Getting started with containers

Singularity

Why singularity?

On a HPC:

- Users have different levels of priviliges

- Users submit jobs with time/cpu/memory restrictions

These are two things Docker doesn't facilitate:

- Requires superuser priviliges

- Docker commands are an API of a deamon (parentless)

Specific singularity features

- UID + permissions are inside the container always the same as outside
- No deamon – container is a child process

Singularity without docker

- The singularity `Dockerfiles` : Singularity recipies (i.e. definition file)
- Singularity hub: https://singularity-hub.org/
- **Note**: installing as root inside container requires root privileges outside container!
- Solutions: --fakeroot or build with external runner

Pipeline development

- Containers are particularly useful for pipelines

- Both snakemake and nextflow support conda, docker and singularity

- Containers are built based on conda environments

- Once your cluster environment is set: ultimate scalability/reproducibility