Introduction to Containers
Advanced Content

featuring Singularity on the Grace cluster

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Outline

- More Container Examples
- Build your own Containers
Learning Resources

- HPRC Wiki  [https://hprc.tamu.edu/wiki/SW:Singularity](https://hprc.tamu.edu/wiki/SW:Singularity)
- HPRC on Youtube  [https://www.youtube.com/c/TexasAMHPRC](https://www.youtube.com/c/TexasAMHPRC)  
  (video of this course will be posted)
- Singularity Manual  [https://apptainer.org/user-docs/3.8/](https://apptainer.org/user-docs/3.8/)
- Docker Manual  [https://docs.docker.com/](https://docs.docker.com/)
- Other container courses:
More Container Examples

With exercises
Singularity with GPU

- Containers should be built with CUDA version compatible with local GPUs (CUDA $\geq 11$)
- 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 \n--gres=gpu:1 --partition=gpu --pty bash -i
$ singularity exec --nv tensorflow_2.4.1-gpu.sif \npython3 tf-gpu-test.py
Num GPUs Available: 1

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 → Grace 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/3.7/user-guide/mpi.html](https://sylabs.io/guides/3.7/user-guide/mpi.html)
LAMMPS MPI Exercise

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.
- Terra and Grace have the wrong version of `mkfs`.
- No problem! We have a container and a script for that.
  - `docker://ubuntu:18.04`
  - `overlay-example.sh`
- On a personal machine that has the correct `mkfs`, Singularity can do the process automatically.
  
  `singularity overlay create <filename>`
Overlay Creation Exercise

Image file: ubuntu-18.04.sif
From docker://ubuntu:18.04
Script file: overlay-example.sh
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’re 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](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/3.7/user-guide/definition_files.html](https://sylabs.io/guides/3.7/user-guide/definition_files.html)
Automatic Singularity Build

You can create an account on Singularity Hub and use it to automatically build and publish your containers.

- Start with a github repository you can push to.
- Commit a singularity recipe file named “Singularity”.
- Link that github repository in Singularity Hub.
- Define what triggers a new build. It can be whenever a new tag is committed, for example.
- Pull your freshly-built container from Singularity Hub.

See [https://singularityhub.github.io/singularityhub-docs/](https://singularityhub.github.io/singularityhub-docs/)
Advanced Content Complete
Conclusion

- Run Containers on clusters! It’s easy.
- HPRC supports Singularity
- Convert Docker to Singularity!
- Expect Charlie Cloud support in the near future
- 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
Learning Resources

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- Singularity Manual [https://apptainer.org/user-docs/3.8/](https://apptainer.org/user-docs/3.8/)
- Docker Manual [https://docs.docker.com/](https://docs.docker.com/)
- Other container courses:
Thank you

Contact: help@hprc.tamu.edu