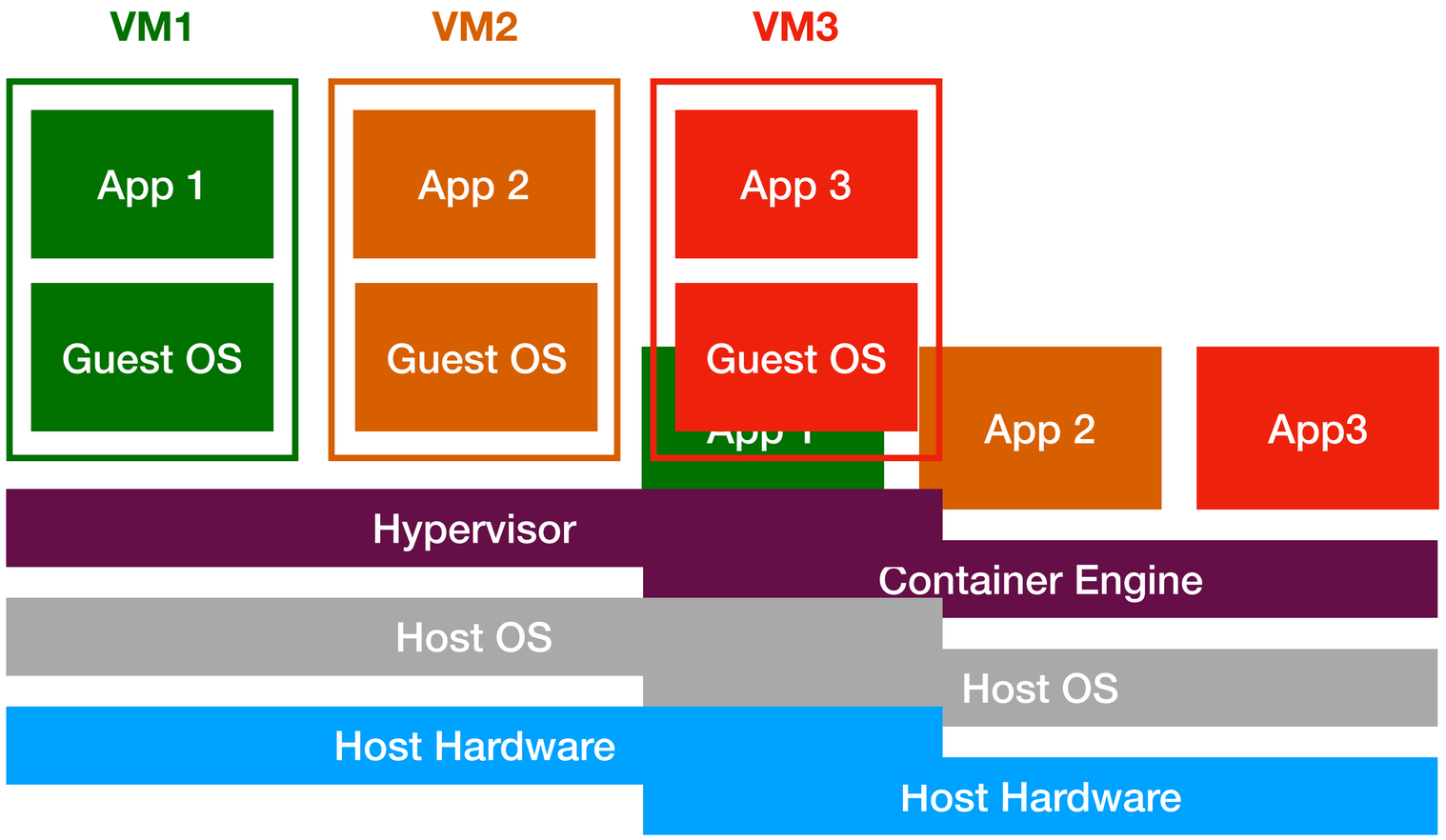
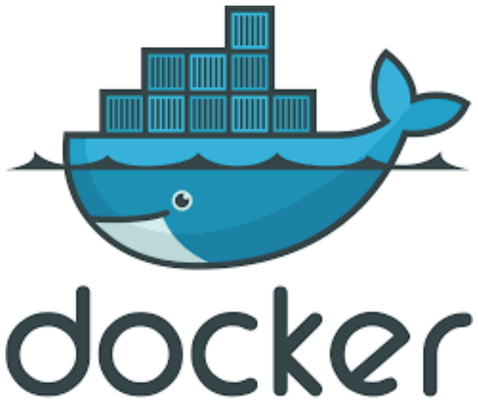
Containerisation


VM1
VM2
VM3
App 1
App 2
App 3
Guest OS
Guest OS
Guest OS
App 2
App3
Hypervisor
Container Engine
Host OS
Host OS
Host Hardware
Host Hardware

Why use a container

- Takes care of dependencies
- Portability of workflow
- Enhance reproducibility
- Help to move between middleware



VS

- **Docker is the industry standard for resource management**
- **Possible for user to escalate privileges to root**
- **Changes made in the container are persistent by default**
- **More mature**

- **Singularity developed specifically with HPC in mind**
- **Does not allow users to escalate to root**
- **Images are read only**
- **Singularity can use docker images**
- **More lightweight**

Singularity workflow

Build Environment → **Production Environment**

- Somewhere you have root privileges eg. Laptop
- Used to develop pipeline/ workflow
- Relevant commands:
  - Sudo singularity build ….

- Where the container will be run eg. GridPP
- User will not generally have root privileges
- Relevant commands:
  - Singularity pull …
  - Singularity run …
  - Singularity exec …

```
BootStrap: yum
OSVersion: 7
MirrorURL: http://mirror.centos.org/centos-%{OSVERSION}/%{OSVERSION}/os/$basearch/
Include: yum wget
```

Header

```
%post
yum -y update
yum -y install yum-utils
yum -y groupinstall development
yum -y install https://centos7.iuscommunity.org/ius-release.rpm
yum -y localinstall --nogpgcheck https://download1.rpmfusion.org/free/el/rpmfusion-free-release-7.noarch.rpm https://download1.rpmfusion.org/nonfree/
el/rpmfusion-nonfree-release-7.noarch.rpm
yum -y install build-essential curl git man vim autoconf libtool debootstrap squashfs-tools
yum -y install python2-pip
yum -y install python-devel
yum -y install fftw fftw-devel
yum -y install libpng libpng-devel
yum -y install cfitsio cfitsio-devel
yum -y install pgplot pgplot-devel
yum -y install qt qt-devel
yum -y install java java-devel
yum -y install libxml2 libxml2-devel
wget http://www.pulsarastronomy.net/psrsoft/psrsoft.tar.gz
tar -xzf psrsoft.tar.gz
cd psrsoft/config
cp profile.example profile
cd ..
cd ..
export PATH=/psrsoft/bin:$PATH
echo 'y' | psrsoft sixproc
echo 'y' | psrsoft psrchive
echo 'y' | psrsoft dspsr

%environment
export PATH=/psrsoft/bin:$PATH
export PSRSOFT_USR=/psrsoft/usr
for env in $PSRSOFT_USR/var/psrsoft/env/bash/* ; do . $env ; done
export PATH=$PSRSOFT_USR/bin:$PATH

%runscript
```

Sections

Header

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- shub (images hosted on Singularity Hub)
- docker (images hosted on Docker Hub)
- localimage (images saved on your machine)
- yum (yum based systems such as CentOS and Scientific Linux)
- debootstrap (apt based systems such as Debian and Ubuntu)
- arch (Arch Linux)
- busybox (BusyBox)
- zypper (zypper based systems such as Suse and OpenSuse)

Sections: %Post

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export PATH=/psrsoft/bin:$PATH
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Sections

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%environment
export PATH=/psrsoft/bin:$PATH
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```

```
%runscript
echo "Starting Tensorflow virtual environment"
source /tensorflow/bin/activate
echo "Arguments received: $*"
exec python "$@"
```

Singularity Commands

- sudo singularity build <image name> <recipe file>
- singularity exec <image> <command>
- singularity run <image> <optional arguments>
- singularity run —nv <image> <optional arguments>
- singularity pull <image in shub>

Example

- shub://TMCantwell/pulsar_timing_containers:pulsar.v1.1
- singularity pull --name pulsar.v1.1.simg shub://TMCantwell/pulsar_timing_containers:pulsar.v1.1
- git clone https://github.com/TMCantwell/pulsar_timing_containers.git
- export SINGULARITY_BINDPATH=$PWD:/mnt
- singularity exec pulsar.v1.1.simg pam -FT -e FT -E /mnt/J1911+37_t2.par /mnt/GBNCC_J1911+37_period.fits
- singularity exec pulsar.v1.1.simg pat -s /mnt/1911+37_820MHz.std -f tempo2 /mnt/GBNCC_J1911+37_period.FT > ToA.txt

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