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Deep Dive into Constructing Containers for Scientific Computing and Gateways: Introduction to Containers

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Outline for the day's events…

Part I

- *Introduction to container technologies (You are here!)*
- *Simple container creation*
- *Docker to Singularity Conversion*
- *First exercise – building and running a scientific workload with Docker and Singularity*

Part II

- *Complex container build (Matlab Compiler Runtime Environment)*
- *Next steps and best practices*
- *Containers for gateways (including an exercise)*
- *Wrap up*

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!*

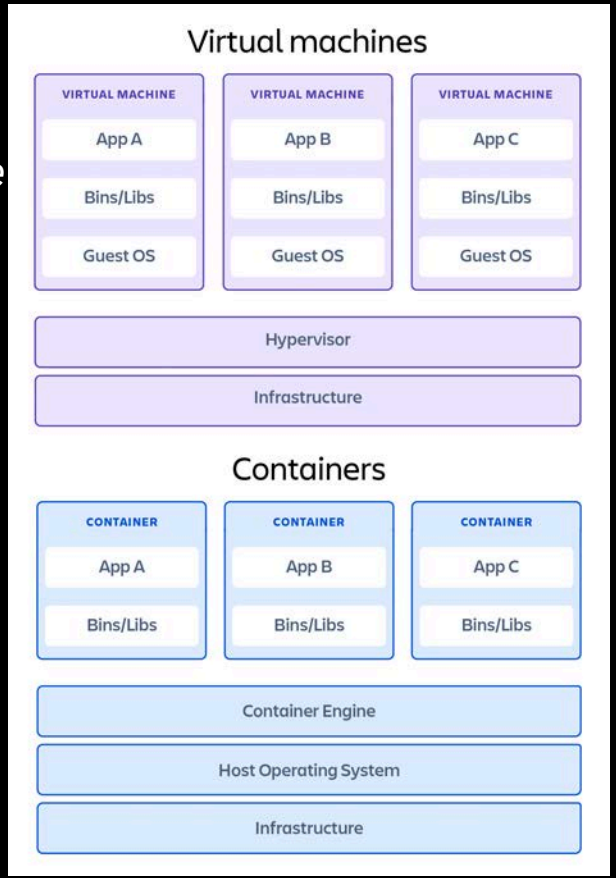
Containers vs. Virtual Machines

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*

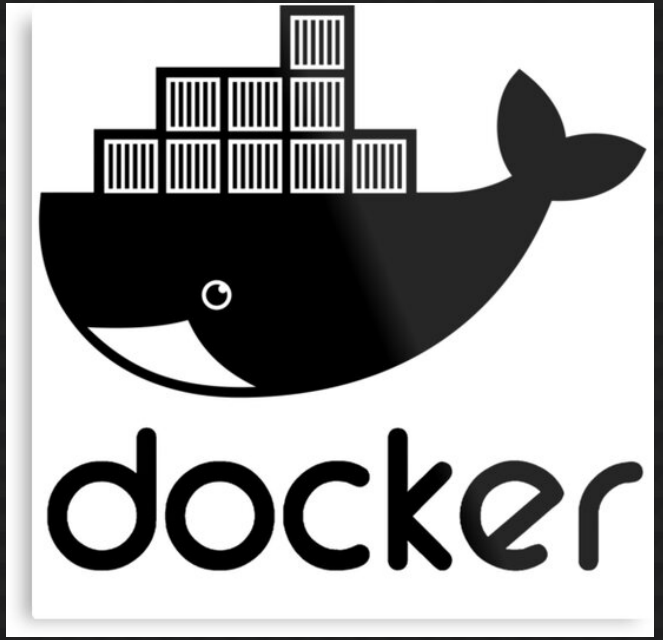
Containers:

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



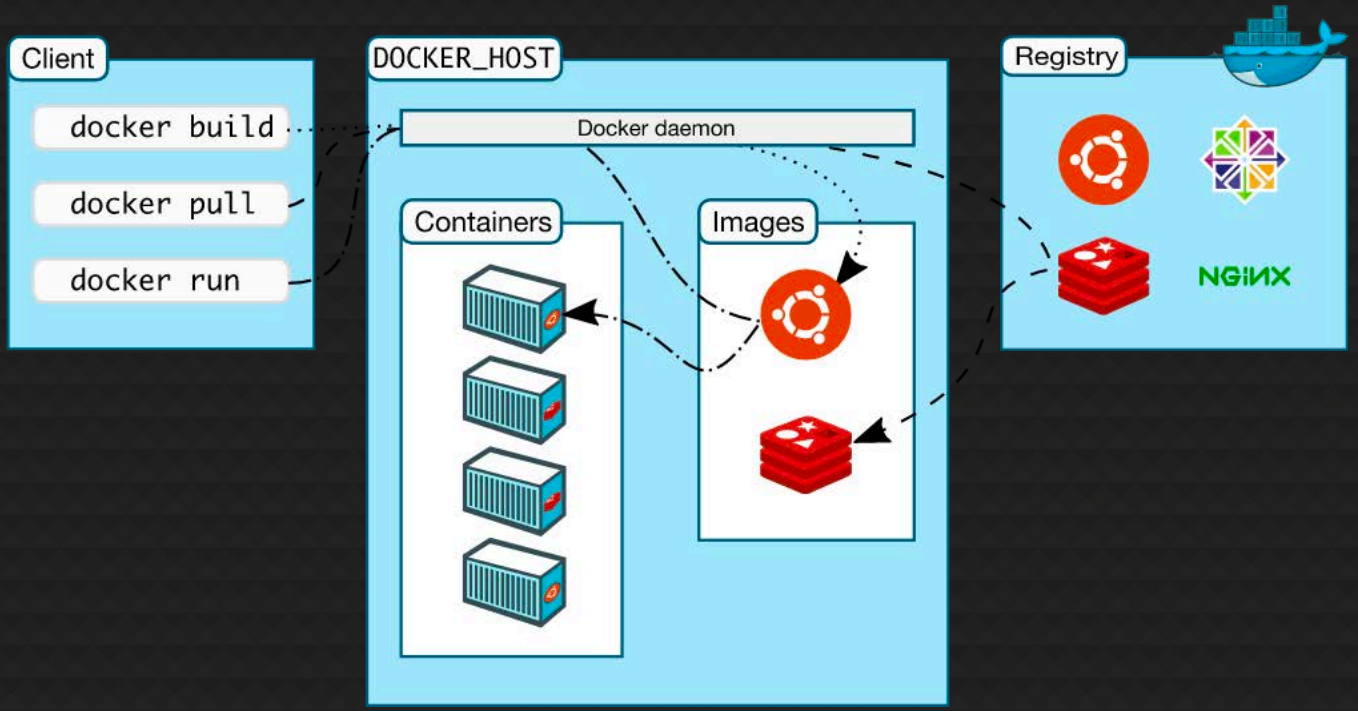
What is Docker

- *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*

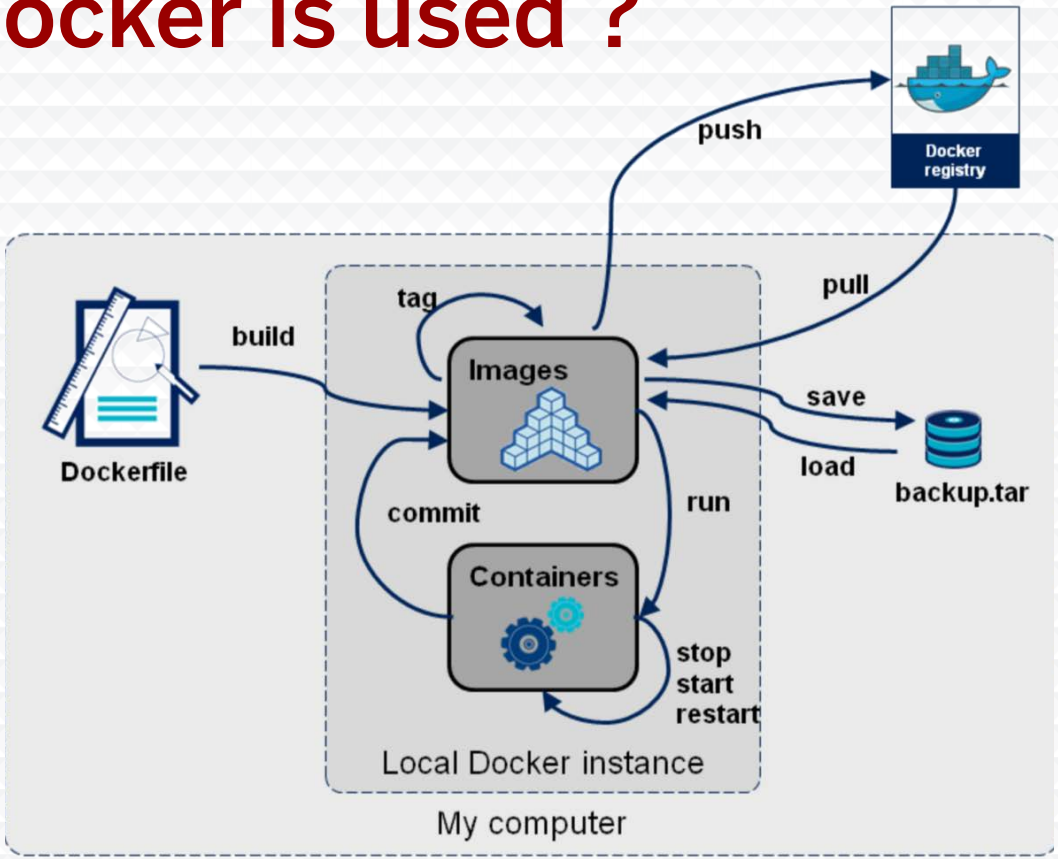


** Even Windows and Mac!

Docker in action...the big picture:



How Docker is 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 the Singularity Hub or Docker containers, even pulling from a Docker registry like Docker Hub*

Moving into the first exercise...

Simple container creation!

Questions?