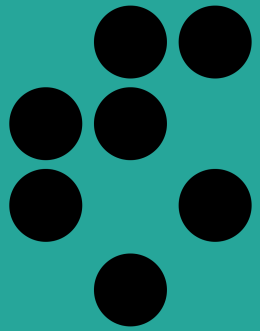

Singularity containers and SLING a tutorial

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Purpose of this tutorial

1. Get to know one of the common pitfalls of research code
2. How to mitigate this issue via dockerization
3. What are Singularity Containers?
4. **Hands-on:** Local builds
5. Cluster execution
6. **Hands-on:** Scaling up with SLING

Part 1

Code replicability and Singularity

The four levels of repositories one finds these days

1. Messy, undocumented code with *no dependency specifications*
2. Code with dependency specifications, *not versioned*
3. Versioned code, dependencies
4. **Code with a replicable environment**

(2) What is Singularity?

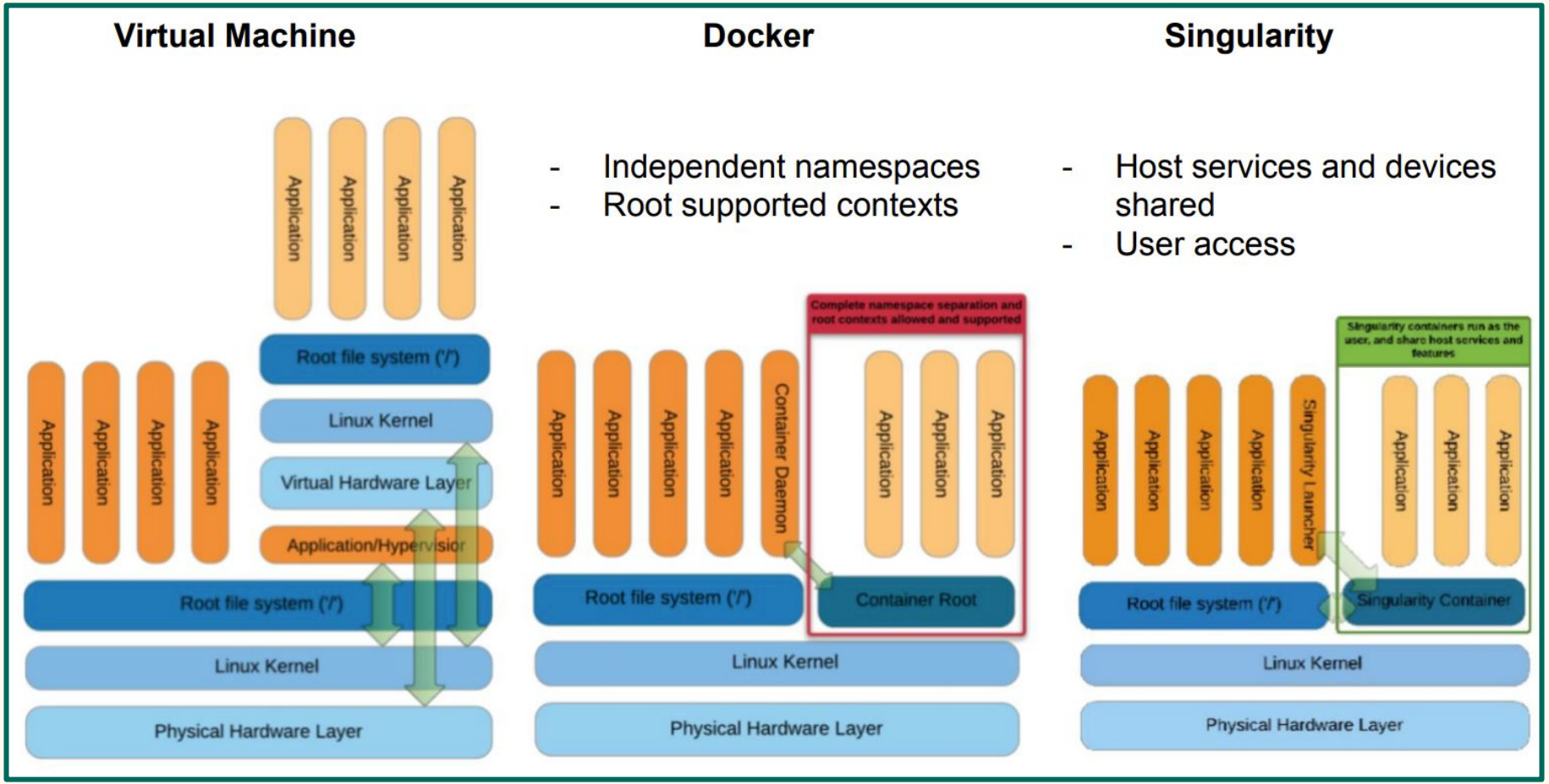
1. It's an environment for **dockerization**. Specifically focused on **scientific** and **HPC** environments.

In other words:

It's the engineering swiss knife suitable for the **fast-paced** (replicable) science**.**

(1) What is Singularity?

1. Assuming you wish to share some code with a colleague
2. What's the minimal effort she/he needs to undergo to run the code?



https://www.bsc.es/support/PATC/2ndDAY/11:00-12:00_Containers-HPC.pdf

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/

Extremely useful for

Deployment on **multiple machines** (HPC).

Quick **replicable** demos and handling dependency problems.

“Oh, this machine is not doing anything, let’s just run this experiment” - type of adventures

Tutorial time - part 1

1. Installation
2. Simple generic replicability case
3. Building containers
4. Using GPUs

Available at: **https://github.com/SkBlaz/singularity-container-tutorial#enter-singularity**

Part 2

Singularity and SLING

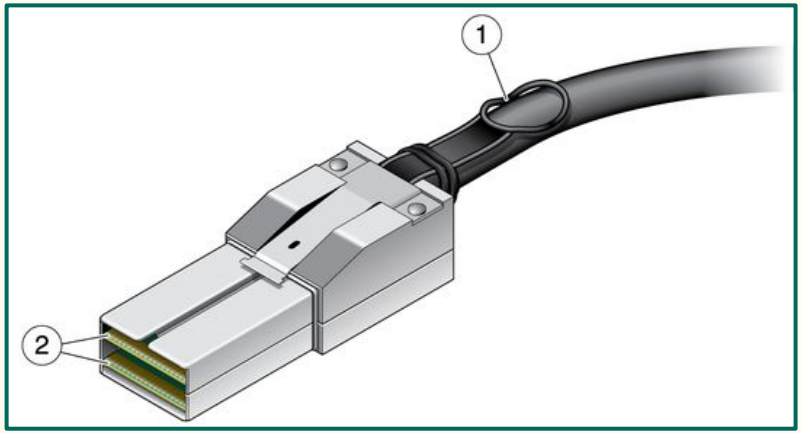
SLING?

Site	CPUs	Load (processes: Grid+local)
ARNES	2048	1845+8
CIPKeBiP	984	144+0
Maister	9872	200+8794
NSC	2880	1424+540
SiGNET	8096	3669+3804
SiGNET	8096	3804+3669
Trdina	536	100+16
UNG	240	232+0
8 sites	*32752*	*11418 + 16831*

Learn more at: http://www.sling.si/sling/en/eurocc/

Why Singularity in this environment?

1. Special support (InfiniBand)
2. No need for customized environments (SysAdmin support for each task)
3. Fast



Source: https://docs.oracle.com/cd/E19654-01/835-0786-02/figures/127163.jpg

Key idea

1. Build the Singularity image locally, copy it to dCache
2. Each job sees the image and executes it (singularity exec [jobStuff])
3. The dCache version of the image can be updated by the user

If it works locally, it will **most likely** work on the grid too.

Tutorial time - part 2

1. Let’s build an image
2. Test it locally
3. Create XRSL job specification
4. Execute, retrieve and inspect the result

Available at:

https://github.com/SkBlaz/singularity-container-tutorial/blob/master/gpu.md
https://github.com/SkBlaz/singularity-container-tutorial/blob/master/optimization.md