Help yourself on a remote server

bioinformatics@age.mpg.de

https://mpg-age-bioinformatics.github.io

Outline

- Connecting to a remote server
- Copying files to/from a remote server
- The modules system
- Shifter/Docker for HPC
- Installing software without `su` access
- Installing R packages
- Installing python packages
- Installing perl packages
- SLURM

Connecting to a remote server

Connecting to a remote server over a Secure Shell (ssh) – ssh username@remote.adress :

```
ssh JBoucas@amalia.age.mpg.de
```

With X forwarding:

```
ssh –X JBoucas@amalia.age.mpg.de
```

Download rc files for your user into your home folder in amalia

```
cd

wget https://raw.githubusercontent.com/mpg-age-
bioinformatics/cluster_first_steps/master/.bashrc

wget https://raw.githubusercontent.com/mpg-age-
bioinformatics/cluster_first_steps/master/.bash_profile

source ~/.bash_profile
source ~/.bashrc

# remember that next time you login this files will be automatically
sourced
```

Copying files to/from a remote server

Copying files over ssh to your home folder on a remote server:

```
scp file.txt UName@ServerAddress:~/
```

Copying files over ssh from your home folder on a remote server:

```
scp UName@ServerAddress:~/file.txt .
```

Both `scp` will only allow you to copy files (not directories) unless you use the `-r` argument for `recursively`. For speed use `-o Cipher=arcfour`.

rsync to a remote server

```
rsync -rtvh -e "ssh -c arcfour" source_folder \
UName@ServerAddress:destination
```

Not all servers will have the less costly cipher arcfour encryption algorithm and therefore you can remove the whole `-e "ssh -c arcfour"` block.

The modules system

A centralized software system.

The modules system **loads software** (version of choice) and changes **environment variables** (eg. LD_LIBRARY_PATH)

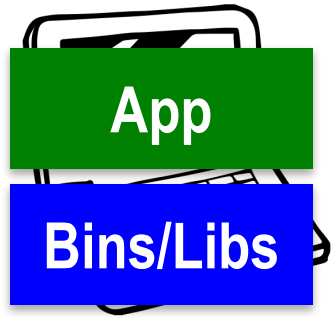
```
module avail             # shows available modules
module whatis SAMtools   # shows a description of the SAMtools module
module show SAMtools     # shows environment changes for SAMtools
module load SAMtools     # loads SAMtools
module list              # lists all loaded modules
module unload SAMtools   # unloads the SAMtools module
module purge             # unloads all loaded modules
```

more on http://modules.sourceforge.net

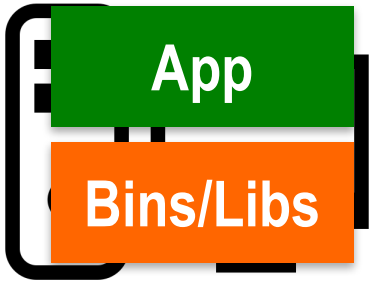
Shifter/Docker for HPC

Mobile, ready to go, reproducible science!

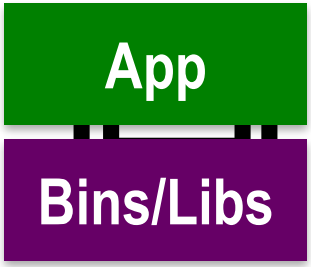
Computers are not all the same



Created by Mike O'Brien
from Noun Project



Created by Mister Pixel
from Noun Project

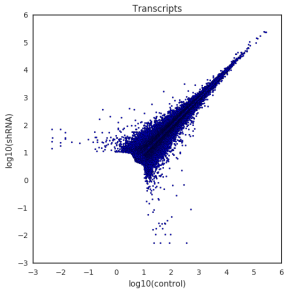


Created by factor[e] design initiative
from Noun Project

The same apparent code can give different results

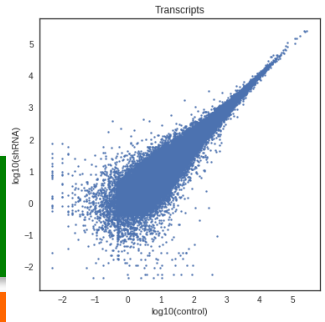
App

Bins/Libs



App

Bins/Libs

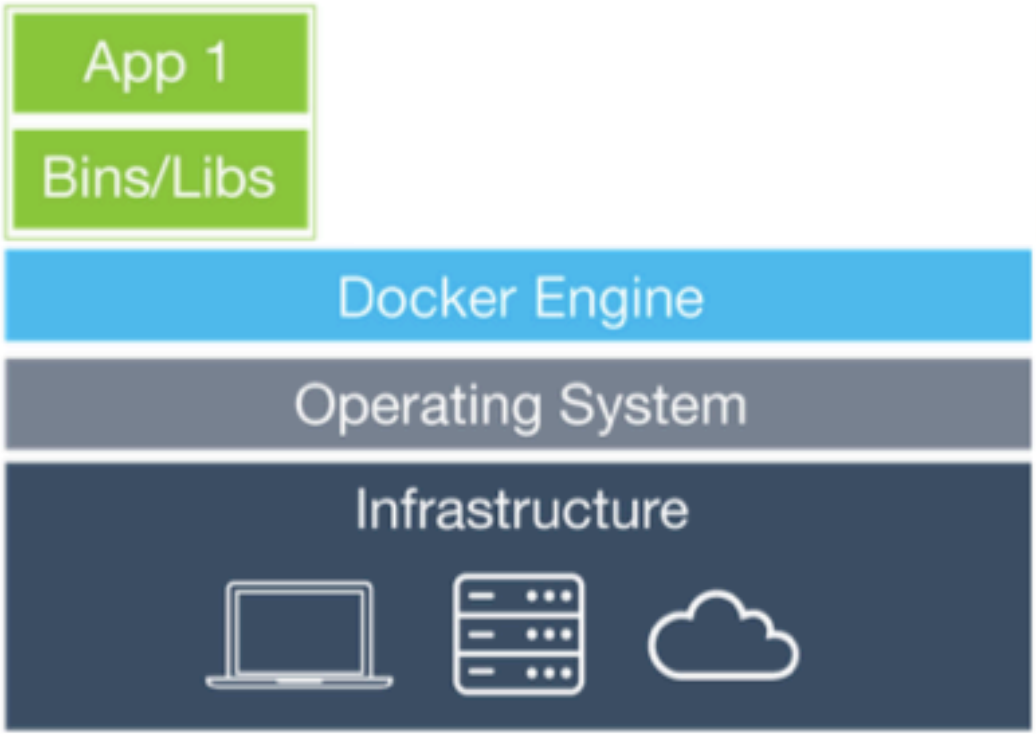


App

Bins/Libs

Different version of dependency in bin/
== different input in one step
== code breaks

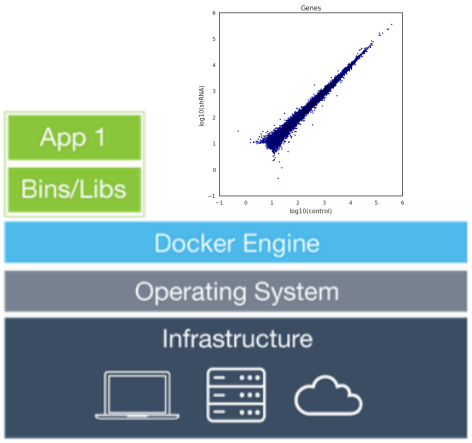
Containers



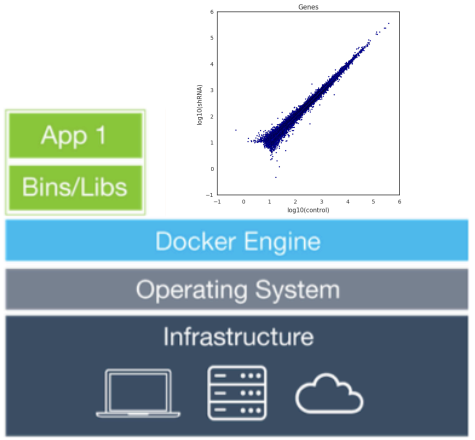
Containers

https://blog.logentries.com/2015/07/an-all-inclusive-log-monitoring-container-for-docker/

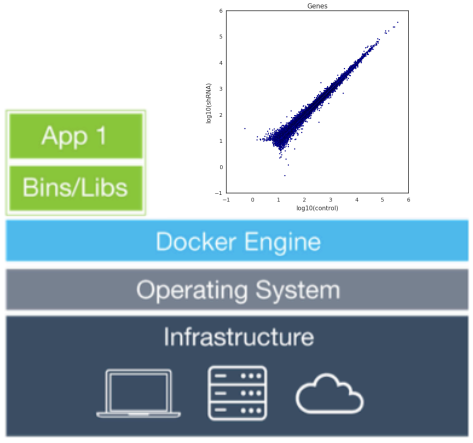
Containers are independent of their host



Containers

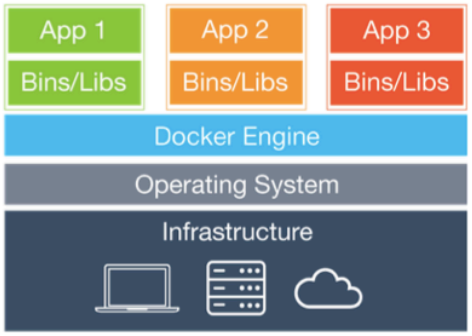


Containers

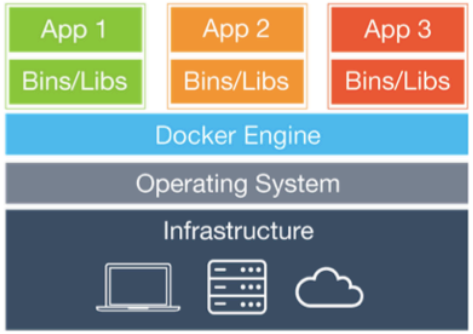


Containers

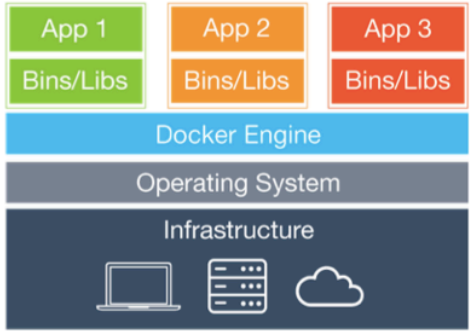
Multiple environments per machine



Containers



Containers



Containers

Shifter/Docker for HPC

```
# load respective module
module load shifter

# list available images
shifterls

# get an interactive shell on ubuntu and check you
# are in the intended image
shifter --image=ubuntu:15.10 bash -login
cat /etc/lsb-release

# use the Bioinformatics image
shifter --image=mpgagebioinformatics/bioinformatics_software:v1.0.0

# run a script inside an image
shifter --image=<provider>/<image_name>:<tag> /path/to/script
```

Working interactively on the mpi age bioinformatics software image

```
module load shifter # load respective module

shifterls # list available images

which R # check if you have R

# login to our software image
shifter --image=mpgagebioinformatics/bioinformatics_software:v1.0.1

pwd

module avail

module load rlang

which R
```

Running a script inside the mpi age bioinformatics software image

Example `~/test.shifter.sh`:

```
#!/bin/bash
source ~/.bashrc

module load rlang python

which python

python << EOF
print "This is python"
EOF

which R

Rscript –e "print('This is R')"
```

Running the script:

```
chmod +x test.shifter.sh
shifter \
    --image=mpgagebioinformatics/bioinformatics_software:v1.0.1 \
    ./test.sh
```

Shifter/Docker for HPC

More infos on

shifter,

docker (eg. for your own laptop),

singularity (running @ draco.mpcdf.mpg.de),

and creation of images on

http://bioinformatics.age.mpg.de/#callout > Jupyter on Docker

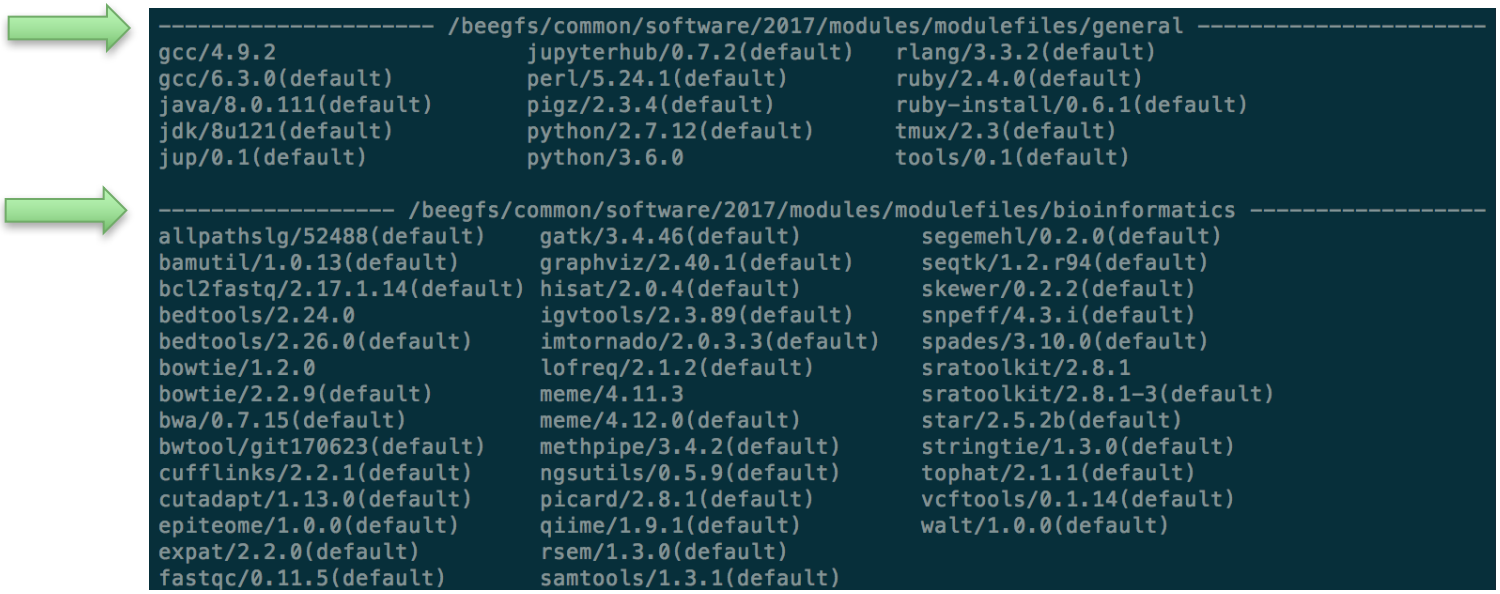
https://github.com/mpg-age-bioinformatics/cluster_first_steps#shifter

More infos on our software image and how to run it on your laptop:

https://github.com/mpg-age-bioinformatics/software_docker#software-container

module avail

Example `module avail` output.



```
---------------------- /beegfs/common/software/2017/modules/modulefiles/general -----------------------
gcc/4.9.2                    jupyterhub/0.7.2(default)    rlang/3.3.2(default)
gcc/6.3.0(default)           perl/5.24.1(default)         ruby/2.4.0(default)
java/8.0.111(default)        pigz/2.3.4(default)          ruby-install/0.6.1(default)
jdk/8u121(default)           python/2.7.12(default)       tmux/2.3(default)
jup/0.1(default)             python/3.6.0                 tools/0.1(default)

------------------- /beegfs/common/software/2017/modules/modulefiles/bioinformatics -------------------
allpathslg/52488(default)    gatk/3.4.46(default)          segemehl/0.2.0(default)
bamutil/1.0.13(default)      graphviz/2.40.1(default)      seqtk/1.2.r94(default)
bcl2fastq/2.17.1.14(default) hisat/2.0.4(default)          skewer/0.2.2(default)
bedtools/2.24.0              igvtools/2.3.89(default)      snpeff/4.3.i(default)
bedtools/2.26.0(default)     imtornado/2.0.3.3(default)    spades/3.10.0(default)
bowtie/1.2.0                 lofreq/2.1.2(default)         sratoolkit/2.8.1
bowtie/2.2.9(default)        meme/4.11.3                   sratoolkit/2.8.1-3(default)
bwa/0.7.15(default)          meme/4.12.0(default)          star/2.5.2b(default)
bwtool/git170623(default)    methpipe/3.4.2(default)       stringtie/1.3.0(default)
cufflinks/2.2.1(default)     ngsutils/0.5.9(default)       tophat/2.1.1(default)
cutadapt/1.13.0(default)     picard/2.8.1(default)         vcftools/0.1.14(default)
epiteome/1.0.0(default)      qiime/1.9.1(default)          walt/1.0.0(default)
expat/2.2.0(default)         rsem/1.3.0(default)
fastqc/0.11.5(default)       samtools/1.3.1(default)
```

Notice the 2 arrows and the two distinct blocks of software being shown.

The distinct blocks are generated by the different paths kept on the `MODULEPATH` variable set like this:

```
export MODULEPATH=/beegfs/common/software/2017/modules/modulefiles\
/general:/beegfs/common/software/2017/modules/modulefiles/bioinformatics
```

The modules system

`module avail` simply lists the contents of the `MODULEPATH` variable.

```
amaliax:~$ tree -L 2 /beegfs/common/software/2017/modules/modulefiles/general
/beegfs/common/software/2017/modules/modulefiles/general
├── gcc
│   ├── 4.9.2
│   └── 6.3.0
├── java
│   └── 8.0.111
├── jdk
│   └── 8u121
├── jup
│   └── 0.1
├── jupyterhub
│   └── 0.7.2
├── perl
│   └── 5.24.1
├── pigz
│   └── 2.3.4
├── python
│   ├── 2.7.12
│   └── 3.6.0
├── rlang
│   └── 3.3.2
├── ruby
│   └── 2.4.0
├── ruby-install
│   └── 0.6.1
├── tmux
│   └── 2.3
└── tools
    └── 0.1

13 directories, 15 files
amaliax:~$ ls -la /beegfs/common/software/2017/modules/modulefiles/general/python
total 8
drwxrwsr-x  2 DRosskopp group_beesw    3 Jun 24 05:15 .
drwxrwsr-x 15 DRosskopp group_beesw   13 Jun 24 05:15 ..
-rw-rw-r--  1 DRosskopp group_beesw 3078 Jun 24 05:15 2.7.12
-rw-rw-r--  1 DRosskopp group_beesw 3058 Jun 24 05:15 3.6.0
-rw-rw-r--  1 DRosskopp group_beesw  137 Jun 24 05:15 .version
```

Example content of a folder in the `MODULEPATH`.

Example content for Python.

The modules system

```
amaliax:~$ ls -la /beegfs/common/software/2017/modules/modulefiles/general/python
total 8
drwxrwsr-x  2 DRosskopp group_beesw    3 Jun 24 05:15 .
drwxrwsr-x 15 DRosskopp group_beesw   13 Jun 24 05:15 ..
-rw-rw-r--  1 DRosskopp group_beesw 3078 Jun 24 05:15 2.7.12
-rw-rw-r--  1 DRosskopp group_beesw 3058 Jun 24 05:15 3.6.0
-rw-rw-r--  1 DRosskopp group_beesw  137 Jun 24 05:15 .version
```

`2.7.12` module file for python 2.7.12

`3.6.0` module file for python 3.6.0

`.version` file defining the default version:

```
#%Module1.0#####################################################################
##
## version file for python
##
set ModulesVersion      "2.7.12"
```

module file

```
#%Module3.2.10#####################################################################
proc ModulesHelp { } {
        global version
        puts stderr "\n\tVersion 2.7.12 of python\n"
}

module-whatis   "Version 2.7.12 of python"

# for Tcl script use only
set     version      "3.2.10"

conflict python
prepend-path PATH /beegfs/common/software/2017/modules/software/python/2.7.12/bin
prepend-path LD_LIBRARY_PATH /beegfs/common/software/2017/modules/software/python/2.7.12/lib
prepend-path CPATH /beegfs/common/software/2017/modules/software/python/2.7.12/include
prepend-path C_INCLUDE_PATH /beegfs/common/software/2017/modules/software/python/2.7.12/include
prepend-path CPLUS_INCLUDE_PATH /beegfs/common/software/2017/modules/software/python/2.7.12/include
prepend-path OBJC_INCLUDE_PATH /beegfs/common/software/2017/modules/software/python/2.7.12/include
prepend-path MANPATH /beegfs/common/software/2017/modules/software/python/2.7.12/share/man
prepend-path INFODIR /beegfs/common/software/2017/modules/software/python/2.7.12/share/man
set home $::env(HOME)
set pythonuser $home/.python/2.7.12/bin
exec /bin/mkdir -p $pythonuser
prepend-path PATH $home/.python/2.7.12/bin
set jupyter_runtime_dir $home/.python/2.7.12/jupyter/run
exec /bin/mkdir -p $jupyter_runtime_dir
setenv JUPYTER_RUNTIME_DIR $home/.python/2.7.12/jupyter/run
set jupyter_data_dir $home/.python/2.7.12/jupyter/data
exec /bin/mkdir -p $jupyter_data_dir
setenv JUPYTER_DATA_DIR $home/.python/2.7.12/jupyter/data
setenv PYTHONHOME /beegfs/common/software/2017/modules/software/python/2.7.12/
setenv PYTHONPATH /beegfs/common/software/2017/modules/software/python/2.7.12/lib/python2.7
setenv PYTHONUSERBASE $home/.python/2.7.12/
exec /bin/mkdir -p $home/.python/2.7.12/pythonpath/site-packages
module load gcc/6.3.0 bzip2/1.0.6 xz/5.2.2 ncurses/6.0 libevent/2.0.22 pcre/8.39 curl/7.51.0 freetype/2.7 openblas/0.2.19
setenv CFLAGS "-I/beegfs/common/software/2017/modules/software/openblas/0.2.19/include -I/beegfs/common/software/2017/modules/software/ncu
rses/6.0/include/ncurses -I/beegfs/common/software/2017/modules/software/libevent/2.0.22/include -I/beegfs/common/software/2017/modules/so
ftware/bzip2/1.0.6/include -I/beegfs/common/software/2017/modules/software/xz/5.2.2/include -I/beegfs/common/software/2017/modules/softwar
e/pcre/8.39/include -I/beegfs/common/software/2017/modules/software/curl/7.51.0/include -I/beegfs/common/software/2017/modules/software/op
enblas/0.2.19/include -I/beegfs/common/software/2017/modules/software/rlang/3.3.2/lib64/R/include"
setenv LDFLAGS "-L/beegfs/common/software/2017/modules/software/openblas/0.2.19/lib -L/beegfs/common/software/2017/modules/software/ncurse
s/6.0/lib -L/beegfs/common/software/2017/modules/software/libevent/2.0.22/lib -L/beegfs/common/software/2017/modules/software/bzip2/1.0.6/
lib -L/beegfs/common/software/2017/modules/software/xz/5.2.2/lib -L/beegfs/common/software/2017/modules/software/pcre/8.39/lib -L/beegfs/c
ommon/software/2017/modules/software/curl/7.51.0/lib -L/beegfs/common/software/2017/modules/software/rlang/3.3.2/lib64/R/lib"
                                                                                                                    15,1          All
```

module file

```
#%Module3.2.10#####################################################################
proc ModulesHelp { } {
        global version
        puts stderr "\n\tVersion 2.7.12 of python\n"
}
```

Help message shown for this modules with `module help python/2.7.12`

```
module-whatis   "Version 2.7.12 of python"
```

Message to be shown by `module whatis python/2.7.12`.

```
# for Tcl script use only
set     version      "3.2.10"
```

Modules system version.

```
conflict python
```

Conflicts. ie. Do not load if a different python version is already loaded.

```
prepend-path PATH /beegfs/common/software/2017/modules/software/python/2.7.12/bin
prepend-path LD_LIBRARY_PATH /beegfs/common/software/2017/modules/software/python/2.7.12/lib
prepend-path CPATH /beegfs/common/software/2017/modules/software/python/2.7.12/include
prepend-path C_INCLUDE_PATH /beegfs/common/software/2017/modules/software/python/2.7.12/include
prepend-path CPLUS_INCLUDE_PATH /beegfs/common/software/2017/modules/software/python/2.7.12/include
prepend-path OBJC_INCLUDE_PATH /beegfs/common/software/2017/modules/software/python/2.7.12/include
prepend-path MANPATH /beegfs/common/software/2017/modules/software/python/2.7.12/share/man
prepend-path INFODIR /beegfs/common/software/2017/modules/software/python/2.7.12/share/man
```

Paths prepended when the module is loaded and removed when the module is unloaded.

module file

```
set home $::env(HOME)
```

`$::env(HOME)` captures the variable HOME from the environment of the user loading the module.

`set home $::env(HOME)` sets a variable `home` to be used within the module with the result of `$::env(HOME)`.

```
set pythonuser $home/.python/2.7.12/bin
```

Sets the python user variable to be used within the module.

```
exec /bin/mkdir -p $pythonuser
```

Executes the command `/bin/mkdir -p $pythonuser` every time the module is loaded.

```
prepend-path PATH $home/.python/2.7.12/bin
```

Prepends `$home/.python/2.7.12/bin` to the user environment PATH variable.

module file

```
setenv PYTHONUSERBASE $home/.python/2.7.12/
exec /bin/mkdir -p $home/.python/2.7.12/pythonpath/site-packages
```

Please notice `PYTHONUSERBASE`

```
module load gcc/6.3.0 bzip2/1.0.6 xz/5.2.2 ncurses/6.0 libevent/2.0.22 pcre/8.39 curl/7.51.0 freetyp
```

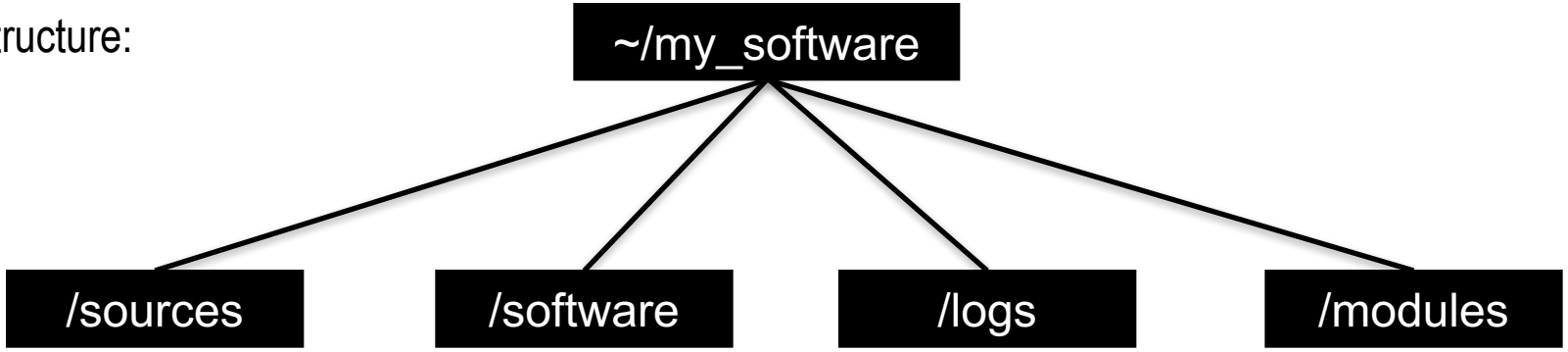
Loads other modules as dependencies when loading the python module.

Installing software without `su` access

Several examples can be obtained from:

https://github.com/mpg-age-bioinformatics/draco_pipelines/blob/master/software/software.sh

Structure:




```
mkdir –p ~/my_software/sources ~/my_software/software \
~/my_software/logs  ~/my_software/modules
```

Installing software without `su` access

Download and edit the script for automatic generation of module files:

```
cd ~/
wget https://raw.githubusercontent.com/mpg-age-bioinformatics/
draco_pipelines/master/software/newmod.sh

sed -i 's/\/u\/jboucas\/modules/~\/my_software/g' newmod.sh
chmod +x newmod.sh
```

Add the `~/my_software/modules` to the MODULEPATH:

```
export MODULEPATH=$MODULEPATH:~/my_software/modules
```

You might want to add this line to your `~/.bashrc`

Installing software without `su` access

```
cd ~/my_software/sources
wget http://zlib.net/pigz/pigz-2.3.4.tar.gz
tar -zxvf pigz-2.3.4.tar.gz
cd pigz-2.3.4
make
mkdir -p ~/my_software/software/pigz/2.3.4/bin
cp pigz unpigz ~/my_software/software/pigz/2.3.4/bin
~/newmod.sh -s pigz -p ~/my_software/modules -v 2.3.4 -d 2.3.4


# TEST #
module avail
module show pigz/2.3.4
module load pigz/2.3.4
which pigz
```

Installing software without `su` access

```
cd ~/my_software/sources
wget http://zlib.net/zlib-1.2.11.tar.gz
tar -zxvf zlib-1.2.11.tar.gz
cd zlib-1.2.11
make
mkdir -p ~/my_software/software/libz/1.2.11
./configure -prefix=~/my_software/software/libz/1.2.11
make
make install
~/newmod.sh -s libz -p ~/my_software/modules -v 1.2.11 -d 1.2.11
```

Installing software without `su` access

```
echo "#!/bin/bash
cd ~/my_software/sources
wget http://zlib.net/zlib-1.2.11.tar.gz
tar -zxvf zlib-1.2.11.tar.gz
cd zlib-1.2.11
make
mkdir -p ~/my_software/software/libz/1.2.11
./configure -prefix=~/my_software/software/libz/1.2.11
make
make install
~/newmod.sh -s libz -p ~/my_software/modules -v 1.2.11 -d 1.2.11
" > ~/my_software/logs/libz-1.2.11.sh
chmod +x ~/my_software/logs/libz-1.2.11.sh
~/my_software/logs/libz-1.2.11.sh 2>&1 | tee \
~/my_software/logs/libz-1.2.11.log
```

Installing software without `su` access

```
if [ ! -f $MODF/general/tmux/2.3 ]; then
    echo 'tmux-2.3'
    echo '#!/bin/bash
    module list
    cd $SOUR && \
    wget -O t.tar.gz https://github.com/tmux/tmux/releases/download/2.3/tmux-2.3.ta
r.gz && \
    mv t.tar.gz tmux-2.3.tar.gz && \
    tar -zxvf tmux-2.3.tar.gz && \
    cd tmux-2.3 && \
    mkdir -p $SOFT/tmux/2.3/ && \
    ./configure --prefix=$SOFT/tmux/2.3/ CFLAGS="-I$SOFT/libevent/2.0.22/include -I
$SOFT/ncurses/6.0/include/ncurses" LDFLAGS="-L$SOFT/libevent/2.0.22/lib -L$SOFT/ncu
rses/6.0/lib" && \
    make && make install
    newmod.sh \
    -s tmux \
    -p $MODF/general/ \
    -v 2.3 \
    -d 2.3
    echo "set home $::env(HOME)" >> $MODF/general/tmux/2.3
    echo "exec /bin/mkdir -p \$home/.tmux.socket" >> $MODF/general/tmux/2.3
    echo "module load ncurses/6.0" >> $MODF/general/tmux/2.3
    echo "module load libevent/2.0.22" >> $MODF/general/tmux/2.3
    echo "setenv TMUX_TMPDIR \$home/.tmux.socket" >> $MODF/general/tmux/2.3
    ' > $LOGS/tmux-2.3.sh
    chmod 755 $LOGS/tmux-2.3.sh
    srun -o $LOGS/tmux-2.3.out $LOGS/tmux-2.3.sh
fi
```

Installing R packages

R standard packages:

```
base  datasets  graphics  grDevices  methods  parallel  stats  stats4
tcltk  tools  utils
```

This are the only packages that should be inside `lib64/R/library`. The `library` folder should have permissions `chmod –R 555 library`. This will enforce the use of the `R_LIBS_USER` variable for installation of new packages.

Alternative (eg. install biomaRt):

```
source("https://bioconductor.org/biocLite.R")
biocLite("biomaRt", lib=Sys.getenv("R_LIBS_USER"))
```

The `lib` argument can also be used in (eg. install packrat):

```
install.packages("packrat", lib=Sys.getenv("R_LIBS_USER"))
```

Installing python packages

Installing the AGEpy package:

```
module load python
pip install AGEpy --user
```

Alternative 1:

```
module load python
git clone https://github.com/mpg-age-bioinformatics/AGEpy
cd AGEpy
pip install ../AGEpy --user
```

Alternative 1b (no package control):

```
cd AGEpy
python setup.py install --user
```

The `--user` argument will make use of the `PYTHONUSERBASE` variable.

Installing perl packages

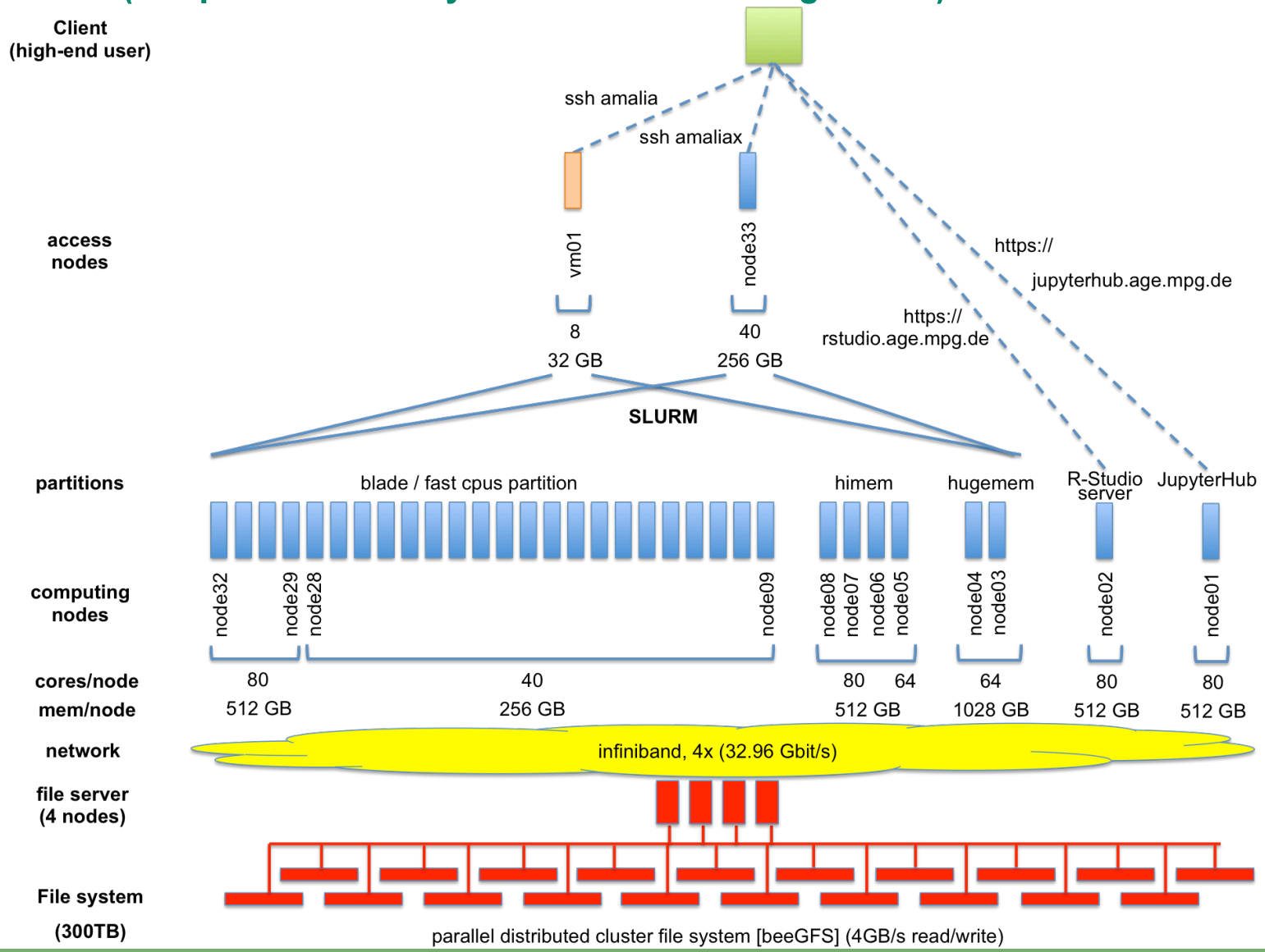
Perl libraries are loaded from the value of `PERL5LIB`. We have added a variable to module perl to ease local installations - `PERLUSER` - check out the content of these two variables.

Example instalation of `Log::Log4perl`:

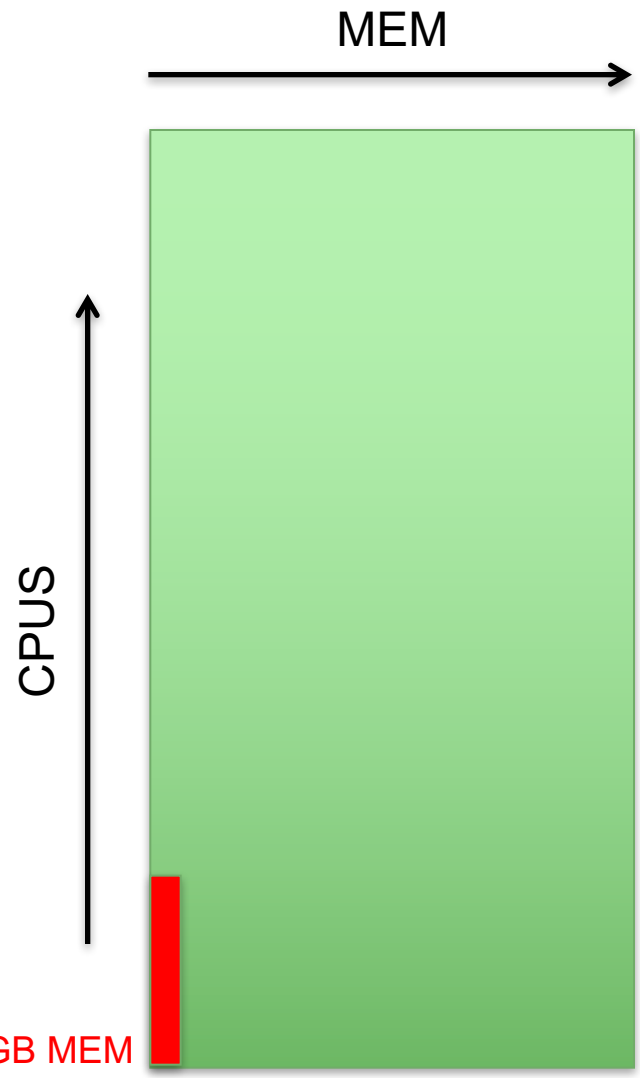
```
module load perl/5.24.1
cpanm Log::Log4perl -l $PERLUSER

# check where it got installed
perldoc -l Log::Log4perl
```

SLURM (Simple Linux Utility for Resource Management)



SLURM: Why an HPC cluster?



One HPC node:

40 CPUS
256 GB MEM

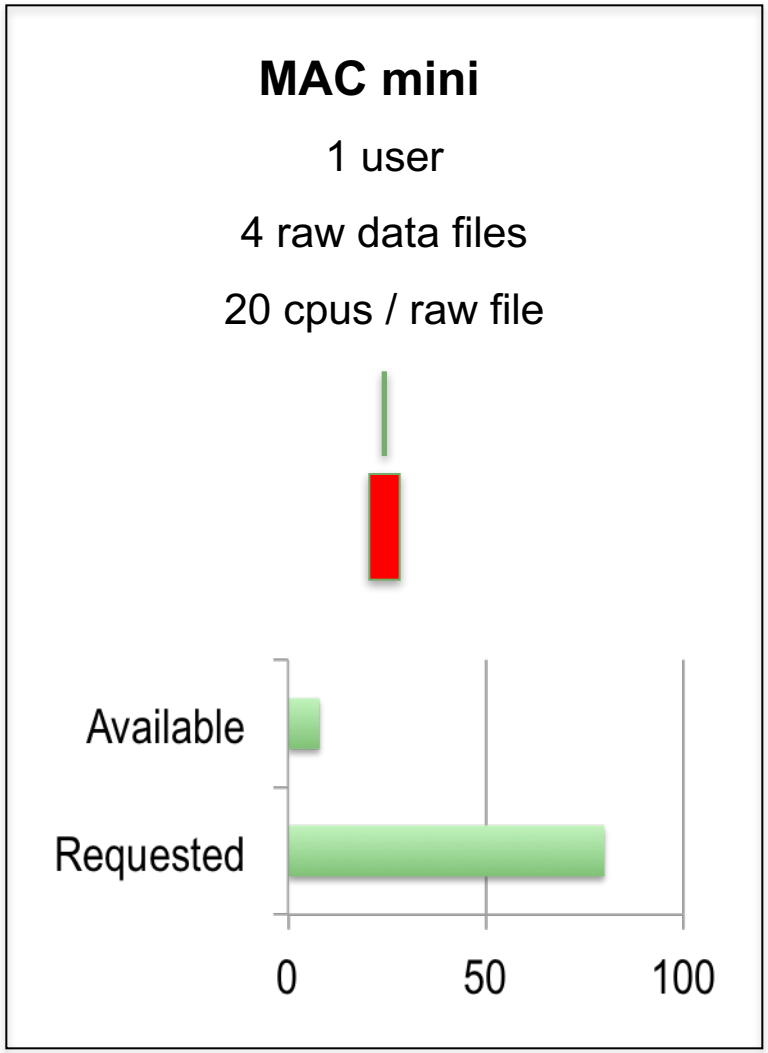
In-house/MPI-AGE

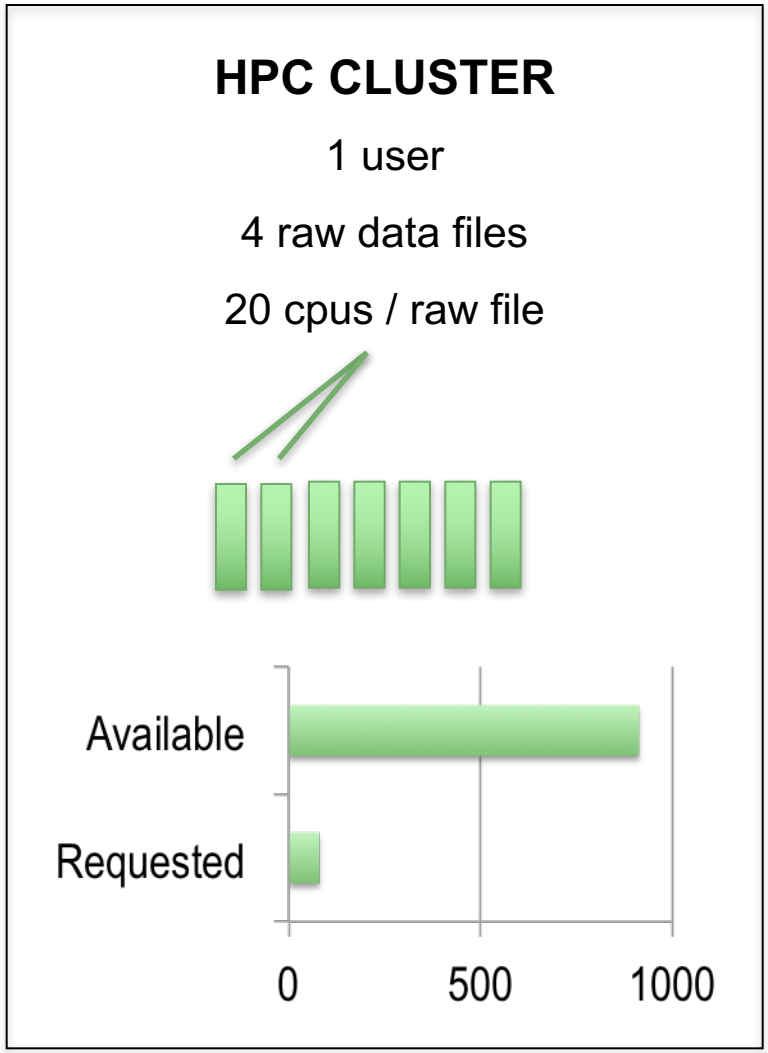
~13 TFlops

Queuing times:
0-20' : 80% of jobs
0-180' : 98% of jobs

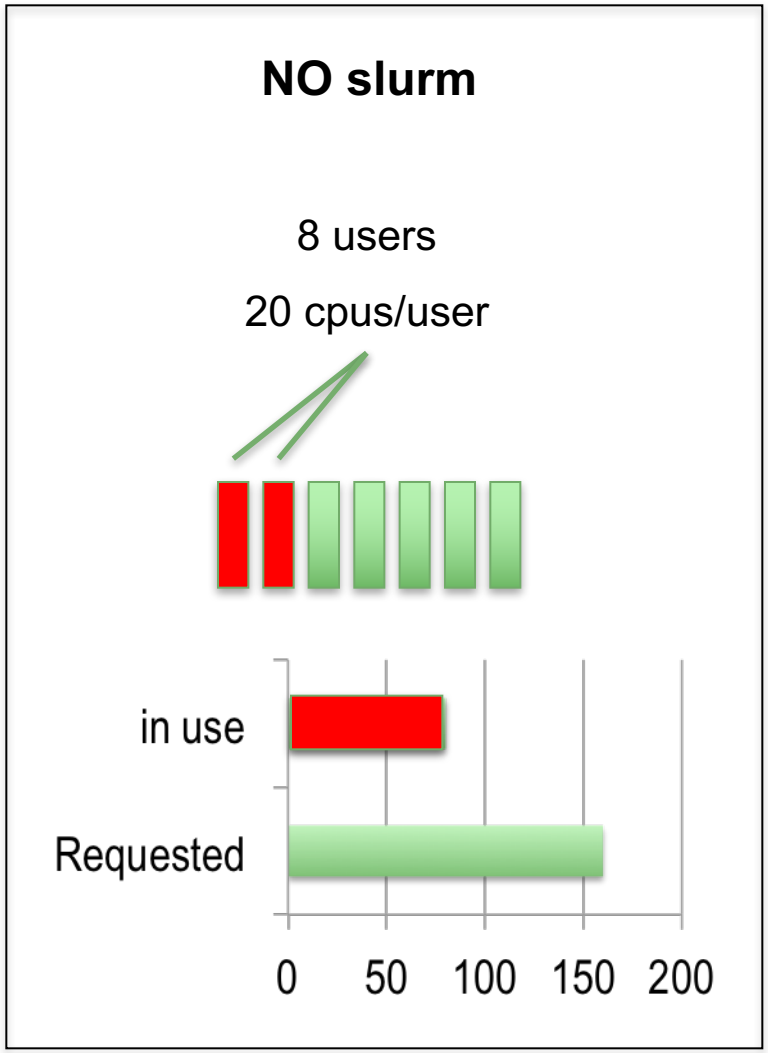
MAC mini: 8 cpus, 16 GB MEM

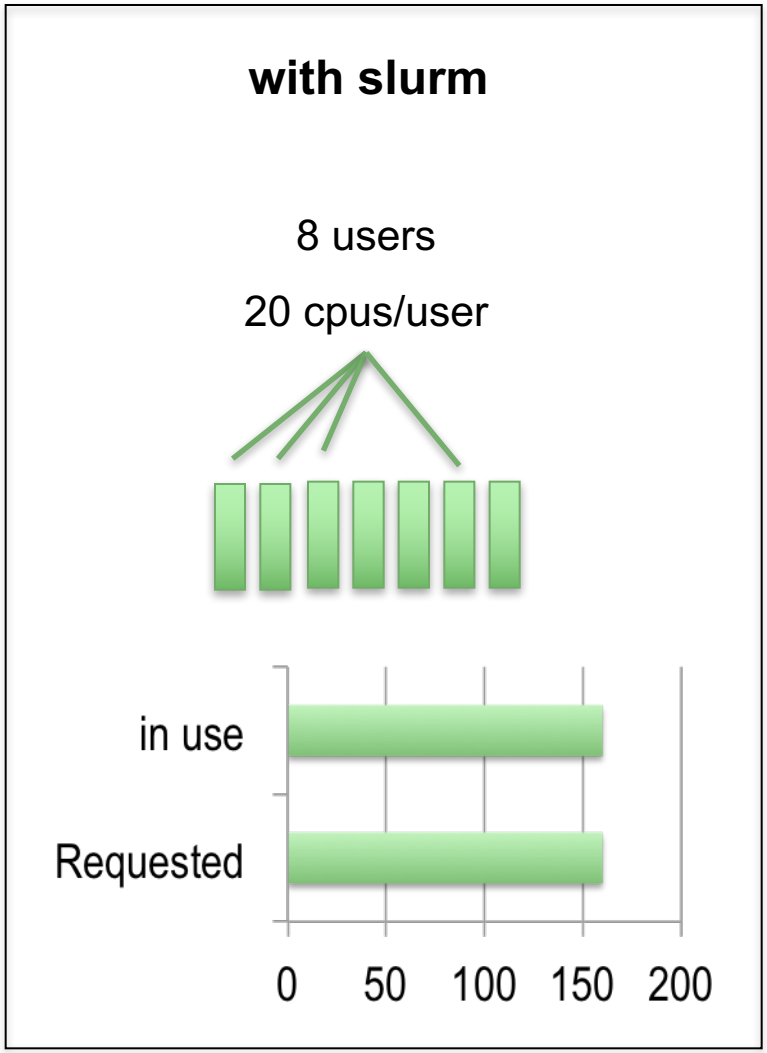
SLURM: Why an HPC cluster?





SLURM: Why SLURM?





SLURM: Why SLURM?

NO slurm

```
bwa mem sample1.fastq
```

with slurm

```
srun bwa mem sample1.fastq
```

SLURM: How to?

NO slurm

```
bwa mem –T 18 sample1.fastq
```

with slurm

```
srun --cpus-per-task=18 \
bwa mem –T 18 sample1.fastq
```

SLURM: How to?

NO slurm

```
bwa mem –T 18 sample1.fastq
```

with slurm

```
srun --cpus-per-task=18 \
--mem=64gb \
bwa mem –T 18 sample1.fastq
```

SLURM: How to?

NO slurm

```
bwa mem –T 18 sample1.fastq
```

with slurm

```
srun --cpus-per-task=18 \
--mem=15gb \
--time=5-24 \
bwa mem –T 18 sample1.fastq
```

(5 days and 24 hours = 6 days

alternative: 144:00:00;

maximum = 14 days)

SLURM: How to?

NO slurm

```
bwa mem –T 18 sample1.fastq
```

with slurm

```
srun --cpus-per-task=18 \
--mem=15gb \
--time=5-24 \
-p blade \
bwa mem –T 18 sample1.fastq
```

SLURM: How to?

NO slurm

```
bwa mem –T 18 sample1.fastq
```

with slurm

```
srun --cpus-per-task=18 \
--mem=15gb \
--time=5-24 \
-p blade \
-o slurm_logs/bwa_1.out \
bwa mem –T 18 sample1.fastq
```

SLURM: How to?

NO slurm

```
./align_1.sh
```

```
#!/bin/bash
bwa mem –T 18 sample1.fastq
exit
```

with slurm

```
sbatch --cpus-per-task=18 \
--mem=15gb \
--time=5-24 \
-p blade \
-o slurm_logs/bwa_1.out \
align_1.sh
```

SLURM: scripting

NO slurm

```
#!/bin/bash
cd ~/project/raw_data
bwa mem –T 18 sample1.fastq
exit


./align_1.sh
```

with slurm

```
#!/bin/bash
#SBATCH --cpus-per-task=18
#SBATCH --mem=15gb
#SBATCH --time=5-24
#SBATCH -p blade
#SBATCH -o slurm_logs/bwa_1.out
cd ~/project/raw_data
bwa mem –T 18 sample1.fastq
exit

sbatch align_1.sh
```

SLURM with modules sytem

```
#!/bin/bash
#SBATCH --cpus-per-task=18
#SBATCH --mem=15gb
#SBATCH --time=5-24
#SBATCH -p blade
#SBATCH -o slurm_logs/bwa_1.out

module load bwa
cd ~/project/raw_data
bwa mem -T 18 sample1.fastq
exit
```

SLURM with shifter & the modules system

```
#!/bin/bash
#SBATCH --cpus-per-task=18
#SBATCH --mem=15gb
#SBATCH --time=5-24
#SBATCH -p blade
#SBATCH -o slurm_logs/bwa_1.out

shifter --image=mpgagebioinformatics/bioinformatics_software:v1.0.1 << SHI
#!/bin/bash
source ~/.bashrc
module load bwa
cd ~/project/raw_data
bwa mem -T 18 sample1.fastq
exit
SHI
```

SLURM: iterating jobs over files

```
#!/bin/bash
cd ~/project/raw_data                                  # go to folder containing files

for f in $(ls *.fastq); do echo "#!/bin/bash           # for each file, echo a script
cd ~/project/raw_data                                  # that goes to folder
bwa mem -T 18 ${f}                                     # executes job on file and
rm ~/project/tmp/${f}.sh                               # once completed removes
" > ~/project/tmp/${f}.sh                              # temporary script

chmod 755 ~/project/tmp/${f}.sh
rm ~/project/slurm_logs/${f}.*.out                     # removes pre-existing logs

sbatch --cpus-per-task=18 --mem=15gb \                 # start batch job
--time=5-24 -p blade \
-o ~/project/slurm_logs/${f}.%j.out \                  # keeps log with job number
~/project/tmp/${f}.sh

done; exit
```

SLURM: iterating jobs over files

```
#!/bin/bash
cd ~/project/raw_data

for f in $(ls *.fastq);
    do rm ~/project/slurm_logs/${f}.*.out

    sbatch --cpus-per-task=18 --mem=15gb --time=5-24 \
    -p blade -o ~/project/slurm_logs/${f}.%j.out << EOF
#!/bin/bash
cd ~/project/raw_data
bwa mem -T 18 ${f}
EOF

done
exit
```

SLURM: iterating without crashing

```
#!/bin/bash
cd ~/project/raw_data
for f in $(ls *.fastq);
   do  rm ~/project/slurm_logs/${f}.*.out

   while [  `squeue –u Jboucas | wc –l` –gt “500” ];
      do echo “sleeping”; sleep 300
   done

   sbatch --cpus-per-task=18 --mem=15gb --time=5-24 \
   –p blade –o ~/project/slurm_logs/${f}.%j.out ~/project/tmp/${f}.sh <<EOF
#!/bin/bash
cd ~/project/raw_data
bwa mem –T 18 ${f}
EOF

done
exit
```

SLURM with shifter

```
#!/bin/bash
cd ~/project/raw_data
for f in $(ls *.fastq);
   do  rm ~/project/slurm_logs/${f}.*.out

   sbatch --cpus-per-task=18 --mem=15gb --time=5-24 \
   -p blade -o ~/project/slurm_logs/${f}.%j.out ~/project/tmp/${f}.sh <<EOF
#!/bin/bash
shifter –image=mpgagebioinformatics/bioinformatics_software:v1.0.1 << SHI
#!/bin/bash
cd ~/project/raw_data
bwa mem –T 18 ${f}
SHI
EOF

done
exit
```

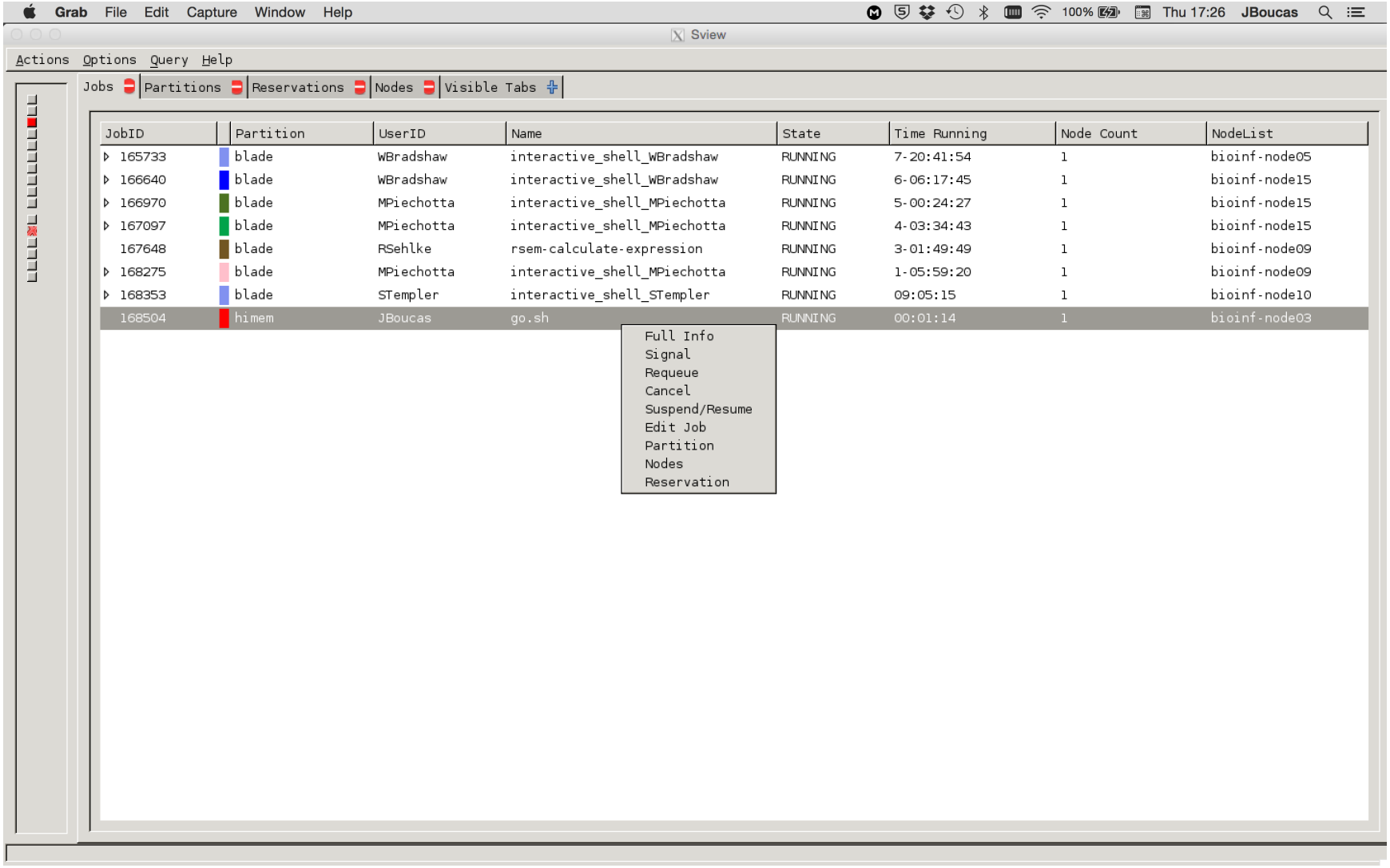
SLURM: other options

```
--mail-type=BEGIN, END,FAIL,REQUEUE,ALL

# Specifies when email is sent to the job owner. The option argument may consist of a
combination of the allowed mail types

--mail-user=username@age.mpg.de
```

SLURM: sview


Grab File Edit Capture Window Help
100% Thu 17:26 JBoucas
Sview
Actions Options Query Help
Jobs Partitions Reservations Nodes Visible Tabs
JobID Partition UserID Name State Time Running Node Count NodeList
165733 blade WBradshaw interactive_shell_WBradshaw RUNNING 7-20:41:54 1 bioinf-node05
166640 blade WBradshaw interactive_shell_WBradshaw RUNNING 6-06:17:45 1 bioinf-node15
166970 blade MPiechotta interactive_shell_MPiechotta RUNNING 5-00:24:27 1 bioinf-node15
167097 blade MPiechotta interactive_shell_MPiechotta RUNNING 4-03:34:43 1 bioinf-node15
167648 blade RSehlke rsem-calculate-expression RUNNING 3-01:49:49 1 bioinf-node09
168275 blade MPiechotta interactive_shell_MPiechotta RUNNING 1-05:59:20 1 bioinf-node09
168353 blade STempler interactive_shell_STempler RUNNING 09:05:15 1 bioinf-node10
168504 himem JBoucas go.sh RUNNING 00:01:14 1 bioinf-node03
Full Info
Signal
Requeue
Cancel
Suspend/Resume
Edit Job
Partition
Nodes
Reservation

SLURM: other useful commands

```
# show the partitions

sinfo


# show information on nodes

sinfo -N -O partitionname,nodehost,cpus,cpusload,freemem,memory


# requires X forwarding and allows viewing and manipulation of submitted jobs

sview


# lists running jobs

squeue


# show the queue for a user

squeue -u <user name>
```

SLURM: other useful commands

```
# cancels job 65673

scancel 65673


# cancels all jobs of user JBoucas

scancel –u JBoucas


# shows detailed resource information on job 43433

scontrol show job 43433


# show information on a partition

scontrol show partition <parition name>


# show information on a node

scontrol show node <node name>
```

SLURM: other useful commands

```
# starts an interactive terminal window on node15

srun –w node15 ––pty bash


# submit a job3 after job1 and job2 are successfully ready

job1=$(sbatch ––parsable <script1>)

job2=$(sbatch ––parsable <script2>)

sbatch –d afterok:${job1}:${job2} <script3>


# attach to a running job and run a command

srun ––jodib <JOBID> ––pty <command>


# change the partitions of a pending job

scontrol update job <job id> partition=<partition1>,<partition2>,<partition3>
```

Notes:

For current information on RStudio server and JupyterHub please check our cluster first steps page:

https://github.com/mpg-age-bioinformatics/cluster_first_steps

SLURM manual:

http://slurm.schedmd.com/man_index.html

Coming soon:

docker on HPC

END

bioinformatics@age.mpg.de

https://mpg-age-bioinformatics.github.io