



New SBNB cluster

Containers & Cluster Rules



Structural Bioinformatics
& Network Biology Group

Why new cluster & Expectations

- ▶ Not flexible
 - ▶ New software always needs to be installed in pac2
 - Users do not have freedom to install what they need
 - ▶ Cluster OS different from desktop computers
-
- ▶ Easy to adapt our needs
 - ▶ Users can install anything they need
 - ▶ OS can be changed easily



Containers

- ▶ Containers offer:
 - Portability
 - Reproducibility
 - Light
 - Fast boot
- ▶ Most popular container: Docker
 - Runs as root
 - Not suitable for HPC
- ▶ HPC Container: Singularity
 - Permissions outside container are the same than inside
 - Designed with performance in mind for HPC applications
 - Supports conversion of Docker images to singularity images



Singularity Workflows

1. Build your own image
2. Use existing image
3. Convert Docker image

Install Singularity

1. <http://singularity.lbl.gov/install-linux>
2. `sudo apt-get install debootstrap`
3. `sudo vi /usr/local/etc/singularity/singularity.conf`
 - a. Change mount home = no to yes
 - b. Add these lines to bind path section:
bind path = /aloy/home
bind path = /aloy/data
bind path = /aloy/scratch
bind path = /home



Build your own image

1. Create image

```
singularity create --size 4000 ubuntu.img
```

2. Bootstrap image

a. Create singularity definition file

b. `sudo singularity bootstrap ubuntu.img <def file>.def`

Singularity definition file

```
Bootstrap: docker
From: ubuntu:latest
```

```
%runscript
```

```
#Pass all args from "singularity run" to python3 interpreter
exec python3 "$@"
```

```
%post
```

```
# Enables acces
mkdir /scratch /data
# Update apt-get's
apt-get -y update
# Install Python3,Numpy, Node and GCC compiler
apt-get -y install python3 python3-numpy python3-nose gcc vim
```

```
%test
```

```
#Run numpy tests
python3 -c "import numpy as np; np.test()"
```

Singularity real case (1)

```
BootStrap: debootstrap
OSVersion: xenial
MirrorURL: http://archive.ubuntu.com/ubuntu/

%post
sed -i 's/main/main restricted universe/g' /etc/apt/sources.list
apt-get update

# Install R, misc. utilities:
apt-get install -y libopenblas-dev r-base-core libcurl4-openssl-dev
openssh-client openssh-server libssh-dev wget vim git nano git cmake
gfortran g++ curl wget python autoconf bzip2 libtool libtool-bin fftw3
software-properties-common python-software-properties libxml2-dev
apt-get clean
ln -sf bash /bin/sh

#Add repo to install R 3.4
add-apt-repository ppa:marutter/rutter
apt-get update
apt-get upgrade -y

mkdir /aloy
mkdir /aloy/home
mkdir /aloy/data
mkdir /aloy/scratch
R --slave -e "source('http://bioconductor.org/biocLite.R'); \
    biocLite('casper')"
```


Singularity real case (2)

```
BootStrap: debootstrap
OSVersion: xenial
MirrorURL: http://archive.ubuntu.com/ubuntu/

%post

# Install R, misc. utilities:
apt-get install -y wget vim git nano git cmake gfortran g++ curl wget python
autoconf bzip2 libtool libtool-bin fftw3 software-properties-common
python-software-properties
apt-get clean
ln -sf bash /bin/sh

wget https://bootstrap.pypa.io/get-pip.py
python get-pip.py
ln -s /usr/local/bin/pip /usr/bin/pip
wget https://repo.continuum.io/miniconda/Miniconda2-latest-Linux-x86\_64.sh
bash Miniconda2-latest-Linux-x86_64.sh

mkdir /aloy
mkdir /aloy/home
mkdir /aloy/data
mkdir /aloy/scratch
```



How to use your container

To modify the container:

1. `sudo singularity shell --writable <image>`
 - Install whatever you want
2. `sudo singularity exec --writable <image> <comand>`

To run scripts:

1. `singularity exec <image> <comand>`
2. `singularity run`

How to use the container in the cluster

```
#!/bin/bash
#
#

# Options for qsub
#$ -S /bin/bash
#$ -r yes
#$ -N wrap_sing
#$ -j yes
#$ -cwd
# End of qsub options

# Loads default environment configuration
if [[ -f $HOME/.bashrc ]]
then
    source $HOME/.bashrc
fi

# Runs the command
singularity exec /aloy/home/tjuan/singularity_img/ubuntu-r.img Rscript wrapKnow.R
```

Containers - Sum up

1. Install singularity in your desktop
2. Create the image that you need
3. Install all you need in that image
4. Test it in your computer
5. Copy it to /aloy/home/....
6. Use it in the cluster

Remember you need to be root in order to bootstrap your image and modify it (2 & 3). That means you can only do that in your own computer and save it in your /home/username



New Cluster

- ▶ The new cluster will contain these resources:
 - 7 nodes (1x44(76), 6x32) -> 268 cores
 - 6 nodes with 64G RAM & 1 node with 256G RAM
- ▶ The cluster head is called: pac-one-head
- ▶ No more pac3 software installed. All you need must be in your container.

New Cluster Rules

1. The cluster is a shared resource. You break it, nobody uses it.
2. You are responsible to control how many processors and how much memory your jobs take. How??

```
#$ -l mem_free=2G,h_vmem=2.5G
```

```
#$ -pe threaded 4
```

A decorative network diagram in the top left corner, featuring a central node with several smaller nodes connected to it, and other nodes further out, all in a light blue color.

Conclusions

New cluster, new life!!

Everybody happy!!!