LUMI

Running containers on LUMI

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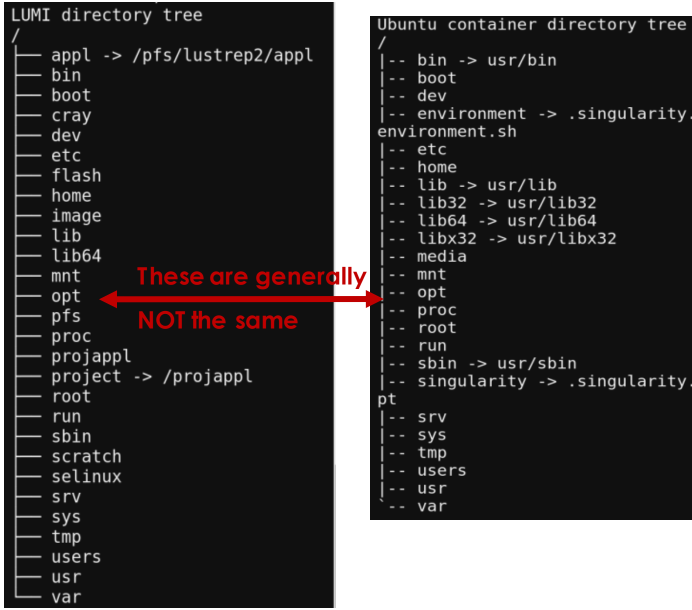
Containers – bring your own user space

- When running containers, the kernel, drivers and hardware is still provided by the host (LUMI) - but the user space (directory tree) changes
- Benefits of using containers:
    - **Enhanced reproducibility**: A fixed (read-only) user space for each computational experiment
        - Have a fully self-contained software environment
        - Pin all versions of the software packages used
        - Version control software environments
    - **Enhanced portability**: Run your container on other systems – as long as the system libraries are compatible
        - Makes the same environment work on all compute platforms – from laptop to supercomputer
        - Makes it easier to share your software environment with others – just share the container
    - **Easily test and trash**: Try a new container – if it doesn't work just trash the container and start over again
    - **Bonus**: Your software environment is a single file (the container) on the Lustre shared filesystems, which is much less stressful to Lustre and more performant, making for a much nicer experience for everyone on LUMI.



```
LUMI directory tree
/
├── appl -> /pfs/lustrep2/appl
├── bin
├── boot
├── cray
├── dev
├── etc
├── flash
├── home
├── image
├── lib
├── lib64
├── mnt
├── opt
├── pfs
├── proc
├── projappl
├── project -> /projappl
├── root
├── run
├── sbin
├── scratch
├── selinux
├── srv
├── sys
├── tmp
├── users
├── usr
└── var
```

These are generally NOT the same

```
Ubuntu container directory tree
/
|-- bin -> usr/bin
|-- boot
|-- dev
|-- environment -> .singularity.
environment.sh
|-- etc
|-- home
|-- lib -> usr/lib
|-- lib32 -> usr/lib32
|-- lib64 -> usr/lib64
|-- libx32 -> usr/libx32
|-- media
|-- mnt
|-- opt
|-- proc
|-- root
|-- run
|-- sbin -> usr/sbin
|-- singularity -> .singularity.
pt
|-- srv
|-- sys
|-- tmp
|-- users
|-- usr
`-- var
```

Running containers on LUMI

- On LUMI, you can run Singularity/Apptainer containers
  - Singularity/Apptainer are HPC container runtimes that allow you to run unprivileged containers, i.e. no need for root or sudo
  - Singularity/Apptainer is not Docker, but if you have an existing Docker container, you can run it using Singularity/Apptainer
- Main singularity commands:
  - Getting (pulling) a container from a container registry

    ```
    singularity pull my_container.sif docker://ubuntu:22.04
    ```
  - Opening a shell inside the container

    ```
    singularity shell my_container.sif
    ```
  - Executing a command inside the container

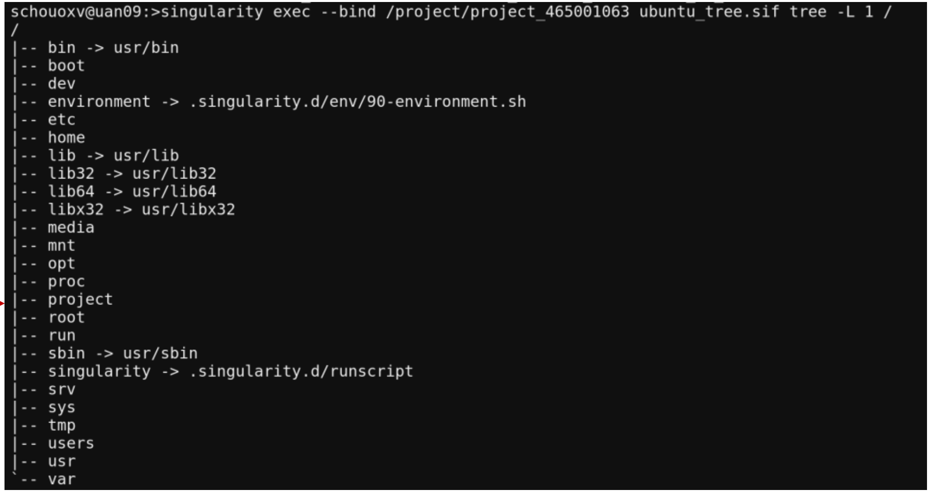
    ```
    singularity exec my_container.sif python3 my_script.py
    ```
- Running containers on compute nodes
  - Launch computation using srun

    ```
    srun <options> singularity exec my_container.sif python3 my_script.py
    ```

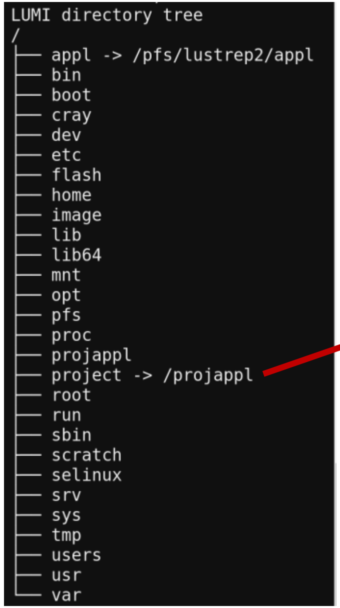
Bind mounting parts of the host file system (1)

- When running a container on LUMI, where is /project, /scratch, etc.?
- You may "inject" parts of the host (LUMI) file system into the container by bind mounting it

```
singularity exec --bind /project/<project_ID>
my_containr.sif tree –L 1 /
```



```
schouoxv@uan09:>singularity exec --bind /project/project_465001063 ubuntu_tree.sif tree -L 1 /
/
|-- bin -> usr/bin
|-- boot
|-- dev
|-- environment -> .singularity.d/env/90-environment.sh
|-- etc
|-- home
|-- lib -> usr/lib
|-- lib32 -> usr/lib32
|-- lib64 -> usr/lib64
|-- libx32 -> usr/libx32
|-- media
|-- mnt
|-- opt
|-- proc
|-- project
|-- root
|-- run
|-- sbin -> usr/sbin
|-- singularity -> .singularity.d/runscript
|-- srv
|-- sys
|-- tmp
|-- users
|-- usr
`-- var
```



```
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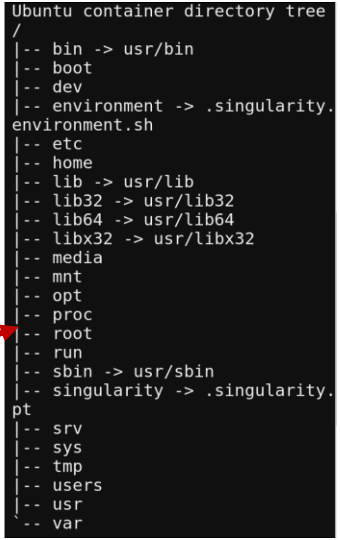
```



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|-- libx32 -> usr/libx32
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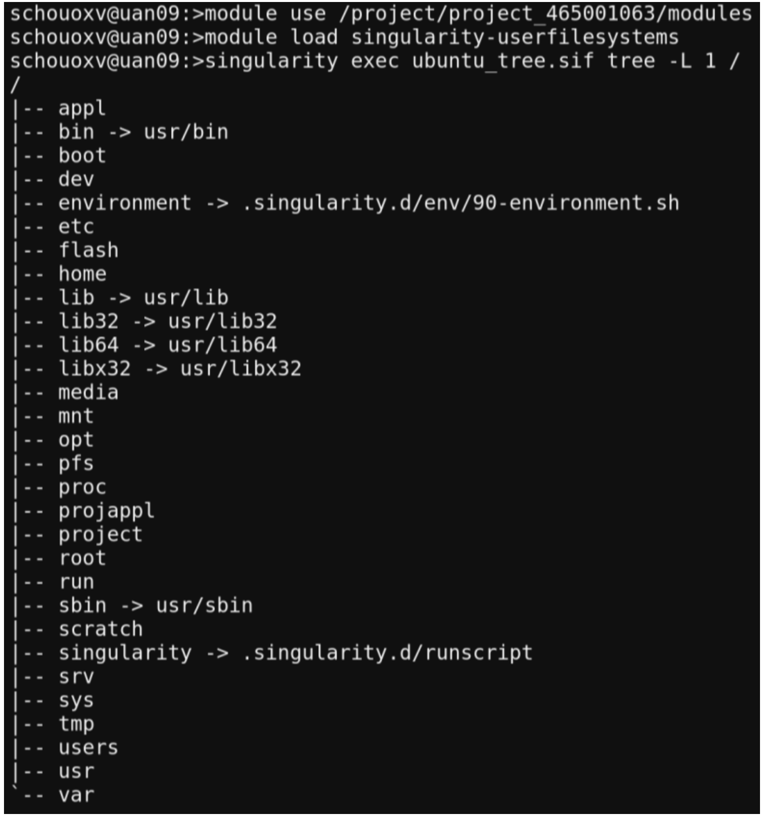
|-- mnt
|-- opt
|-- proc
|-- root
|-- run
|-- sbin -> usr/sbin
|-- singularity -> .singularity.
pt
|-- srv
|-- sys
|-- tmp
|-- users
|-- usr
`-- var
```

Bind mounting parts of the host file system (2)

- You typically want to bind mount your project folders (/project, /scratch, /flash). A shortcut is:

```
module use /appl/local/training/modules/AI-20240529
module load singularity-userfilesystems
```

- You may need to bind mount some of the host libraries to fully exploit the hardware
  - On LUMI you need this to get optimal performance when using the Slingshot 11 interconnect
  - **WARNING**: Be careful when bind mounting libraries from the host system. You can easily end up in a broken state if mixing the container libraries with host libraries.



```
schouoxv@uan09:>module use /project/project_465001063/modules
schouoxv@uan09:>module load singularity-userfilesystems
schouoxv@uan09:>singularity exec ubuntu_tree.sif tree -L 1 /
/
|-- appl
|-- bin -> usr/bin
|-- boot
|-- dev
|-- environment -> .singularity.d/env/90-environment.sh
|-- etc
|-- flash
|-- home
|-- lib -> usr/lib
|-- lib32 -> usr/lib32
|-- lib64 -> usr/lib64
|-- libx32 -> usr/libx32
|-- media
|-- mnt
|-- opt
|-- pfs
|-- proc
|-- projappl
|-- project
|-- root
|-- run
|-- sbin -> usr/sbin
|-- scratch
|-- singularity -> .singularity.d/runscript
|-- srv
|-- sys
|-- tmp
|-- users
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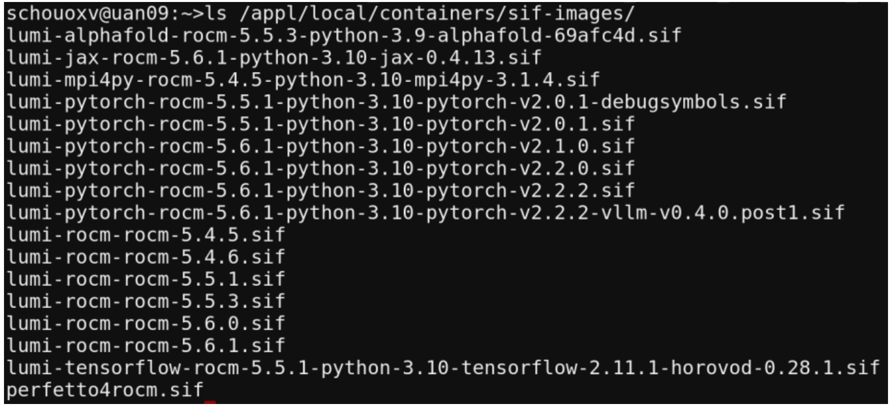
`-- var
```

The LUMI (FakeCPE) containers (1)

- Official LUMI containers available on LUMI under /appl/local/containers/sif-images
- Application images:
  - Alphafold
  - JAX
  - mpi4py
  - PyTorch
  - Tensorflow + Horovod
- Base images:
  - Lumi-rocm-rocm-X.Y.Z.sif: ROCm + aws-ofi-rccl + MI250X (gfx90a) MIOpen kernels + rccltest
- Remember to copy these to your project folder
  - We may remove/replace the container under /appl/local/containers/sif-image at any time!
  - If you like EasyBuild and modules, we also provide a set of easyconfigs to "install" the containers.



```
schouoxv@uan09:~>ls /appl/local/containers/sif-images/
lumi-alphafold-rocm-5.5.3-python-3.9-alphafold-69afc4d.sif
lumi-jax-rocm-5.6.1-python-3.10-jax-0.4.13.sif
lumi-mpi4py-rocm-5.4.5-python-3.10-mpi4py-3.1.4.sif
lumi-pytorch-rocm-5.5.1-python-3.10-pytorch-v2.0.1-debugsymbols.sif
lumi-pytorch-rocm-5.5.1-python-3.10-pytorch-v2.0.1.sif
lumi-pytorch-rocm-5.6.1-python-3.10-pytorch-v2.1.0.sif
lumi-pytorch-rocm-5.6.1-python-3.10-pytorch-v2.2.0.sif
lumi-pytorch-rocm-5.6.1-python-3.10-pytorch-v2.2.2.sif
lumi-pytorch-rocm-5.6.1-python-3.10-pytorch-v2.2.2-vllm-v0.4.0.post1.sif
lumi-rocm-rocm-5.4.5.sif
lumi-rocm-rocm-5.4.6.sif
lumi-rocm-rocm-5.5.1.sif
lumi-rocm-rocm-5.5.3.sif
lumi-rocm-rocm-5.6.0.sif
lumi-rocm-rocm-5.6.1.sif
lumi-tensorflow-rocm-5.5.1-python-3.10-tensorflow-2.11.1-horovod-0.28.1.sif
perfetto4rocm.sif
```

The LUMI (FakeCPE) containers (2)

- These LUMI containers are built against the Cray Programming Environment (CPE) However, the CPE is NOT included in the container due to license restrictions
- To fully utilize the Slingshot 11 interconnect with these containers, you need to bind mount parts of the CPE when running the container

  ```
  singularity exec --bind /var/spool/slurmd,/opt/cray,/usr/lib64/libcxi.so.1,
   /usr/lib64/libjansson.so.4 <program>
  ```

  - For the containers making use of MPI (mpi4py and Horovod), this is required
  - For all other containers it is optional. If you don't include it, RCCL internode communication falls back to using slower TCP/IP sockets
  - Shortcut to getting the binds right:

    ```
    module use /appl/local/training/modules/AI-20240529
    module load singularity-CPEbits
    ```

- For the LUMI application containers, you need to run $WITH_CONDA in the container to activate the conda environment in which the application, e.g. PyTorch, is installed

Further reading

- LUMI Docs running containers page: https://docs.lumi-supercomputer.eu/runjobs/scheduled-jobs/container-jobs/
- LUMI (EasyBuild) Software Library: https://lumi-supercomputer.github.io/LUMI-EasyBuild-docs/