Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Containers @ BSC: Singularity

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PATC Systems Workshop: Programming MareNostrum4

Index

- **Introduction**
  - Why containers in HPC
  - Introducing singularity
- **Availability in BSC machines**
- **How to:**
  - Execute
  - Build
  - Path binding
  - MPI
- **Questions**

Introduction to Singularity

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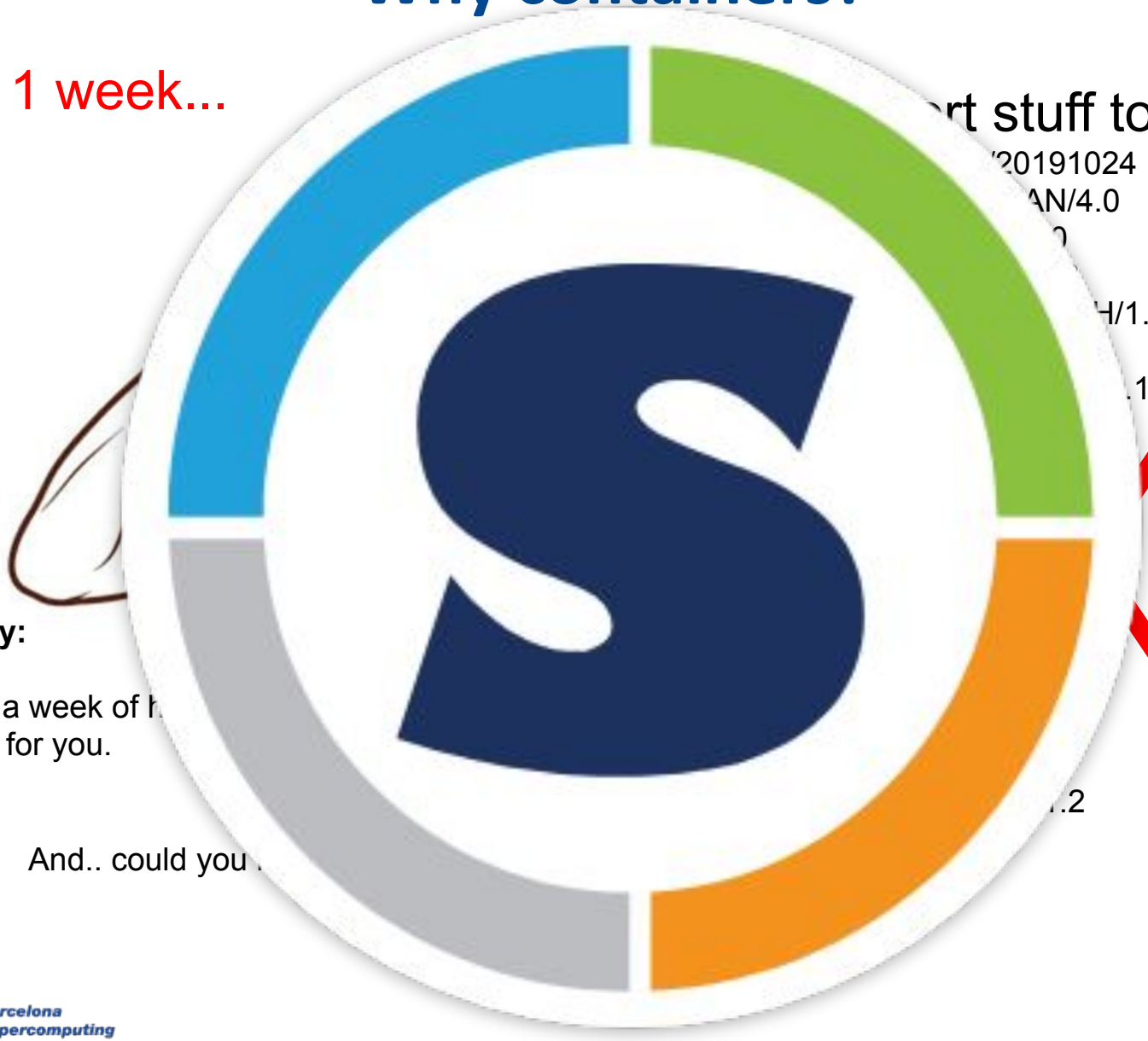
Why containers?

After 1 week...



rt stuff to install:

20191024

AN/4.0

H/1.0

.1

.2

Support guy:

Finally after a week of h
and running for you.

And.. could you

Introducing Singularity

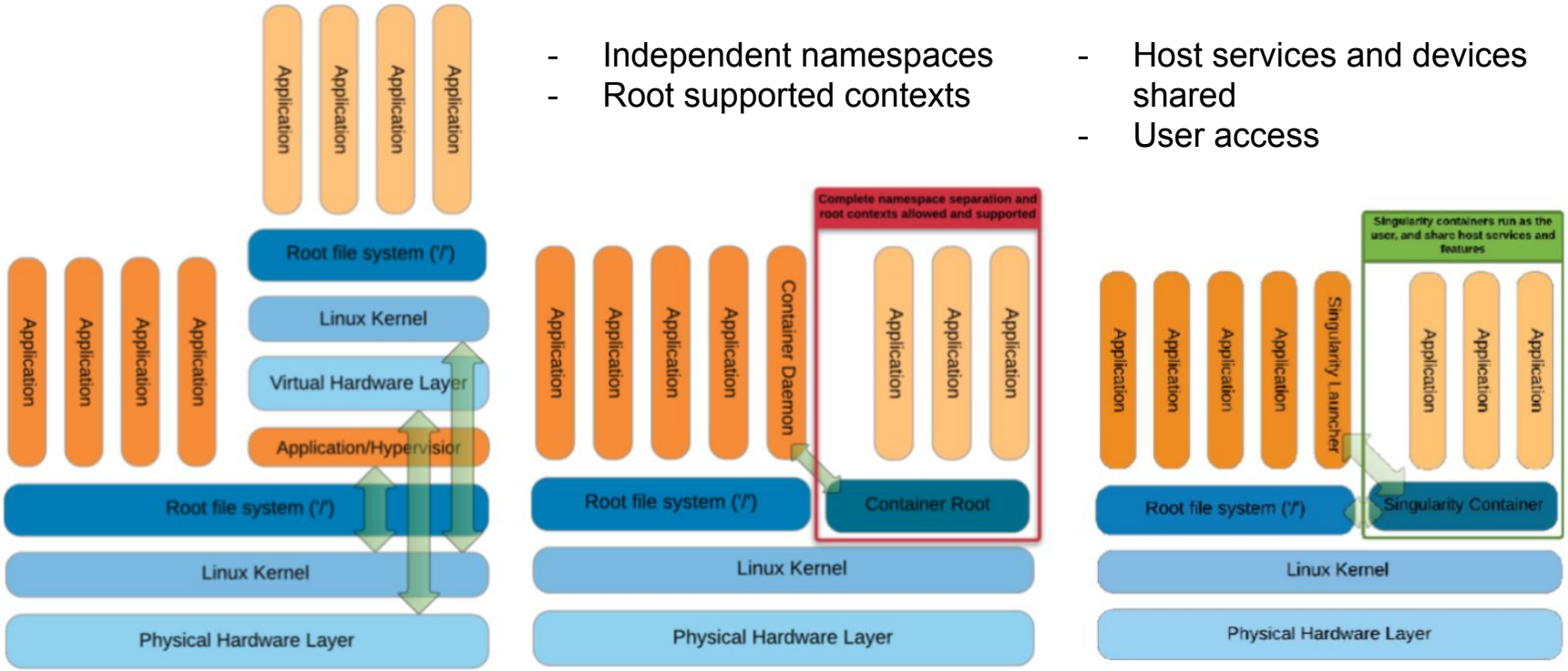
Virtual Machine

Docker

- Independent namespaces
- Root supported contexts

Singularity

- Host services and devices shared
- User access



[From] Arango, Carlos et al. "Performance Evaluation of Container-based Virtualization for High Performance Computing Environments." *ArXiv* abs/1709.10140 (2017): n. pag.

Introducing Singularity

- **Container:**

  File containing all software and dependencies needed to run your applications.

- **Container platform:**

  Run Build Edit + Containers at + Marenostrum4 Nord3 Minotauro ....

- Not ideal : Architecture dependant
  X86 container do not run at Power9

Availability and usage

Availability at BSC

Marenostrum4

x86_64 General purpose cluster. 48 core per Node

$ module load singularity/3.5.2

Availability at BSC

Marenostrum4 **CTE-Power9**

PPC architecture + 4x nvidia volta (v100) GPUs

$ module load singularity/3.4.1

Availability at BSC

Marenostrum4 CTE-Power9 **Nord3**

x86_64 General purpose cluster. 16 core per Node

$ module load SINGULARITY/3.2.0

Availability at BSC

Marenostrum4 CTE-Power9 Nord3 **Minotauro**

x86_64 16 cores per Node + 4 x Nvidia tesla (K80) GPUs

$ module load SINGULARITY/2.5.1

How to...

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How to… Execute

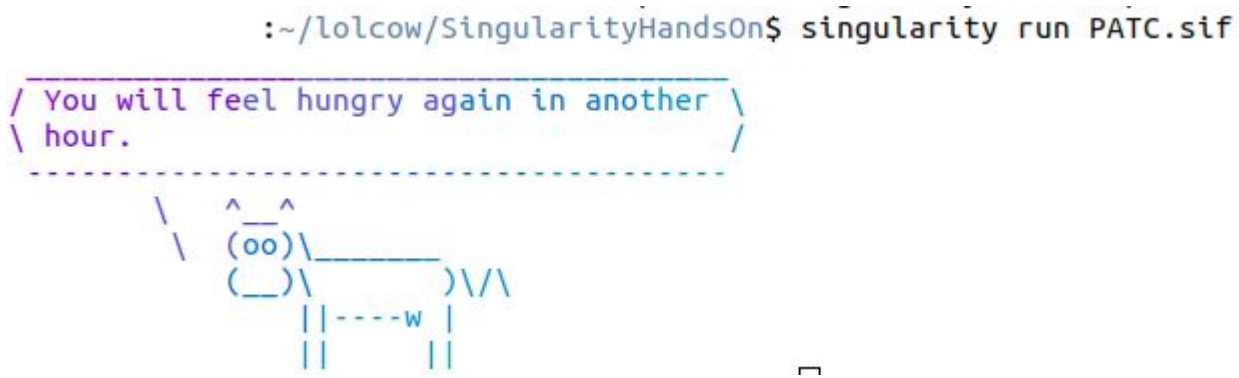
- **Singularity run**

  Runs container default command

  Only one command may be specified by container

- *Usage: (assume our container is called demo.sif)*

  $ singularity run demo.sif



How to… Execute

- **Singularity exec**

  Allows to run any command/software/tool

  It must be available within the container

- *Usage:*

  $ singularity exec demo.sif “command”

```
:~/lolcow/SingularityHandsOn$ singularity exec PATC.sif cowsay "Kill me pls :)"
 _________________
< Kill me pls :) >
 -----------------
        \   ^__^
         \  (oo)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
```

How to… Execute

- **Singularity shell**

  Shell into the container environment

  Inspect/Modify the container interactively

- *Usage:*

  $ singularity shell demo.sif

How to… Execute

- **Singularity shell**

```
             :~/lolcow/SingularityHandsOn$ cat /etc/os-release
NAME="Ubuntu"
VERSION="18.04.4 LTS (Bionic Beaver)"
ID=ubuntu
ID_LIKE=debian
PRETTY_NAME="Ubuntu 18.04.4 LTS"
VERSION_ID="18.04"
HOME_URL="https://www.ubuntu.com/"
SUPPORT_URL="https://help.ubuntu.com/"
BUG_REPORT_URL="https://bugs.launchpad.net/ubuntu/"
PRIVACY_POLICY_URL="https://www.ubuntu.com/legal/terms-and-policies/privacy-policy"
VERSION_CODENAME=bionic
UBUNTU_CODENAME=bionic
             :~/lolcow/SingularityHandsOn$ singularity shell PATC.sif
Singularity PATC.sif:~/lolcow/SingularityHandsOn> cat /etc/os-release
NAME="Ubuntu"
VERSION="14.04.5 LTS, Trusty Tahr"
ID=ubuntu
ID_LIKE=debian
PRETTY_NAME="Ubuntu 14.04.5 LTS"
VERSION_ID="14.04"
HOME_URL="http://www.ubuntu.com/"
SUPPORT_URL="http://help.ubuntu.com/"
BUG_REPORT_URL="http://bugs.launchpad.net/ubuntu/"
Singularity PATC.sif:~/lolcow/SingularityHandsOn>
```

How to… Create

- **Singularity build**

Allows building of images from different sources:

- URI beginning with **library://** to build from the Container Library
- URI beginning with **docker://** to build from Docker Hub
- URI beginning with **shub://** to build from Singularity Hub
- path to a **existing container** on your local machine
- path to a **directory** to build from a sandbox
- path to a Singularity definition file

How to… Create

- **Singularity build (Use cases)**

  Building from dockerhub - immutable container

  $ singularity build test.sif docker://ubuntu

  Building from dockerhub - editable container

  $ singularity build --sandbox test docker://ubuntu

  Editable from immutable and vice versa

  $ singularity build --sandbox test test.sif

How to… Create

- **Singularity build (Use cases)**

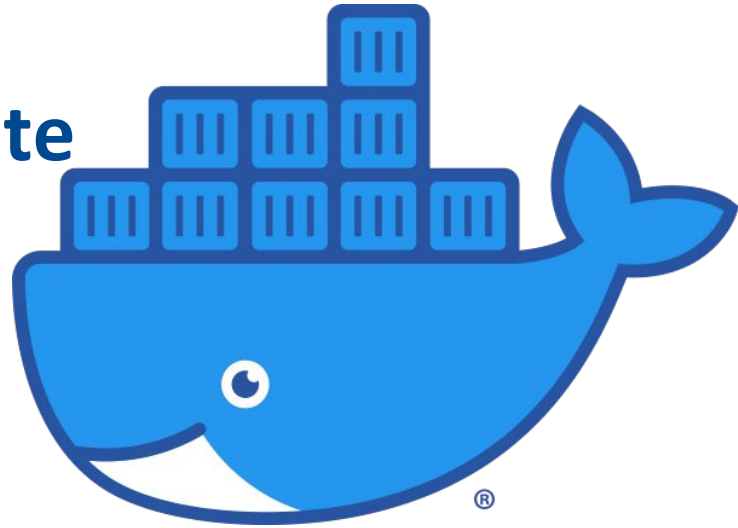
Building from definition file

```
BootStrap: library
From: ubuntu:14.04

%post
    apt-get -y update
    apt-get -y install fortune cowsay lolcat

%environment
    export LC_ALL=C
    export PATH=/usr/games:$PATH

%runscript
    fortune | cowsay | lolcat
```

$ sudo singularity build test.sif DEFINITION_FILE

Warn: Build from scratch may require root privileges

How to… Create



- **Singularity and docker**

  If it is on dockerhub:

  $ singularity build test.sif docker://ubuntu

  Converting local docker images to singularity:

  docker2singularity

  $ docker run quay.io/singularity/docker2singularity

  Info: https://github.com/singularityhub/docker2singularity

How to… Edit

- **Modify container content (--writable)**

  Install new tools, modify config files...

  $ singularity shell --writable test

  Tips:

  Preferably to be run with root permission

  $ sudo singularity shell --writable test

  Container must be in sandbox mode

  $ sudo singularity build --sandbox test test.sif

  $ sudo singularity shell --writable test

How to… Edit

- **Modify container environment**

  Set default environment variables

  $ sudo singularity shell --writable test

  Edit the following file:

```
#!/bin/sh
#Custom environment shell code should follow
```

  $ vi /environment

```
export LC_ALL=C
export PATH=/usr/games:$PATH
```

  We can configure our custom paths, as example:

  export MY_APP_PATH=/apps/myAPP

How to… Bind

- **Bind container paths (--bind/-B)**

  One path

  $ singularity run -B /data:/mnt test.sif

  Several paths “,” as separator

  $ singularity run -B /opt,/data:/mnt test.sif

How to… Bind

- **Bind container paths (--bind/-B)**

  One path

  $ singularity run -B /data:/mnt test.sif

  Several paths “,” as separator

  $ sudo singularity run -B /opt,/data:/mnt test.sif

  Tips:

  Create bind directories inside container

  $ sudo singularity exec --writable test mkdir /apps

  $ singularity exec -B /apps test /apps/myapp

How to… MPI

- **Running MPI applications**

  MPI in singularity is supposed to work seamlessly

  Proved to work:

  $ mpirun -np 4 singularity exec test.sif ./mpiapp

  Don't usually work:

  $ singularity exec test.sif mpirun -np 4 ./mpiapp

How to… MPI

- **Running MPI applications**

MPI in singularity is supposed to work seamlessly

Proved to work:

$ mpirun -np 4 singularity exec test.sif ./mpiapp

Tips:

Sometimes binding host MPI libraries improves compatibility with the site HPC network and libs

*$ srun -B /usr/lib64/:/.singularity.d/libs *
singularity exec ./mpiapp test.sif

How to… MPI

- **Jobscript example (MN4)**

```
#!/bin/bash

#SBATCH --ntasks=96
#SBATCH --time=00:20:00
#SBATCH --job-name=mpi-test
#SBATCH --error=%j.err
#SBATCH --output=%j.out


module purge
module load gcc openmpi/3.1.1 singularity

mpirun singularity exec ~/MPI.sif mpi_hello_world
```

How to… GPUs

- **Running on GPUs (--nv)**

  GPUs supported by default

How to… GPUs

- **Running on GPUs (--nv)**

  GPUs supported by default

  $ singularity exec --nv test.sif ./GPUapp

  Cluster necessary libraries are mounted on the container to be used

Summary

When to use it

Testing

- Unstable releases
- Proof of concept executions
- Punctual data preproces

Reproducibility

- Complex software stacks

When NOT to use it

Production

- Architecture aware software

  GROMACS, NAMD, CPMD...
- Frequent HPC applications

Not available soft?

- Request it to the support team

Detailed info at: https://sylabs.io/docs/

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Thank you!

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