Uni.lu HPC School 2021
PS7: HPC Containers with Singularity

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`http://hpc.uni.lu`

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Computing &
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Latest versions available on Github:

UL HPC tutorials: https://github.com/ULHPC/tutorials

UL HPC School: hpc.uni.lu/education/hpcschool

PS7 tutorial sources: ulhpc-tutorials.rtfd.io/en/latest/virtualization/singularity

Summary

Main Objectives of this Session

- **Discussion on container systems**
  - $\hookrightarrow$ what they are and where they help
  - $\hookrightarrow$ common container systems
  - $\hookrightarrow$ will focus on **Singularity** container system

The tutorial will show you...

- how to use **Singularity** containers on the UL HPC platform
  - $\hookrightarrow$ how to build containers from a definition file
  - $\hookrightarrow$ how to import pre-existing containers
  - $\hookrightarrow$ how to use applications embedded in containers
- containerized parallel applications execution
- Please go to readthedocs – singularity

Summary

1 **Introduction**

2 **HPC Containers**

A brief intro. to containers

- **Application portability**
  - ↪ containers bundle together an entire runtime env. (OS to apps.)
  - ↪ easy replication of environments
- **Services isolation**
  - ↪ separate microservices in different containers
- **Do more with less**
  - ↪ fast instantiation and tear-down
  - ↪ little memory/CPU overhead
- **OS-level virtualization** - **light virtualization**
  - ↪ don't spin up a full virtual machine
- **Close to native bare metal speed**
  - ↪ user software and libraries run on host kernel

Common container systems

- **Docker** https://www.docker.com
  - ↪ A new (2013-) take on containers (OpenVZ and LXC came before)
  - ↪ High uptake in Enterprise (microservices) & science (reproducibility)
  - ↪ In use everywhere (esp. DevOps), available on most Cloud infra.
- **Shifter** https://github.com/NERSC/shifter
  - ↪ *Linux containers for HPC*, developed at NERSC
  - ↪ Uses Docker functionality but makes it safe in shared HPC systems
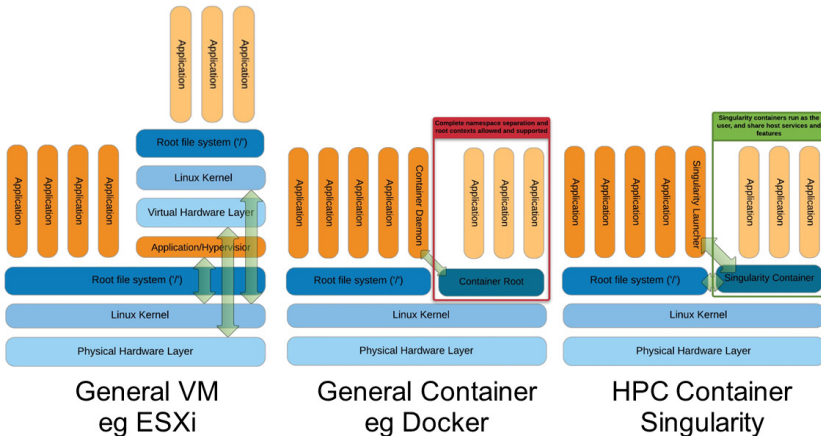 - ↪ Image gateway used to convert Docker images before use
- **Singularity** https://github.com/sylabs/singularity
  - ↪ *Containers for science*, initially developed at LBNL
  - ↪ Not based on Docker, but can directly import/run Docker images
  - ↪ Also HPC oriented, diff. take to running MPI software than Shifter
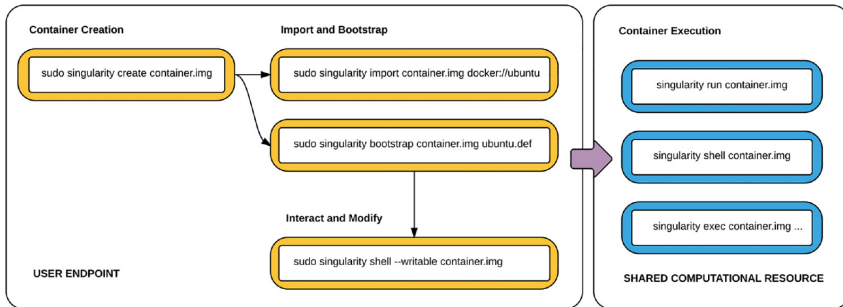 - ↪ Provides an Image Registry https://github.com/singularityhub/sregistry

High level view of containers vs full virt.

General VM
eg ESXi

General Container
eg Docker

HPC Container
Singularity

Sources:
Greg Kurtzer keynote slides at HPC Advisory Council 2017 @ Stanford (highly recommended read!)

Singularity in a nutshell

Many changes in newest v3 Singularity but workflow still similar.

user endpoint: your workstation (admin. privileges required)
shared computational resource: UL HPC clusters

Tutorials

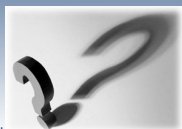### Now it's time to try ...

- Please go to readthedocs – singularity

Thank you for your attention...

Questions?

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1. **Introduction**
2. **HPC Containers**

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