Introduction to Containers Advanced Content

featuring Singularity on the FASTER cluster

by Richard Lawrence

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High Performance Research Computing
DIVISION OF RESEARCH

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Outline

- More Container Examples
- Build your own Containers

Learning Resources

- HPRC Wiki https://hprc.tamu.edu/wiki/SW:Singularity
- HPRC on Youtube https://www.youtube.com/c/TexasAMHPRC
  (video of this course will be posted)
- Singularity Manual https://apptainer.org/user-docs/3.8/
- Docker Manual https://docs.docker.com/
- Other container courses:
  NBIS
  https://nbis-reproducible-research.readthedocs.io/en/latest/singularity/
  Arizona https://learning.cyverse.org/projects/Container-camp-2020/
  TACC https://learn.tacc.utexas.edu/mod/page/view.php?id=95

More Container Examples

With exercises

Singularity with GPU

- Containers should be built with CUDA version compatible with local GPUs (CUDA ≧ 11)
- Just add the `--nv` flag to your singularity command

Many repositories on Docker Hub have GPU-ready images. Search for images with “gpu” in tags

The nvidia cloud also provides GPU-ready images. See: https://hprc.tamu.edu/wiki/SW:Singularity:Examples#NVIDIA_GPU_Cloud

TensorFlow GPU Exercise

Image file: `tensorflow_2.4.1-gpu.sif` from docker://tensorflow/tensorflow:2.4.1-gpu

Located at `/scratch/data/Singularity/images/`

Also: `tf-gpu-test.py` in the same location.

```
$ srun --mem=512m --time=01:00:00 \
--gres=gpu:1 --partition=gpu --pty bash -i
$ singularity exec --nv tensorflow_2.4.1-gpu.sif \
python3 tf-gpu-test.py
Num GPUs Available:  1
```

Following along live? add `--reservation=training`

If error "couldn't find `tf-gpu-test.py`" try using `--bind` and/or specify full path to the file.

Containers in HPRC Portal

Container support for Interactive Apps on the HPRC Portal

Currently:

- Jupyter Notebook (a popular Python IDE)

Will extend container support to other Apps. If you would like something, please ask help@hprc.tamu.edu

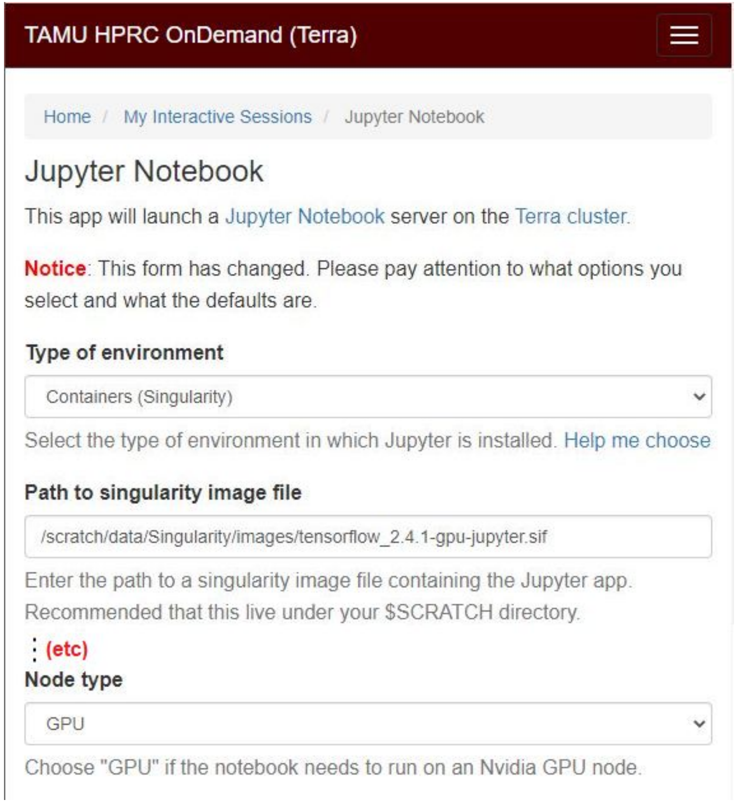
Jupyter Exercise

- Choose an image file on disk that contains Jupyter
- Image file: `tensorflow_2.4.1-gpu-jupyter.sif` from docker://tensorflow/tensorflow:2.4.1-gpu-jupyter

  Located at `/scratch/data/Singularity/images/`

Jupyter Exercise

- Navigate to HPRC Portal → FASTER OnDemand → Interactive Apps → Jupyter Notebook
- Select “Containers (Singularity)” from “Type of environment” drop-down menu
- Enter the path to the image file.



Singularity with MPI

There are several ways to containerize MPI.

Check with your container source to see how it is meant to be used.

- MPI installed and run inside container.
  `singularity exec <sif> mpirun <exe>`
- MPI installed and run outside container.
  `mpirun singularity exec <sif> <exe>`
- MPI installed outside, run inside.
  `singularity exec --bind /dir <sif> /dir/mpirun <exe>`

See https://sylabs.io/guides/3.8/user-guide/mpi.html

LAMMPS MPI Exercise

Image file: `lammps-stable_29Oct2020[...].sif` from docker://lammps/lammps:stable_29Oct2020[...]

Located at `/scratch/data/Singularity/images/`

Also: `lammps-test-input.txt` in the same location.

```
$ srun --ntasks=4 --nodes=1 --mem=2560m --time=01:00:00 \
--pty bash -i

$ singularity run --bind "/scratch,$TMPDIR:/work" \
lammps-stable_29Oct2020_ubuntu20.04_openmpi_py3.sif mpirun -np 4 \
/bin/lmp_mpi -in lammps-test-input.txt
```

Biocontainers Exercise

Image file: `bcbio-nextgen-1.2.8.sif`
From docker://quay.io/biocontainers/bcbio-nextgen
https://biocontainers.pro/tools/bcbio-nextgen
Located at `/scratch/data/Singularity/images/`

```
$ srun --mem=512m --time=01:00:00 --pty bash -i
$ singularity exec bcbio-nextgen-1.2.8.sif bcbio_nextgen.py --help
usage: bcbio_nextgen.py [...]
$ singularity exec bcbio-nextgen-1.2.8.sif python -c \
 "import pysam; print(pysam.__version__)"
0.16.0.1
```

Singularity with Writable Filesystem

Problem:

- You want to save your work or add things *inside* the container - but not the real, local filesystem
- Example: an application creates millions of files

Reminder:

- Singularity images are **immutable**.
- Singularity filesystem is **ephemeral** (does not *persist*)

Solution:

- A second file called an **overlay** that is user writable.

Overlay Creation Tool

- The tools `dd` and `mkfs` create a virtual filesystem.
  - The version of `mkfs` matters.
  - FASTER has the correct `mkfs`
- Singularity can do the process automatically.

```
singularity overlay create <filename>
```

Overlay Creation Exercise

```
$ srun --mem=512m --time=01:00:00 --pty bash -i
$ singularity overlay create --size 256 $TMPDIR/my_overlay
```

Result: blank virtual filesystem `my_overlay` of size 256 MB
(`cp` to `$SCRATCH` if you want to keep it)

Overlay Creation Tool

- The tools `dd` and `mkfs` create a virtual filesystem.
  - The version of `mkfs` matters.
  - Some machines have the wrong version of `mkfs`.
- No problem! We have a *container* and a *script* for that case.
  - `docker://ubuntu:18.04`
  - `overlay-example.sh`

Overlay Creation Exercise (Alternative)

Image file: `ubuntu-18.04.sif`
From docker://ubuntu:18.04
Script file: `overlay-example.sh`
Both located at `/scratch/data/Singularity/images`

```
$ srun --mem=512m --time=01:00:00 --pty bash -i
$ singularity exec ubuntu-18.04.sif bash overlay-example.sh
```

Result: blank virtual filesystem `my_overlay`, size 200 MB.
(`cp` to `$SCRATCH` if you want to keep it)

Overlay Usage Exercise

Run your container image together with the overlay file.

```
singularity --overlay <overlay file>
```

Any files you create (outside the mounted filesystems) will go in the overlay file virtual filesystem and *persist*.

```
$ srun --mem=512m --time=01:00:00 --pty bash -i
$ singularity shell --overlay /path/to/my_overlay ubuntu-18.04.sif
> mkdir /new_dir
> touch /new_dir/new_file
> exit
$ singularity shell --overlay /path/to/my_overlay ubuntu-18.04.sif
> ls /new_dir
```

Build your own Containers

Overview, no exercises

Singularity Image Formats

Singularity has two image formats:

- A compressed read-only file (extension `.sif`)
- A writable directory structure called “sandbox”.

Singularity `build` command can convert from one to the other. This is mainly useful for modifying images, such as installing new software.

Installing new software usually requires root privileges, which must be done on your personal machine.

Modify Container Example

Starting with an existing image located at `<source>`

```
$ singularity build --sandbox <sandbox-name> <source>
```

This creates a directory `<sandbox-name>/` that works the same as an image file, except it can be used in write mode.

```
$ sudo singularity shell --writable <sandbox-name>/
```

Now you install software in the root directories, as the root user. When you are done, you exit the sandbox and:

```
$ singularity build <final-name>.sif <sandbox-name>/
```

This creates the read-only file suitable for production use.

See https://sylabs.io/guides/3.7/user-guide/build_a_container.html

Container Recipe

Singularity `build` can build containers from a recipe.
A recipe might contain these facts:

- “Bootstrap”: what your build starts from. It could be an existing recipe or image, or it could be from scratch.
- What software to install in the container and how.
- “Runscript”: what your container does by default.

Once you have the recipe file defined:

```
$ sudo singularity build <container> <recipe-file>
```

See https://sylabs.io/guides/3.8/user-guide/definition_files.html

Advanced Content Complete

Conclusion

- Run Containers on clusters! It’s easy.
- HPRC supports Singularity
- Convert Docker to Singularity!
- Charlie Cloud support also available.
- Ask for help!

Survey

Please fill out the survey to let us know how you feel about this short course. This will help us improve.

Questions

?

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  TACC https://learn.tacc.utexas.edu/mod/page/view.php?id=95

Thank you

Contact: help@hprc.tamu.edu