

Uni.lu HPC School 2020

PS6: HPC Containers: Singularity

Uni.lu High Performance Computing (HPC) Team

E. Kieffer

University of Luxembourg (UL), Luxembourg

<http://hpc.uni.lu>



High Performance
Computing &
Big Data Services



LU  **EMBOURG**
LET'S MAKE IT HAPPEN

uni.lu
UNIVERSITÉ DU
LUXEMBOURG

Latest versions available on Github:



UL HPC tutorials:

<https://github.com/ULHPC/tutorials>

UL HPC School:

<http://hpc.uni.lu/hpc-school/>

PS6 tutorial sources:

ulhpc-tutorials.rtf.d.io/en/latest/virtualization/singularity





Summary

1 Introduction

2 HPC Containers

Main Objectives of this Session



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

The tutorial will show you...

- how to use **Singularity** containers on the UL HPC platform
 - ↳ how to build containers from a definition file
 - ↳ how to import pre-existing containers
 - ↳ 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

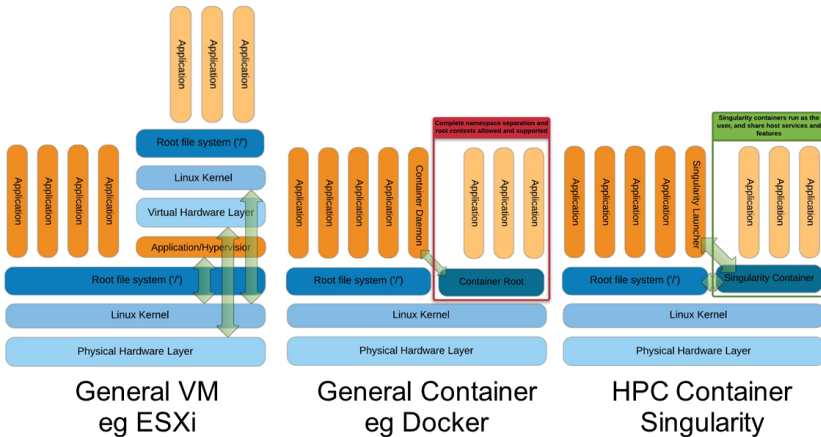
• Singularity

<https://github.com/sylabs/singularity>

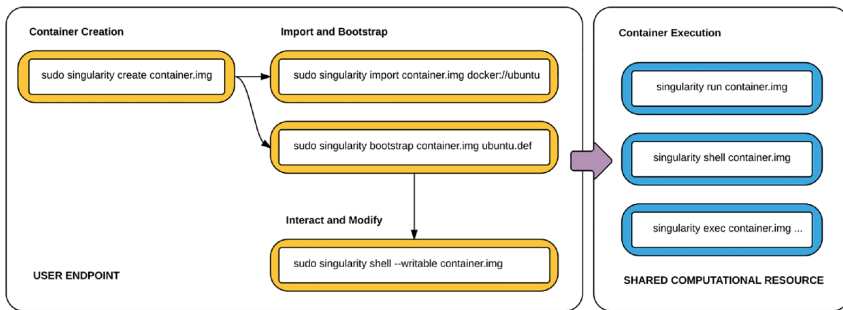
- *Containers for science*, initially developed at LBNL
- Not based on Docker, but can directly import/run Docker images
- Also HPC oriented, diff. take to running MPI software than Shifter
- Provides an Image Registry

<https://github.com/singularityhub/sregistry>

High level view of containers vs full virt.



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



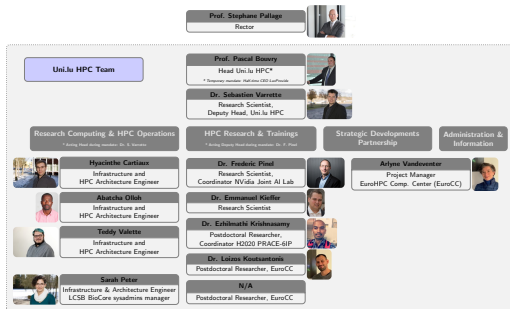
Now it's time to try ...

- Please go to [readthedocs – singularity](#)

Thank you for your attention...

Questions?

High Performance Computing @ Uni.lu



University of Luxembourg, Belval Campus
Maison du Nombre, 4th floor
2, avenue de l'Université
L-4365 Esch-sur-Alzette
mail: hpc@uni.lu

- 1 Introduction
- 2 HPC Containers



<https://hpc.uni.lu>