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Containers for Scientific Computing and Gateways: Introduction to Containers

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SGCI Coding Institute 2021 (Virtual Edition) - June 23rd, 2020

Outline of events

Morning

- Introduction to container technologies (You are here!)
- Environment introduction
- Docker container build
- Singularity Overview

Afternoon

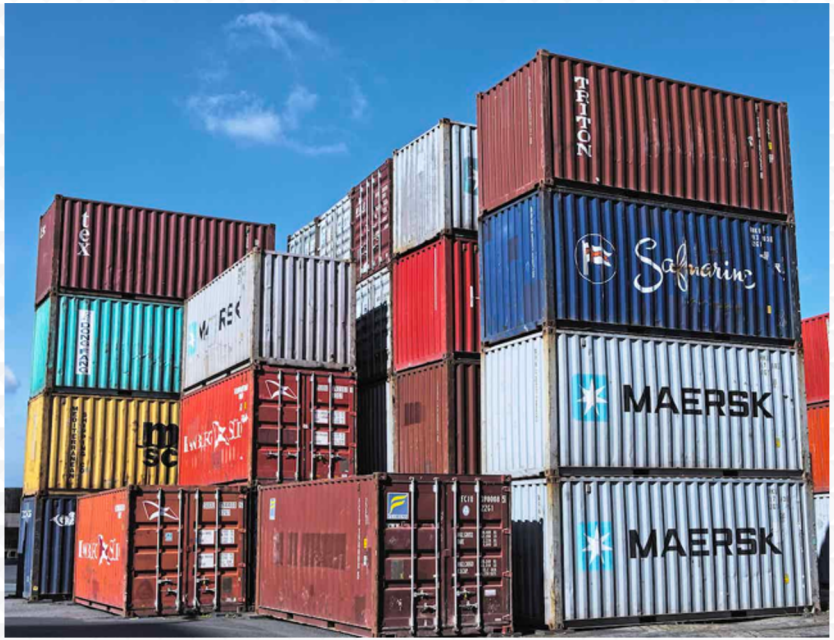
- Docker to Singularity Conversion
- 2nd exercise – building and running a scientific workload with Singularity
- Next steps and best Practices

Introduction

…or how I learned to stop worrying and love ~~the bomb~~ containers…

What are containers?

- Born from a simple idea (chroot)
- Evolved over time into various forms of container services (e.g. BSD Jails, Solaris Zones)
- LXC (LinuX Containers) was released in 2008
- Docker came on the scene in 2013
- Other technologies evolved – Shifter, CharlieCloud, Singularity
- Upping the ante – Docker Compose and container orchestration

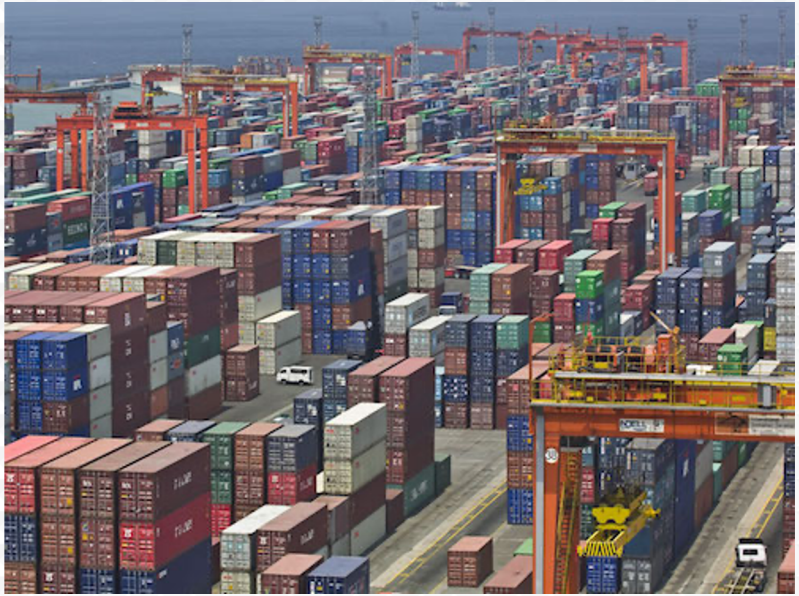


…and why would I want to use one

- Consistency
- Portability
- Ability to package and run on HPC
- “Just in time” instantiation and updating on the fly
- Creating microservices
- Run legacy code/obsolete OSes
- Reproducible Science!

Why bother with containers on a gateway?

- Consistency
- Reproducibility
- Easily integrate new applications (especially legacy applications)
- More easily manage many applications that may have complex requirements
- Portability of applications between gateways and individuals and HPC



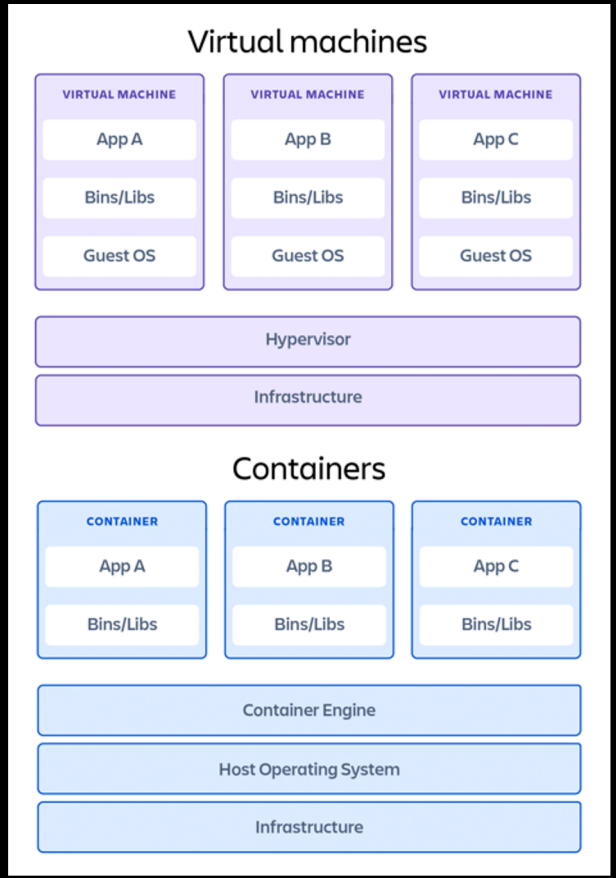
Containers vs. Virtual Machines

VMs:

- VMs are fully contained – everything you need is there
- VMs are independent of the host operating system
- All OS resources and tools are available

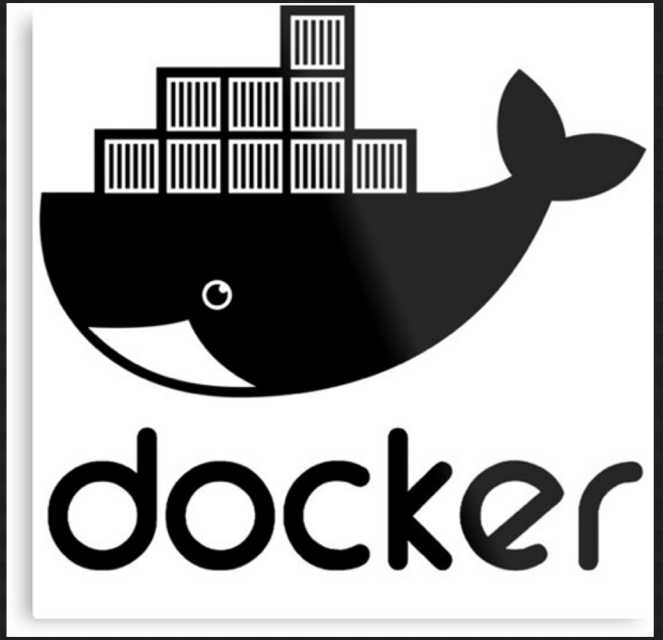
Containers:

- Compact – minimal OS parts to run, rely on host
- Compact nature makes them more portable
- Robust ecosystem – many pre-made containers available



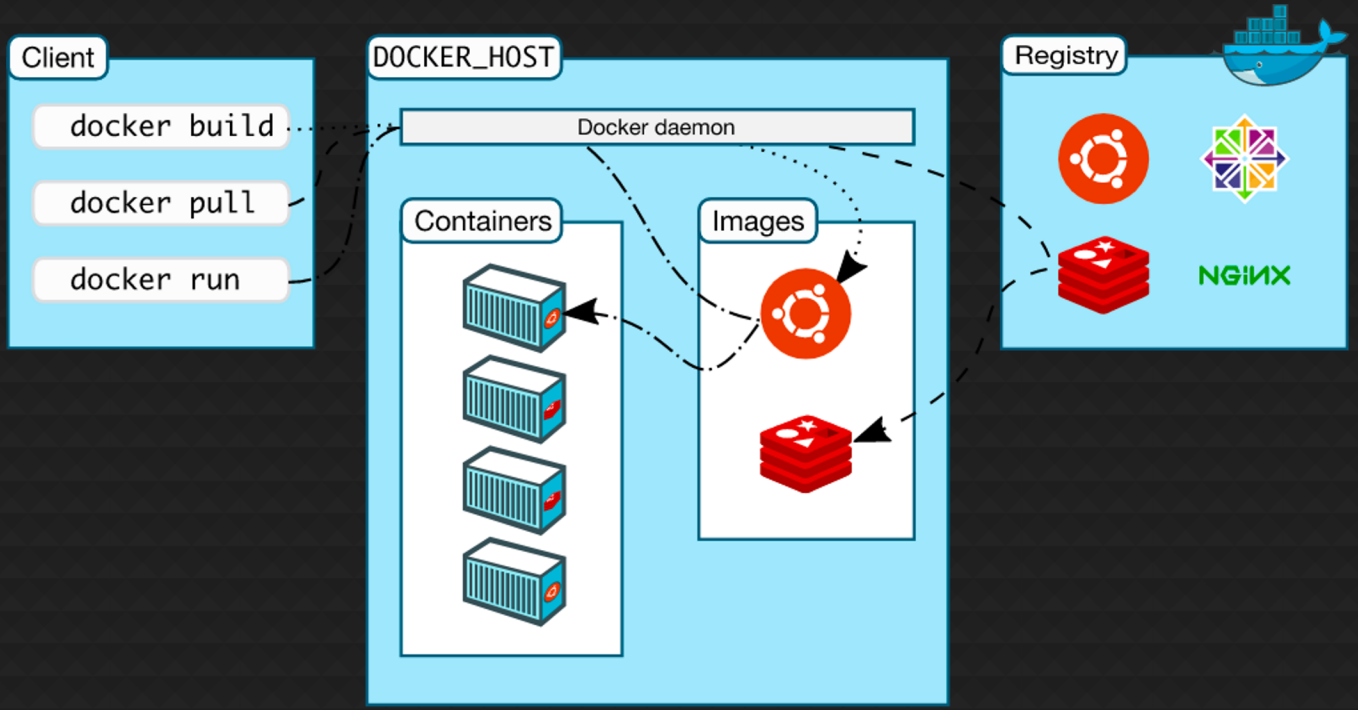
What is Docker

- Docker is a container technology tool to create, deploy, and run applications
- Low overhead, uses the running kernel
- Lets a creator package all of the software needed to run an application in a reasonably compact and run it on any other Docker-capable machine**
- Uses a client (*docker)* to talk over a REST API to the docker daemon (*dockerd)* either locally or remotely
- Has a large public repository of objects (containers, images, etc) at DockerHub -- and other repos are available
- It allows users to develop applications, package (ship) them into containers which can then be deployed anywhere

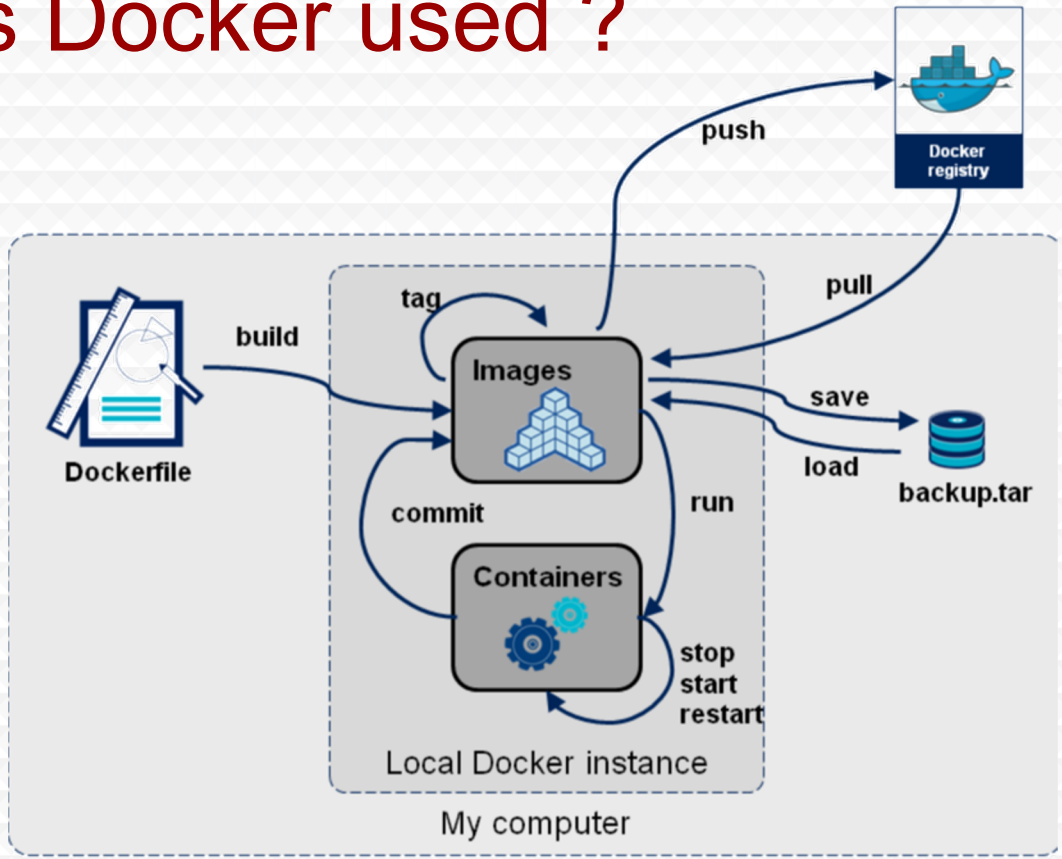


** Even Windows and Mac!

Docker in action…the big picture:



How is Docker used ?



What is Singularity?

- YACP (Yet another container platform)
- Why are we talking about Singularity at all?
- How is it different from Docker?
- How does this all come together?
- Singularity can use Singularity containers from a registry or Docker containers, even pulling from a Docker registry like Docker Hub

Moving into the first exercise…

Simple container creation!

Questions?