
  - This is much more efficient than every environment running independently

Why use Containers?

In General:

- Personalized functionality that is portable and performant

Specific:

- Provide full environment for reproducibility
- Keep files intended for /home on faster storage
- Easily install and test library updates
- Include exact third party library versions & compilations with code versions
- Provide an isolated environment for individual tests and code development
- Avoid home directory usage for conda environment performance
- Containerfiles can be used as a lightweight method for sharing complicated compilation instructions
- Allow for consistent libraries between multiple development sites
- Share environments between users for clean and rapid development
- Easily deploy applications onto multiple disparate compute resources
- Allow for simple testing across a variety of environments
- Utilize cloud-based resources for testing
- Functionality test across multiple distros before code publication

The Rest of the Talk

General Overview of Containers

- Walk through basic workflow and terminology
- Clear up misunderstood terms

Running Containers at NERSC

- Shifter
- podman-hpc

General Containers Overview

Getting an Image

Containerfile: a file that specifies how an image should be built

- Human readable
- Specify the OS and install libraries
- Get and compile files

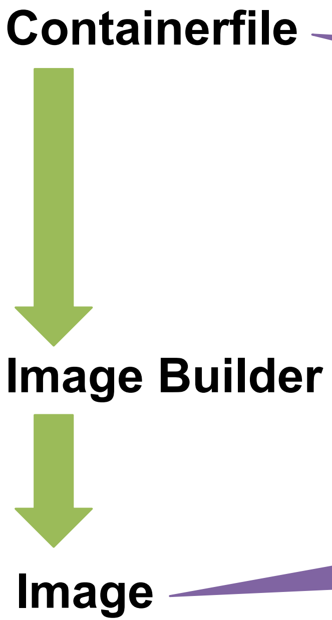
Image Builder: a program that builds an image from a container file

- Either a separate program or a part of a container engine

Image: an archive of the environment, application, and data

- Binary file

Notes on Getting an Image



Containerfile

Image Builder

Image

Containerfiles are commonly called **Dockerfiles**

- Docker was the first widely used container solution
- Docker nomenclature is still common even Docker isn't being used

Images can be stored in an **image registry**

- Public or private
  - Dockerhub, quay.io, registry.nersc.gov
- Share your images or grab others already available
- Most registries include the image builder

Running a Container

Image (either built by you, shared with you, or pulled from a registry)

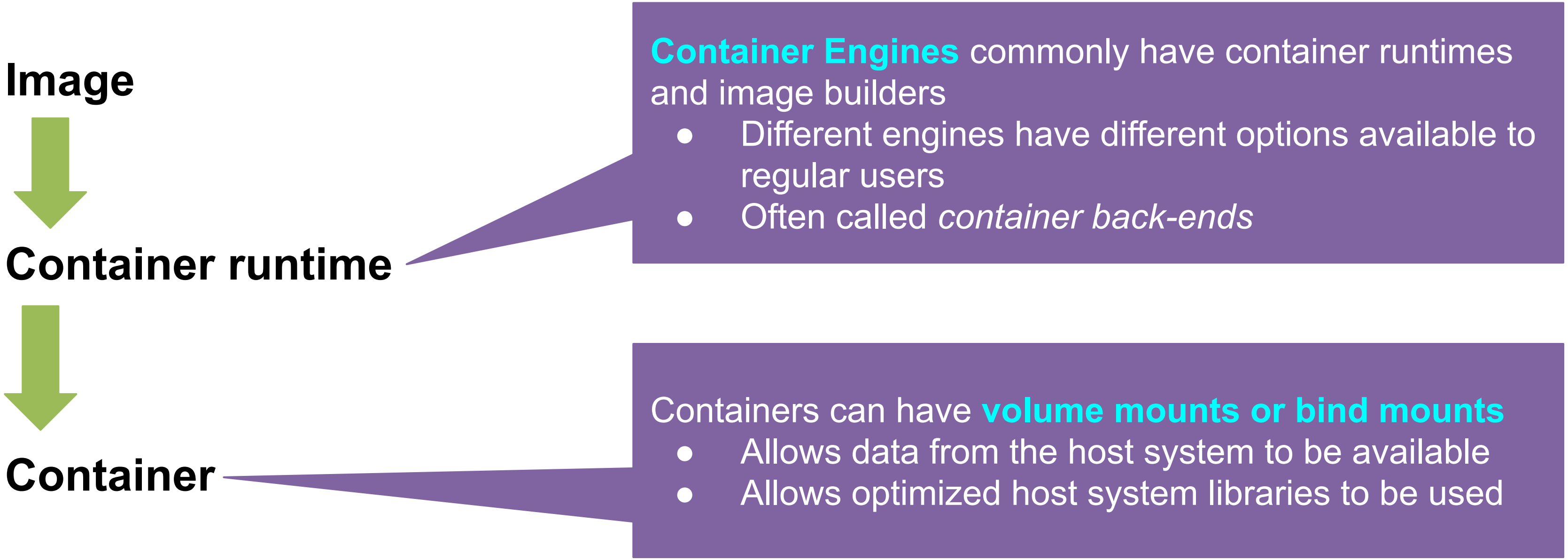
Container runtime: software used to launch containers

- This is likely the command you use to launch a container

Container: an image that is running

- Application that you built and instructions for the run
- Likely includes ephemeral filesystem

Notes on Running a Container



Image

Container runtime

Container

Container Engines commonly have container runtimes and image builders

- Different engines have different options available to regular users
- Often called *container back-ends*

Containers can have **volume mounts or bind mounts**

- Allows data from the host system to be available
- Allows optimized host system libraries to be used

Clarifying Related Topics

Open Container Initiative (OCI): Standards body pushing for standardization across container engines

Virtual Machines (VMs): Similar to containers but use their own kernel

- More isolated from the host machine
- More overhead associated with the applications

Kubernetes: An open source container orchestrator standard

- Used to deploy, scale and manage containers
- Many implementations: K8s, K3s, OpenShift, Rancher, Swarm, …
- Governed by Cloud Native Computing Foundation (CNCF)

Slurm: A job scheduler used on HPC systems

- Allocate resources for a particular job which may contain a container

Running Containers at NERSC

Containers for HPC

HPC Applications:

- Are often sensitive to filesystem performance
- May be communication intensive
- Often use system tuned libraries for peak performance
- Are run on shared (untrusted) systems
- Typically use batch schedulers

NERSC container engines and tools are built to do this well.

Changes from standard container engines for these purposes are denoted with an HPC mark

Containers at NERSC

Shifter is a NERSC built container engine

- Built by NERSC to address HPC needs
- Popular at NERSC but not widely adopted elsewhere
- *Requires images to be built elsewhere*

podman-hpc is a NERSC built wrapper for podman

- HPC additions to a community supported container engine
- NERSC is building the HPC additions
- *Able to build images as a user*

Pulling an Image in Shifter

Get an image from dockerhub:

```
$ shifterimg pull docker:godlovedc/lolcow:latest
```

- Pull an image and put it in shifter format
  - Intended to improve filesystem performance **HPC**
- Repository
- Username
- Container name
- Version number

```
Pulling Image: docker:godlovedc/lolcow:latest, status: READY
```

Viewing Images in Shifter

Show available images:

```
$ shifterimg images | grep lolcow
```

- Show all of the images available
- Only show the lines containing lolcow
  - There will be a lot of images! Grep is your friend

```
perlmutter docker     READY    a692b57abc   2024-02-21T03:00:52 godlovedc/lolcow:latest
```

Shifter on Login nodes

Run the image on the log-in node:

```
$ shifter  --image=godlovedc/lolcow:latest --entrypoint
```

- Use shifter to start a container
- Choose this image to start
- Run this
  - “entrypoint” is a standard way to set up your container
  - You control this in the containerfile when building the container

```
/ Think twice before speaking, but don't \
\ say "think think click click".         /
 ----------------------------------------
        \   ^__^
         \  (oo)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
```

Note: Shifter requires the container executable to run as a regular user$^{\text{HPC}}$. If your container appears to hang when you start it, it may be configured to run using root. See the NERSC docs for more information.

Interactive Shifter Jobs

Run the image in an interactive job:

```
$ salloc -N 1 -t 60 -C cpu -q interactive --image=godlovedc/lolcow:latest
```

- Request a job
- Requirements for the request (1 node, 60 minutes, CPU partition, interactive node)
- Preload this image$^{\text{HPC}}$

```
salloc: Granted job allocation 42
salloc: Waiting for resource configuration
salloc: Nodes nid42 are ready for job
```

```
$ srun shifter --entrypoint
```

- Run shifter within the job
- Run this within the preloaded container

Our cow and a lol will show up, but without color, indicating that we are within a job.

```
$ exit
```

Batch Shifter Jobs

Create a submission script and submit using sbatch:

```
#!/bin/bash
#SBATCH -q regular
#SBATCH -N 1
#SBATCH -t 10:00
#SBATCH -C cpu
#SBATCH -o %x_%j.out
#SBATCH -e %x_%j.err
#SBATCH --image=godlovedc/lolcow:latest

srun -n $SLURM_NNODES shifter --entrypoint
```

The .out file will contain our lolcow

- Most of this is the same as our salloc options
- Create output and error files based on the submission script name and jobID
- Preload the image
- Run as before, including the number of nodes

Using Shifter Options

```
--volume=/pscratch/sd/u/user:/scratch
```

- Make external storage available within your container

```
--clearenv
```

- Ignore the external environment

```
--env=MYENV=1234
```

- Set environment variables

```
--workdir=/work
```

- Set up a work directory within the container

Using Shifter Modules HPC

These are not the same as lmod modules (eg module load gcc)

```
--module=XYZ # Use this performance module
```

Options:

More info is available on the NERSC docs.

`mpich` - Use the Cray MPI

`cvmfs` - Enable CVMFS filesystem

`gpu` - Provides CUDA user driver and tools

`cuda-mpich` - Provides CUDA-aware MPI

`nccl-2.18` - Provides NCCL plugin for CUDA

`none` - Turn off all modules

Shifting to podman-hpc

Shifter was built for NERSC needs

- podman-hpc is OCI compliant
  - Shifter has some capabilities loaded by default
  - Manually loaded with podman-hpc
- podman-hpc development guided by Shifter

podman-hpc controls access using namespaces

- Users can build containers on Perlmutter with podman-hpc
- Executables within containers can run as root

Building a Container with podman-hpc

Create a Containerfile (and call it Containerfile):

```
FROM docker.io/library/ubuntu:latest

ENTRYPOINT echo "no lols here"
```

- Start with a base operating system
- What will automatically run when you start the container

Create the container:

```
$ podman-hpc build -t nolols:1.0 .
```

Note: you must be in the same directory as Containerfile

- Use podman-hpc to build a container
- Tag this container with a name and version
- Build this container using a file called Containerfile found here

More podman-hpc Functionality

View your container:

```
$ podman-hpc images
localhost/nolols          1.0          59551900ead8  3 minutes ago  80.4 MB
docker.io/library/ubuntu  latest       3db8720ecbf5  8 days ago     80.4 MB
```

- View the images

Note: you do this for performance$^{\text{HPC}}$ reasons

Migrate the container to scratch:

```
$ podman-hpc migrate nolols:1.0
```

- Use podman-hpc to move the container to scratch
- Which container we are migrating
  - Note that if you update your container on the login node you must remigrate

Running Basic podman-hpc Containers

On the log-in node:

```
$ podman-hpc run --rm nolols:1.0
no lols here
```

- Use podman-hpc to run the container
- Clean up the used container when we are done
- Container name and version number

Interactively on the batch nodes:

```
$ salloc -N 1 -t 60 -C cpu -q interactive
```

```
$ podman-hpc run --rm nolols:1.0
```

- We don't specify the container name here, but the rest is the same as Shifter
- Run as before

Note: you also don't include the image name in a submission script

Extending podman-hpc

Use the same flags as Shifter for extended functionality:

`--volume=/pscratch/sd/u/user:/scratch`

- Make external storage available within your container

`--net host`

- Use the host network (off by default)

Shifter’s modules are now flags:

See more details about podman-hpc performance$^{\text{HPC}}$ flags in the NERSC docs.

`--mpi` - Use the Cray MPI

`--cvmfs` - Enable the CVMFS filesystem

`--gpu` - Provides CUDA user driver and tools

`--cuda-mpi` - Provides CUDA-aware MPI

Next Steps

Where to go from here?

- NERSC documentation and examples
  - Shifter
  - podman-hpc
- Registries
  - NERSC registry (and docs page): private and free with NERSC account
  - DockerHub: free public or paid private
  - Quay.io: free public or paid private
- More detailed Shifter training
- Submit NERSC Help tickets via the portal
- NERSC user appointment: nersc.as.me

Thank you!

NERSC

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