Introdution to Singularity containers

Jan P. Buchmann
jan.buchmann@sydney.edu.au

The University Of Sydney

2018-11-29

Just in case...

Download https://www.sylabs.io/singularity/get-singularity/

Manual https://www.sylabs.io/guides/3.0/user-guide.pdf

Singularity: Containers for HPC

Containers are encapsulated system enviroments

Not a microservice: Scientific focus, e.g. whole pipelines

Single file: The image is a single file easily share, archive, reproduce, good for parallel file sytems, e.g. Lustre

Run as user: root to create, user to run

Access HPC resources: MPI, GPUs, InfiniBand/Network, file systems

Biggest difference to Docker

Privileges

You run the container as the user who invokes singularity. You can only be root in the container if you run it as root. Not your usual HPC experience.

Daemon

There is no deamon required, Singularity image is mounted as a loopback. Docker swarms need a DockerEngine on each node or instance they run.

Runs closer to the host

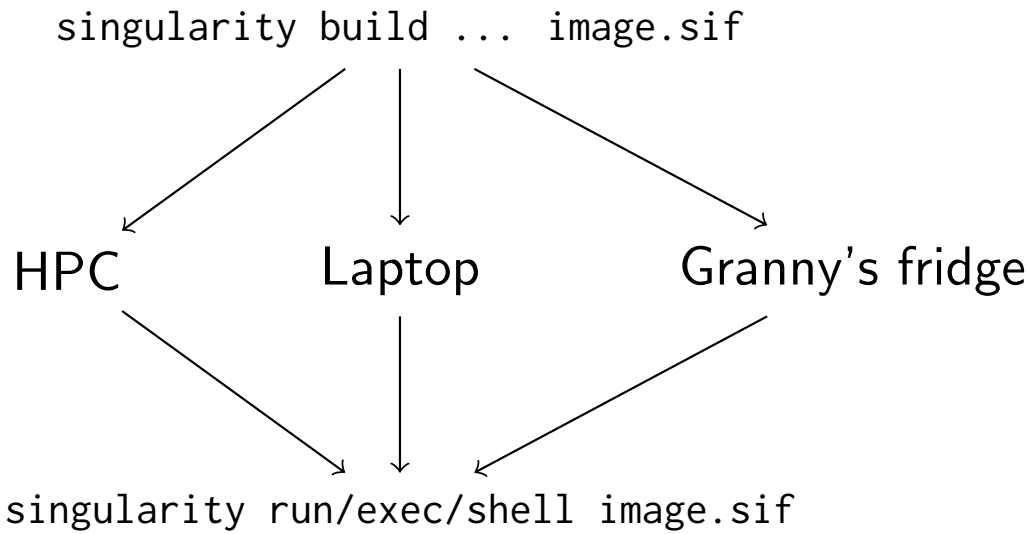
Running a singularity container bind mount your $HOME, /dev, /sys, and /proc automatically by default.

Singularity Image Format (SIF) ($\geq$3.0)

Image container format resembling a general file system whoch will allow PGP signing, block encryption, partitions accomodating multiple OSes, fast metadata access.

Speed

Overall singularity workflow



Building singularity containers

Docker Hub (docker://) singularity build lolcow.simg
docker://godlovedc/lolcow

Container Library (library://) singularity build lolcow.simg
library://sylabs-jms/testing/lolcow

Singularity Hub (shub://) singularity build demo.simg
shub://jasongallant/singularity_demosingularity

Singularity receipe files Roll your own

Invoking singularity

```
singularity [global options] command [command options]
singularity -v build --sandbox /tmp/ubuntu docker://ubuntu:latest
```

Workflow: Build enviroment (root)

Interactive

- singularity build –sandbox /tmp/ubuntu docker://ubuntu:latest
- singularity exec –writeable /tmp/ubuntu apt-get install python
- singularity build /tmp/ubuntu.sif /tmp/ubuntu

Workflow: Build enviroment (root)

Receipe

Production enviroment (user)

singularity receipe files

Bind paths

Overlays