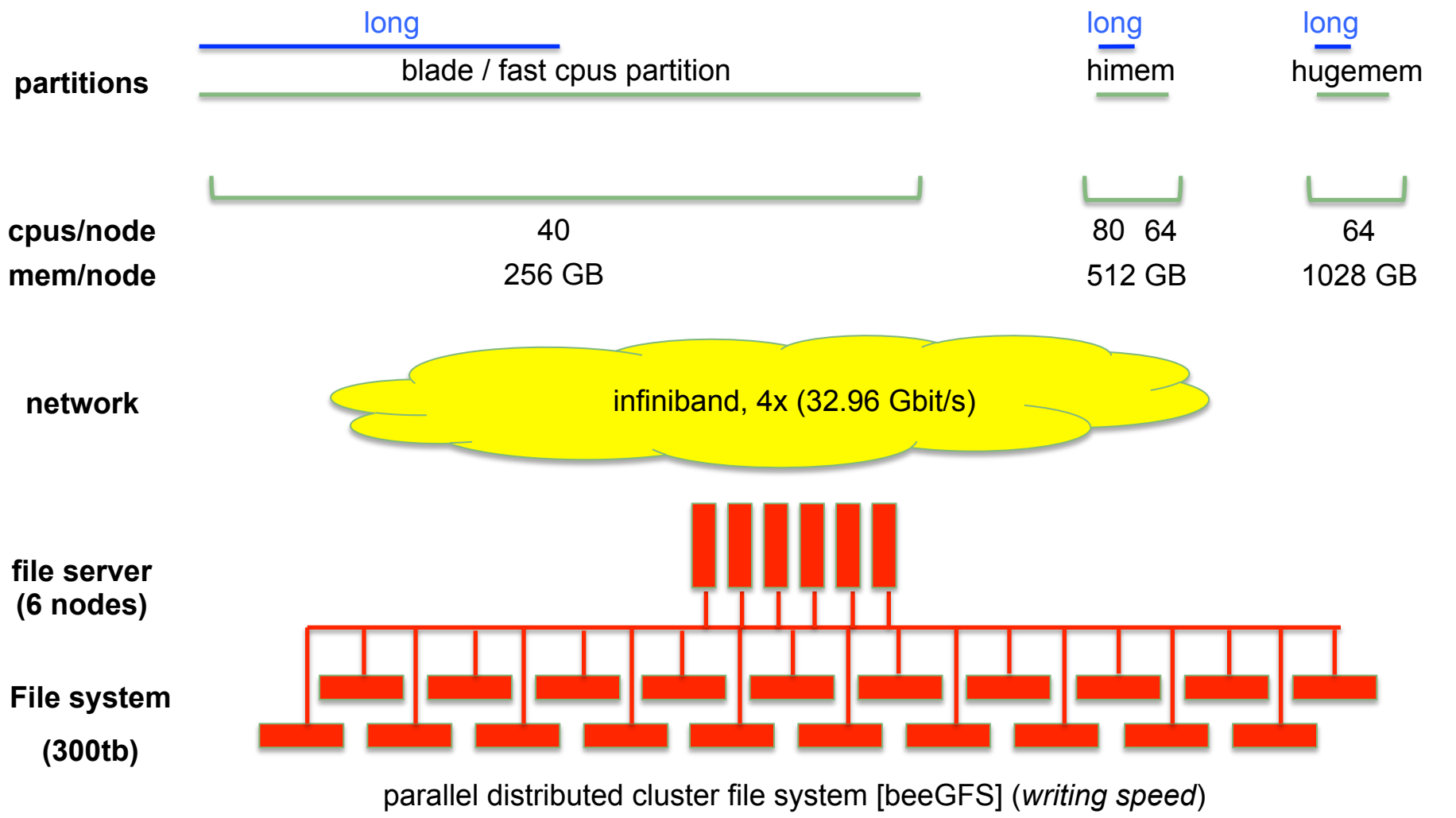
MAX PLANCK INSTITUTE FOR **BIOLOGY OF AGEING**

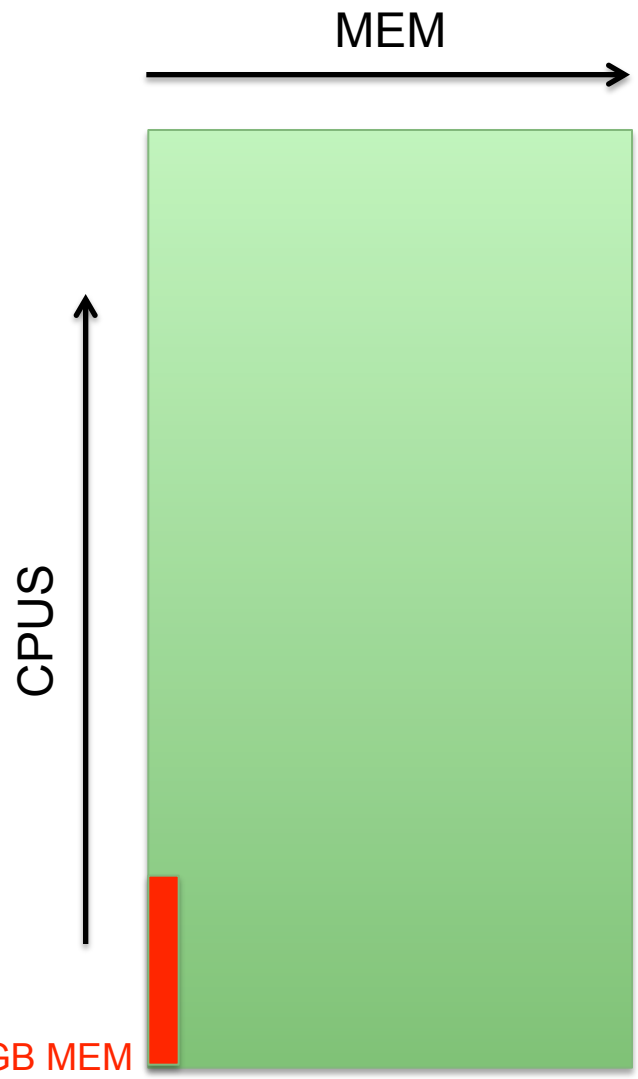
High Performance Computing

and the Simple Linux Utility for Resource Management (SLURM)

Architecture



Why a 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

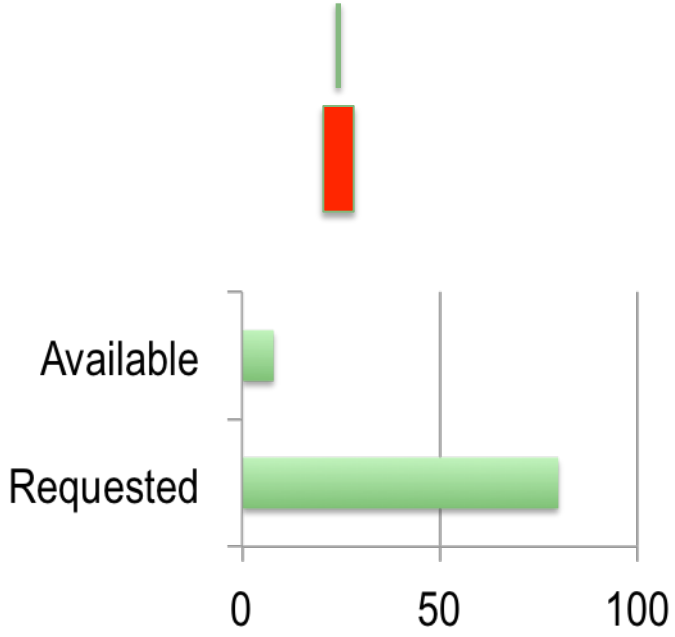
Why a HPC cluster?

MAC mini

1 user

4 raw data files

20 cpus / raw file

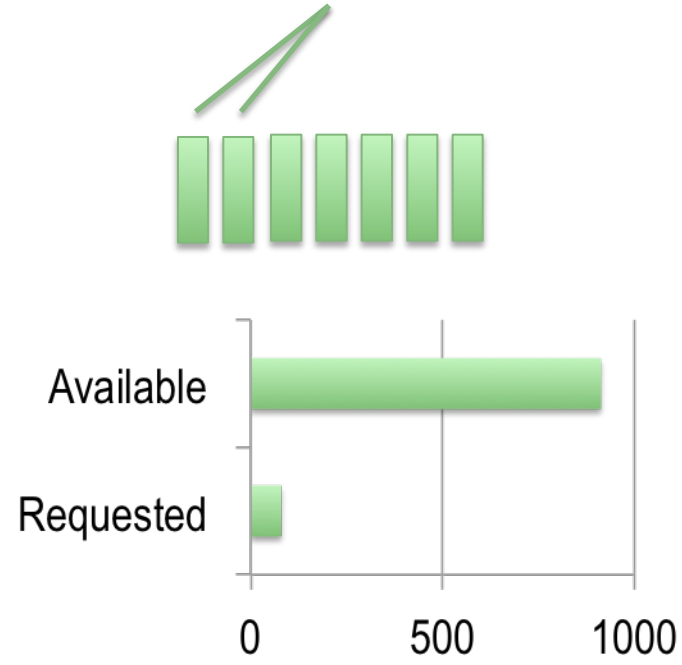


HPC CLUSTER

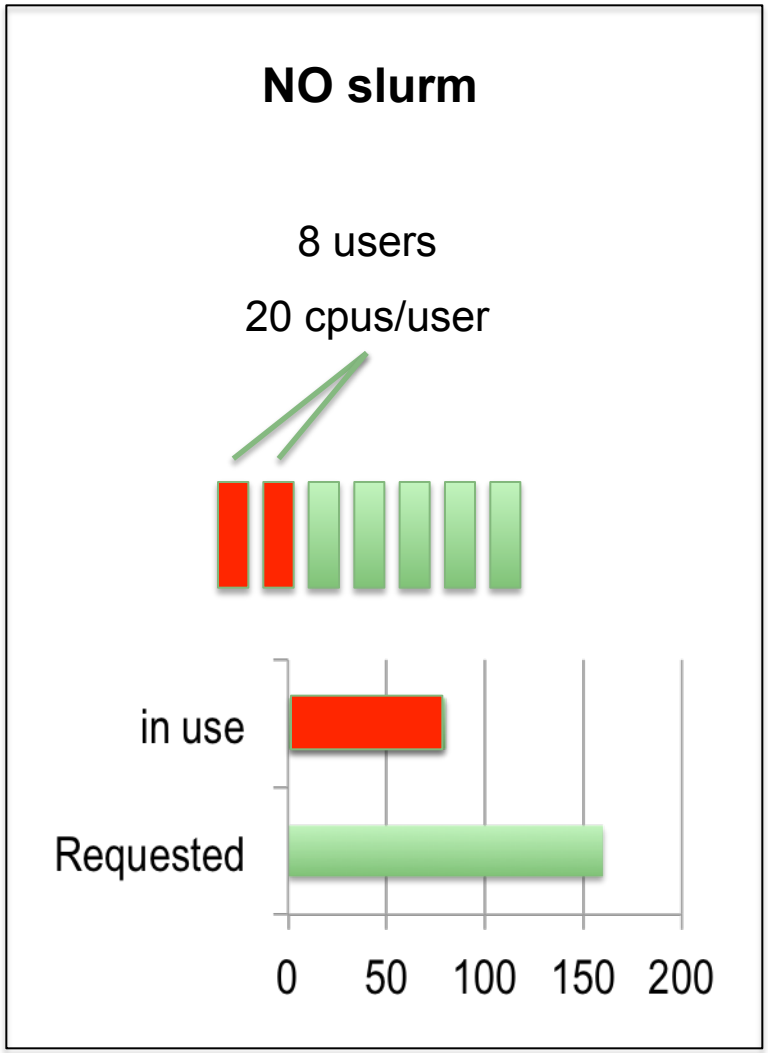
1 user

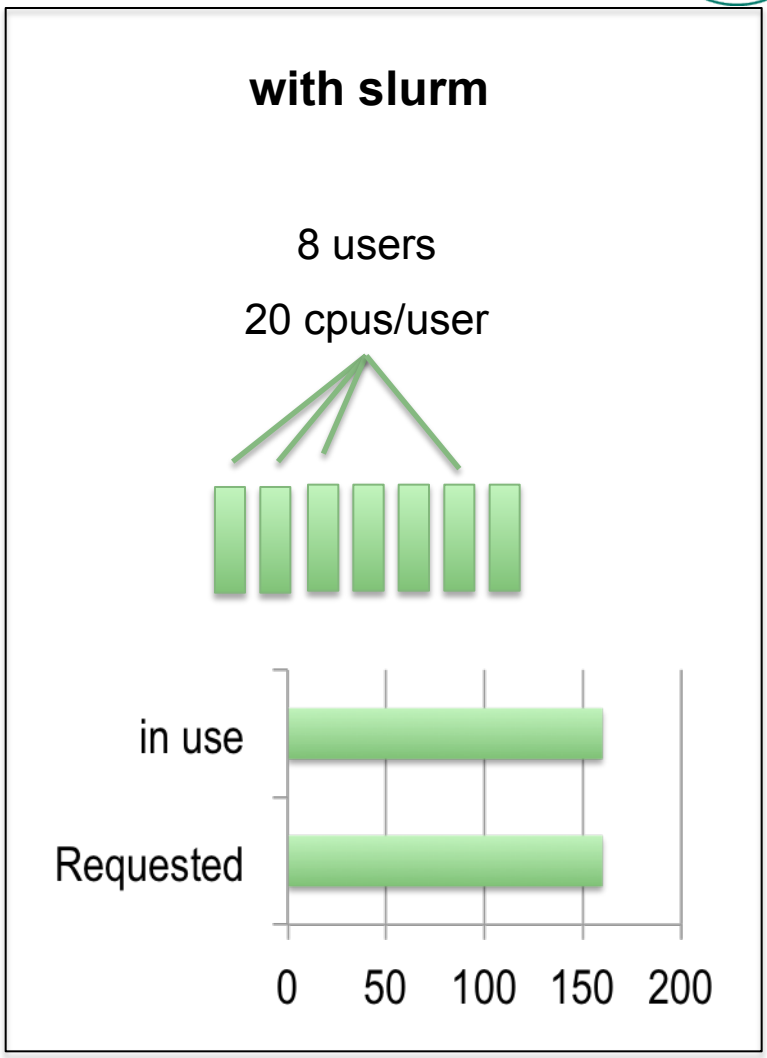
4 raw data files

20 cpus / raw file



Why SLURM?


NO slurm
8 users
20 cpus/user
in use
Requested
0
50
100
150
200


with slurm
8 users
20 cpus/user
in use
Requested
0
50
100
150
200

HOW TO use SLURM

NO slurm

> bwa mem sample1.fastq

with slurm

> **srun** bwa mem sample1.fastq

HOW TO use SLURM

NO slurm

```
> bwa mem –T 18 sample1.fastq
```

with slurm

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

HOW TO use SLURM

NO slurm

> bwa mem –T 18 sample1.fastq

with slurm

> srun --cpus-per-task=18 \

--mem=64gb \

bwa mem –T 18 sample1.fastq

HOW TO use SLURM

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)

HOW TO use SLURM

NO slurm

```
> bwa mem –T 18 sample1.fastq
```

with slurm

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

HOW TO use SLURM

NO slurm

```
> bwa mem –T 18 sample1.fastq
```

with slurm

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

HOW TO use SLURM

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,himem **

**-o slurm_logs/bwa_1.out **

align_1.sh

HOW TO use SLURM inside your scripts

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,himem
#SBATCH -o slurm_logs/bwa_1.out
cd ~/project/raw_data
bwa mem –T 18 sample1.fastq
exit

> sbatch align_1.sh
```

iterating SLURM 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
```

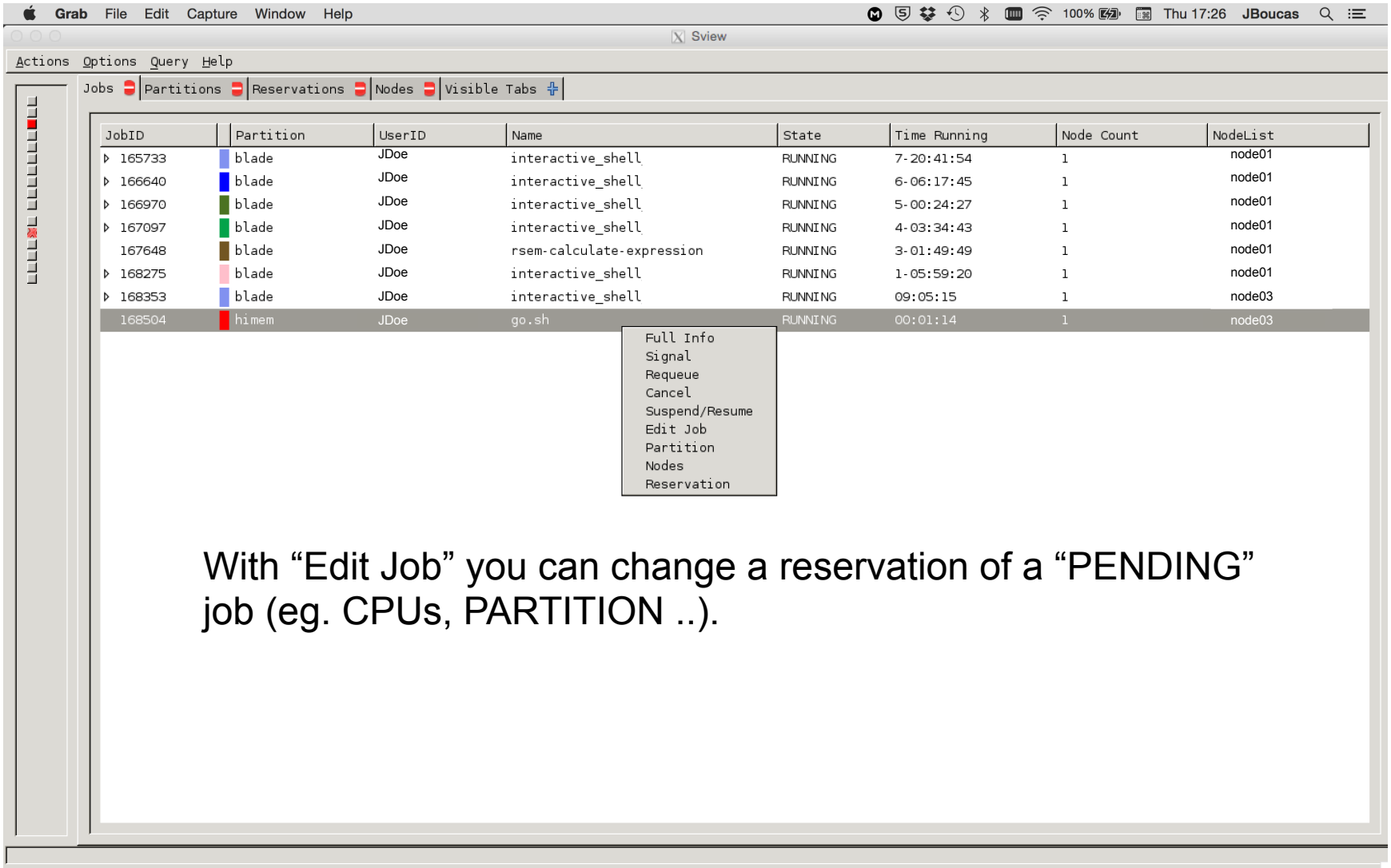
other options

--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*

useful slurm commands



With “Edit Job” you can change a reservation of a “PENDING” job (eg. CPUs, PARTITION ..).

useful slurm commands

```
> sview                    # requires X forwarding and allows viewing and
                           manipulation of submitted jobs
> squeue                   # lists running jobs
> scancel 65673            # cancels job 65673
> scancel -u JDoe          # cancels all jobs of user JDoe
> scontrol show job 43433  # shows detailed resource information on job 43433
```

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

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

NO BACKUP

! Data in the HPC / beeGFS is not backed up !

In HPC terabytes of intermediary and/or non-usable data can be generated in the space of a few hours..

! You are responsible for backing up your data !

copying data in and out of the beeGFS

scp

scp file.txt JDoe@my_ip_address:~/Desktop

Filezilla

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

/beegfs/common

✓ **JDoe@cluster:/beegfs/common$** tree -L 1

```
.
|-- databases
|-- example
|-- galaxy
|-- genomes
|-- shared_data
`-- software
```

/beegfs/common

✓ **JDoe@cluster:.../common/databases$** tree -L 1

```
.
|-- BLAST
|-- DATABASE_VERSION_LIST
|-- GOMo
|-- hmdb
|-- Motif
|-- new
|-- Pfam
|-- README
|-- SequencingAdapters
|-- SwissProt
`-- UniRef90
```

/beegfs/common

✓ **JDoe@cluster:.../common/genomes$** tree -L 1

```
.
|-- adapters
|-- caenorhabditis_elegans
|-- drosophila_melanogaster
|-- homo_sapiens
|-- mus_musculus
|-- TrueSeqAdapters.fa
`-- x
```

/beegfs/common

```
|-- chromosomes
|-- cuffcmp_GTF.GRCh38.81.gtf
|-- GRCh38.81.abinitio.gtf
|-- GRCh38.81.gtf
|-- GRCh38.dna.primary_assembly.fa
|-- GRCh38.dna.toplevel.fa
|-- logs
|-- primary_bowtie2
|-- primary_bwa
|-- primary_hisat
|-- primary_star
|-- primary_tophat_cuffcmp_GTF_index
|-- primary_tophat_GTF_index
|-- toplevel_bowtie2
|-- toplevel_bwa
|-- toplevel_hisat
|-- toplevel_star
|-- toplevel_tophat_cuffcmp_GTF_index
`-- toplevel_tophat_GTF_index
```

Contacts and links

ssh UName@cluster	# HPC cluster address
https://mpg-age-bioinformatics.github.io	# external
https://github.com/mpg-age-bioinformatics/cluster_first_steps	
bioinformatics@age.mpg.de	# bioinformatics core facility email
hpc@age.mpg.de	# hpc users mailing list
https://github.molgen.mpg.de	# git at the MPI-MOLGEN
https://rstudio.age.mpg.de	# r-studio server on beegfs
daniel.rosskopp@age.mpg.de ; tel. 257	# Systems Administrator
jorge.boucas@age.mpg.de ; tel. 312	# Head of Bioinformatics