IOWA STATE UNIVERSITY

High Performance Computing

Workshop: Building and using containers on the HPC clusters

Yasasvy Nanyam

Robert Grandin

14 October 2021

Container Images and Samples

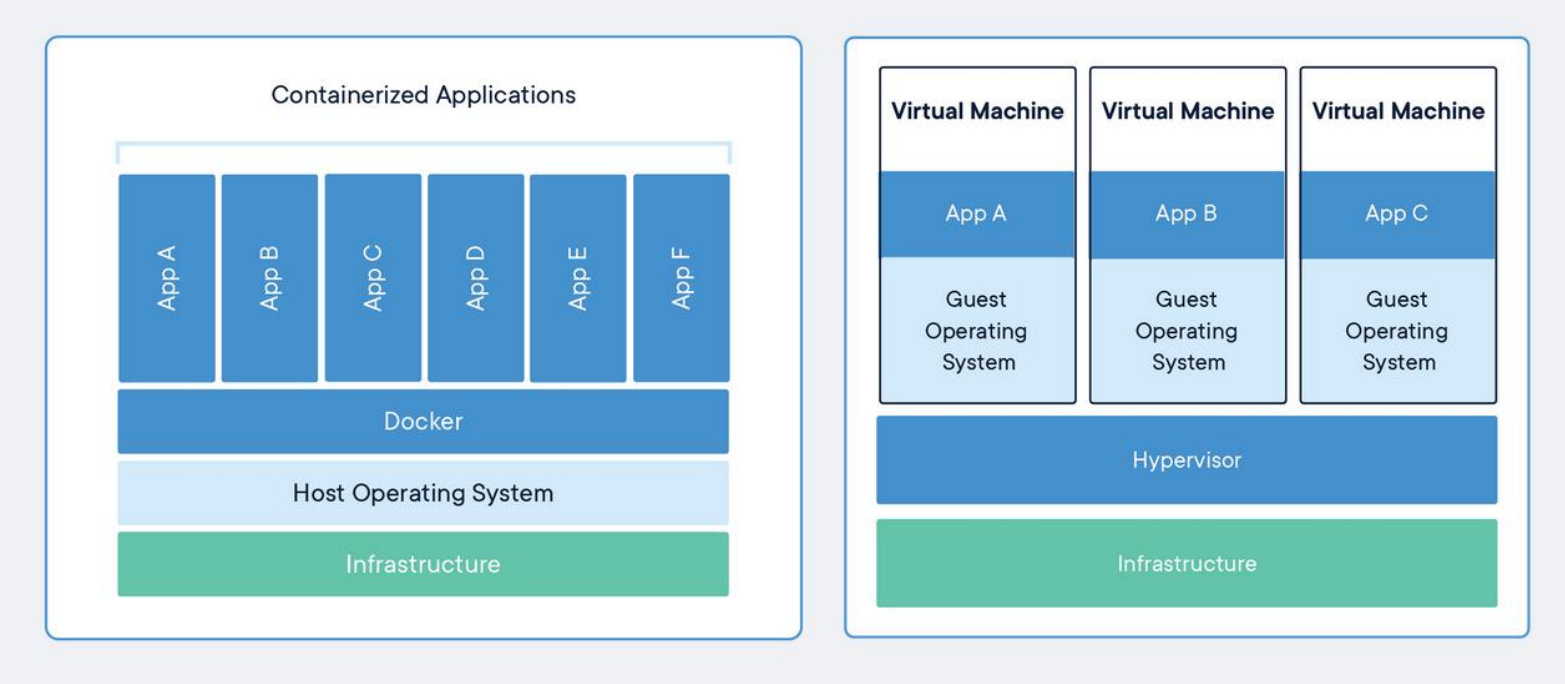
- All samples, test codes, container images and these presentation slides are available on hpc-class at

```
/ptmp/containers-workshop-october-2021
```

Outline

- Introduction to Containers
- Introduction to Singularity
- Singularity and HPC clusters
- Important Singularity commands
- Singularity and MPI
- Singularity recipes
- Demonstrate possible use cases
- Q&A, hands-on session

Introduction to Containers



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

Introduction to Containers

		
DOCKER	**SINGULARITY**	**PODMAN**
Daemon-based	Daemonless	Daemonless
Requires admin privileges	No special privileges	No special privileges
Persistent services (web services, database)	User-space applications	Will likely replace docker when HPC transitions to RHEL8

Introduction to Singularity

- Compatible with most stand-alone OCI images(includes Docker)
- Can build containers on local machine and copy to cluster
- Devices and directories are also visible inside the container
  - accelerator cards, networks, work directories, etc.
- User outside = user inside (No contextual changes)
- Maintain your existing workflow
  - works with SLURM, MPI
- Little to no overhead

Overhead

Calculate the number of prime numbers until 1024^2

Host	Container
The number of processes is 16 N Pi Time 1048576 82025 **18.524753**	The number of processes is 16 N Pi Time 1048576 82025 **18.505317**

```
Host
[ynanyam@hpc-class05 openmpi-4.0.2]$ mpirun -np $SLURM_NTASKS ./prime_mpi

Container
[ynanyam@hpc-class05 openmpi-4.0.2]$ mpirun -np $SLURM_NTASKS \
                                     singularity exec openmpi_4.0.2.sif ./prime_mpi
```

Singularity use cases

- **BYOE** – Bring Your Own Environment
- **Reproducibility** – version control, custom scripts and workflows
- Legacy programs that require specific environment

Limitations

- **Architecture** – limited by CPU architecture. The containers used in this workshop only work with x86_64 arch.
- **Portability** – requires glibc and kernel compatibility between host and container.
- **User space** – Not all containers available in docker hub are usable

Important Singularity Commands

- `pull` Get container images from repositories
- `exec` Run command in the container
- `shell` “Login to” the container for debugging
- `build` Create container from recipe

Important Singularity Variables

- SINGULARITY_CACHEDIR
- SINGULARITY_TMPDIR

Limited space in home directories.
Set to $TMPDIR to avoid quota limits.

```
export SINGULARITY_CACHEDIR=$TMPDIR
export SINGULARITY_TMPDIR=$TMPDIR
```

Singularity `pull`

- Pull (download) container images from “hubs”
  - Docker - https://hub.docker.com/
  - Singularity - https://cloud.sylabs.io/library
  - Quay (Bioinformatics) - https://quay.io/search
  - Nvidia NGC - https://ngc.nvidia.com/catalog/containers

```
singularity pull <library>://<image>[:<tag>]
singularity pull docker://gcc:8.3.0
```

Note: Only use the compute nodes to pull containers.

Singularity pull

```
[ynanyam@hpc-class05 container-workshop]$ singularity pull docker://gcc:8.3.0
INFO:    Converting OCI blobs to SIF format
INFO:    Starting build...
Getting image source signatures
Copying blob 50e431f79093 done
Copying blob dd8c6d374ea5 done
------------------------------
Writing manifest to image destination
Storing signatures
2021/10/13 16:49:01  info unpack layer:
sha256:50e431f790939a2f924af65084cc9d39c3d3fb9ad2d57d183b7eadf86ea46992
INFO:    Creating SIF file...

[ynanyam@hpc-class05 container-workshop]$ ls
gcc_8.3.0.sif
```

Singularity exec

- Spawn a command within a container image
- Recommended way to use containers in HPC as it facilitates batch submissions and can be included as a part of your SLURM script.

```
singularity exec [options] image.simg command [command-args]
```

Singularity exec

- Useful options
  - `--nv`: Leverage GPUs
  - `--bind`: Bind mount directories to the containers
    - **Note:** `/home` is mounted by default. `/work` `/ptmp` and `$TMPDIR` need to mounted manually.
    - **Note:** SINGULARITY_BIND can also be used
  - `--contain/--containall`: Better isolate the container runtime from the host
  - `--cleanenv`: Clean the environment
  - `--pwd`: Initial working directory within the container

- Issue `singularity exec --help` to see all options

Singularity exec

```
[ynanyam@hpc-class05 ~]$ which gcc; gcc --version
/usr/bin/gcc
gcc (GCC) 4.8.5 20150623 (Red Hat 4.8.5-36)
Copyright (C) 2015 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.


[ynanyam@hpc-class05 ~]$ singularity exec gcc_8.3.0.sif gcc --version
gcc (GCC) 8.3.0
Copyright (C) 2018 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
```

Singularity exec

By default, only `/home/$USER` and `/tmp` is bind mounted within the container

```
[ynanyam@hpc-class05 container-workshop]$ singularity exec gcc_8.3.0.sif df -hT
Filesystem                                      Type      Size  Used Avail Use% Mounted on
overlay                                         overlay    16M   20K   16M   1% /
devtmpfs                                        devtmpfs   63G     0   63G   0% /dev
tmpfs                                           tmpfs      63G     0   63G   0% /dev/shm
/dev/mapper/rhel-rootvol                        xfs        20G  3.9G   16G  20% /tmp
hpc-class-stor02:/hpc-class-stor02/home/ynanyam nfs4       10T  1.2T  8.8T  12% /home/ynanyam
tmpfs                                           tmpfs      16M   20K   16M   1% /etc/group
```

Singularity exec

```
[ynanyam@hpc-class05 container-workshop]$ export SINGULARITY_BIND=/ptmp,$TMPDIR

[ynanyam@hpc-class05 container-workshop]$ singularity exec gcc_8.3.0.sif df -hT
Filesystem                                      Type      Size  Used Avail Use% Mounted on
overlay                                         overlay    16M   20K   16M   1% /
devtmpfs                                        devtmpfs   63G     0   63G   0% /dev
tmpfs                                           tmpfs      63G     0   63G   0% /dev/shm
/dev/mapper/rhel-rootvol                        xfs        20G  3.9G   16G  20% /tmp
hpc-class-stor02:/hpc-class-stor02/home/ynanyam nfs4       10T  1.2T  8.8T  12% /home/ynanyam
tmpfs                                           tmpfs      16M   20K   16M   1% /etc/group
hpc-class-stor02:/hpc-class-stor02/ptmp         nfs4       47T  2.2T   45T   5% /ptmp
/dev/mapper/rhel-local                          xfs       2.5T  779M  2.5T   1% /scratch/ynanyam/101051
```

```
[ynanyam@hpc-class05 container-workshop]$ singularity exec –B /ptmp –B $TMPDIR gcc_8.3.0.sif df -hT
```

Binding `$TMPDIR` is required for MPI jobs

Singularity shell

- Interactively access the container image
- Similar to logging-in to a machine via SSH
- Useful for debugging during interactive sessions (e.g., salloc), not suitable for batch submissions

Singularity + MPI

- OPENMPI available both inside and on the host

```
[ynanyam@hpc-class05 openmpi-4.0.2]$ export SINGULARITY_BIND=/ptmp,$TMPDIR
[ynanyam@hpc-class05 openmpi-4.0.2]$ module load gcc/7.3.0-xegsmw4 openmpi

[ynanyam@hpc-class05 openmpi-4.0.2]$ mpirun -np $SLURM_NTASKS singularity exec openmpi_4.0.2.sif ./hello_mpi
P0:  HELLO_MPI - Master process:
P0:    C/MPI version
P0:    An MPI example program.
P0:    The number of processes is 16.
P0:    'Hello, world!'
P0:    Elapsed wall clock time = 0.000029 seconds.
P1:    'Hello, world!’
----------------------
P11:    'Hello, world!'
P12:    'Hello, world!'
P13:    'Hello, world!'
P14:    'Hello, world!'
P15:    'Hello, world!'
P0:  HELLO_MPI - Master process:
P0:    Normal end of execution: 'Goodbye, world!'
```

Singularity `build`

- Build on Singularity Cloud library. Requires a GitHub account.
  - Relatively slow, resource limits can require splitting container into "layers" and building piece-by-piece.
  - Great for publishing/distributing the final container
- Build locally. Requires administrator privileges on the build machine. (not possible on ISU HPC systems)
  - Often faster to iterate and debug the container-build process
  - If you don't have admin privileges, ask for a VM to use
- Once added to Singularity Cloud, containers can be pulled by any machine where singularity is installed

Singularity recipe

- Builds upon other containers
- Utilize package managers to install software into container
  - apt, yum
  - spack

```
Bootstrap: docker
From: centos:7

%post

    echo "Installing Development Tools YUM group"
    yum -y groupinstall "Development Tools"

    echo "Installing OpenMPI into container..."
    # Here we are at the base, /, of the container
    git clone https://github.com/open-mpi/ompi.git
    cd ompi

    # Now at /ompi
    git checkout cb5f4e7 #4.0.2

    ./autogen.pl
    ./configure --prefix=/usr/local

    make
    make install

    /usr/local/bin/mpicc examples/ring_c.c -o /usr/bin/mpi_ring
```

CentOS-based container with locally-built OpenMPI

Singularity recipe

- Builds upon other containers
- Utilize package managers to install software into container
  - apt, yum
  - spack

```
Bootstrap:shub
From:ResearchIT/spack-singularity:spack

%labels
MAINTAINER ynanyam@iastate.edu
APPLICATION trinity

%help
This container provides trinity

%environment
source /etc/profile.d/modules.sh
module load trinity

%post
export SPACK_ROOT=/opt/spack
export PATH=$SPACK_ROOT/bin:$PATH

yum -y install bc paste
yum clean all

export FORCE_UNSAFE_CONFIGURE=1
source $SPACK_ROOT/share/spack/setup-env.sh
spack install trinity

%runscript
exec Trinity "$@"
```

Containerized Trinity, built via spack

For more information…

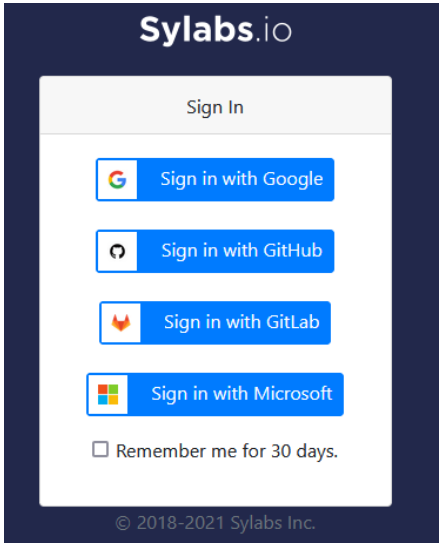
- https://www.hpc.iastate.edu/guides/containers
- https://opencontainers.org/about/overview/
- https://sylabs.io/guides/latest/user-guide/
- https://spack.readthedocs.io
- https://cloud.sylabs.io
- https://hub.docker.com
- https://quay.io/search
- https://ngc.nvidia.com/catalog
- As always: hpc-help@iastate.edu

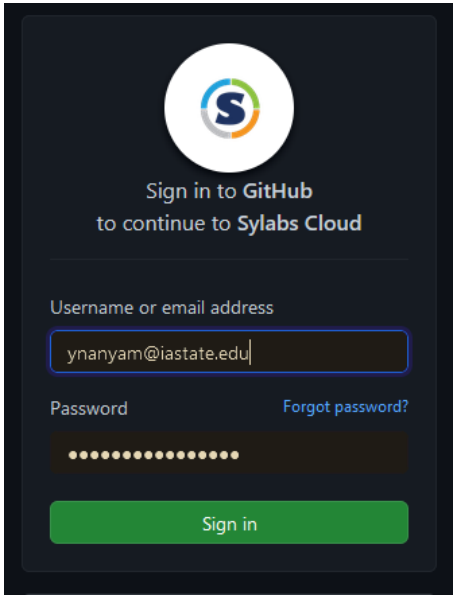
Hands-On

- Demonstrations
  - Getting started with Singularity Cloud
  - Using Singularity Cloud to build a container from a recipe
  - Building locally from a recipe
  - Using containers
    - Compiling with GCC 8.3
    - Running TensorFlow on a GPU
    - Running Hisat2
- Workshop, Q&A

Using Singularity Cloud to Build

- Create a GitHub account
- Go to https://cloud.sylabs.io/home and click sign-in





Using Singularity Remote Builder

- Creates OpenMPI 4.0.2 container image
- ~15min to build on remote builder

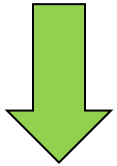
```
Bootstrap: docker
From: centos:7

%post

    echo "Installing Development Tools YUM group"
    yum -y groupinstall "Development Tools"

    echo "Installing OpenMPI into container..."
    # Here we are at the base, /, of the container
    git clone https://github.com/open-mpi/ompi.git
    cd ompi

    # Now at /ompi
    git checkout cb5f4e7 #4.0.2

    ./autogen.pl
    ./configure --prefix=/usr/local

    make
    make install

    /usr/local/bin/mpicc examples/ring_c.c -o /usr/bin/mpi_ring
```

Building Locally from a Recipe

```
Bootstrap:docker
From: makaho/hisat2-zstd

%labels
MAINTAINER rgrandin@iastate.edu
APPLICATION hisat2

%help
This container provides hisat2

%runscript
exec hisat2 "$@"
```

hisat2.def

```
{root@d5q4v2g2} # singularity build hisat2.sif hisat2.def
```



1.75 minutes

```
{root@d5q4v2g2} # ls -alh
total 319M
drwxr-xr-x.  2 root     root    4 Mar 27 09:06 .
drwxr-xr-x. 10 rgrandin root   10 Mar 27 09:06 ..
-rwxr-xr-x.  1 root     root 319M Mar 27 09:01 hisat2.sif
-rw-r--r--.  1 root     root  170 Mar 27 08:59 hisat2.def
```

Demo: Compiling with GCC 4.8.5

```
1  //#include <stio.h>
2
3  int main()
4  {
5      printf("Hello, world!\n");
6      return 0;
7  }
```

Missing #include

hello.c

```
{rgrandin@hpc-class06}> gcc hello.c –o hello
hello.c: In function ‘main’:
hello.c:5:5: warning: incompatible implicit declaration of
built-in function ‘printf’ [enabled by default]
     printf("Hello, world!\n");
     ^
```

Compilation using system gcc (v4.8.5)

Demo: Compiling with GCC 8.3.0

Typical warnings

Suggested Fix

```
{rgrandin@hpc-class06}> singularity exec -B /ptmp gcc-8.3.0.sif gcc hello.c -o hello
hello.c: In function 'main':
hello.c:5:5: warning: implicit declaration of function 'printf' [-Wimplicit-function-declaration]
     printf("Hello, world!\n");
     ^~~~~~
hello.c:5:5: warning: incompatible implicit declaration of built-in function 'printf'
hello.c:5:5: note: include '<stdio.h>' or provide a declaration of 'printf'
hello.c:1:1:
+#include <stdio.h>
 //#include <stio.h>
hello.c:5:5:
     printf("Hello, world!\n");
```

Compilation using containerized gcc (v8.3.0)

Running TensorFlow

```
import tensorflow as tf


# Create some tensors
a = tf.constant([[1.0, 2.0,
3.0], [4.0, 5.0, 6.0]])
b = tf.constant([[1.0, 2.0],
[3.0, 4.0], [5.0, 6.0]])
c = tf.matmul(a, b)

print(c)
```

tf-test.py

- Create basic functionality test
- Does not require use of GPU

Running TensorFlow

```
[ynanyam@hpc-class05 tensorflow]$ singularity exec tensorflow_2.1.0-gpu.sif python tf-test.py
2021-10-13 18:44:04.580698: I tensorflow/stream_executor/platform/default/dso_loader.cc:53]
Successfully opened dynamic library libcudart.so.11.0
2021-10-13 18:44:07.056091: W tensorflow/stream_executor/platform/default/dso_loader.cc:64] Could not
load dynamic library 'libcuda.so.1'; dlerror: libcuda.so.1: cannot open shared object file: No such
file or directory; LD_LIBRARY_PATH: /usr/local/cuda/lib64:/.singularity.d/libs
2021-10-13 18:44:07.056132: W tensorflow/stream_executor/cuda/cuda_driver.cc:326] failed call to
cuInit: UNKNOWN ERROR (303)
2021-10-13 18:44:07.056175: I tensorflow/stream_executor/cuda/cuda_diagnostics.cc:156] kernel driver
does not appear to be running on this host (hpc-class05): /proc/driver/nvidia/version does not exist
2021-10-13 18:44:07.056537: I tensorflow/core/platform/cpu_feature_guard.cc:142] This TensorFlow binary
is optimized with oneAPI Deep Neural Network Library (oneDNN) to use the following CPU instructions in
performance-critical operations:  SSE3 SSE4.1 SSE4.2 AVX AVX2 FMA
To enable them in other operations, rebuild TensorFlow with the appropriate compiler flags.
[5 12 21 32]
```

Run the test script inside the container – NO GPU

Print() statement outputs

Error that CUDA device is unavailable (container built with GPU expectation)

Running TensorFlow on GPU

```
[ynanyam@hpc-class-gpu05 tensorflow]$ singularity exec --nv -B /ptmp tensorflow_2.1.0-gpu.sif python tf-test.py
2021-10-13 21:09:01.086951: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1555] Found device 0 with
properties:
pciBusID: 0000:82:00.0 name: Tesla K20m computeCapability: 3.5
coreClock: 0.7055GHz coreCount: 13 deviceMemorySize: 4.63GiB deviceMemoryBandwidth: 193.71GiB/s
2021-10-13 21:09:01.404166: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1697] Adding visible gpu
devices: 0
2021-10-13 21:09:01.414724: I tensorflow/core/platform/profile_utils/cpu_utils.cc:94] CPU Frequency: 2000005000
Hz
2021-10-13 21:09:03.460912: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1096] Device interconnect 2021-
10-13 21:09:03.461007: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1102]      0
2021-10-13 21:09:03.461026: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1115] 0:   N
2021-10-13 21:09:03.462978: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1241] Created TensorFlow device
(/job:localhost/replica:0/task:0/device:GPU:0 with 4339 MB memory) -> physical GPU (device: 0, name: Tesla
K20m, pci bus id: 0000:82:00.0, compute capability: 3.5)
2021-10-13 21:09:03.465466: I tensorflow/stream_executor/platform/default/dso_loader.cc:44] Successfully opened
dynamic library libcublas.so.10
tf.Tensor(
[[22. 28.]
 [49. 64.]], shape=(2, 2), dtype=float32)
```

Print() statement outputs

Info about CUDA device used

hisat2

```
[ynanyam@hpc-class05 ]$ cp -r /ptmp/containers-workshop-october-2021/hisat2 .
[ynanyam@hpc-class05 ]$ cd hisat2
[ynanyam@hpc-class05 hisat2]$ mkdir HS_out
[ynanyam@hpc-class05 hisat2]$ module load parallel
[ynanyam@hpc-class05 hisat2]$ singularity exec -B /ptmp hisat2_2.2.1.sif hisat2-
build Arabidopsis_thaliana.TAIR10.dna.chromosome.1.fa At_chr1
[ynanyam@hpc-class05 hisat2]$ parallel -j 4 "singularity exec -B /ptmp
hisat2_2.2.1.sif hisat2 -p 4 -x At_chr1 -1 {1} -2 {2} -S HS_out/{1/.}.sam >&
HS_out/{1/.}.log" ::: samples/*_1.* :::+ samples/*_2.*
[ynanyam@hpc-class05 hisat2]$ ls -altr HS_out/
total 16831
drwxr-xr-x. 4 ynanyam domain users      14 Oct 13 20:12 ..
-rw-r--r--. 1 ynanyam domain users 5406097 Oct 13 20:12 SRR4420295_1.fastq.sam
-rw-r--r--. 1 ynanyam domain users 5521927 Oct 13 20:12 SRR4420296_1.fastq.sam
-rw-r--r--. 1 ynanyam domain users     587 Oct 13 20:12 SRR4420295_1.fastq.log
---------------------------- SNIP -------------------------
```

Q&A – Hands-on Session

- Questions?

- Try to run these examples yourself
  - Compute nodes: `salloc -N 1 -n 4 -t 15:00`
  - GPU nodes: `salloc -N 1 -n 4 -t 15:00 --gres gpu:1`

  - Be considerate with resource requests.
    We have to share the cluster.