

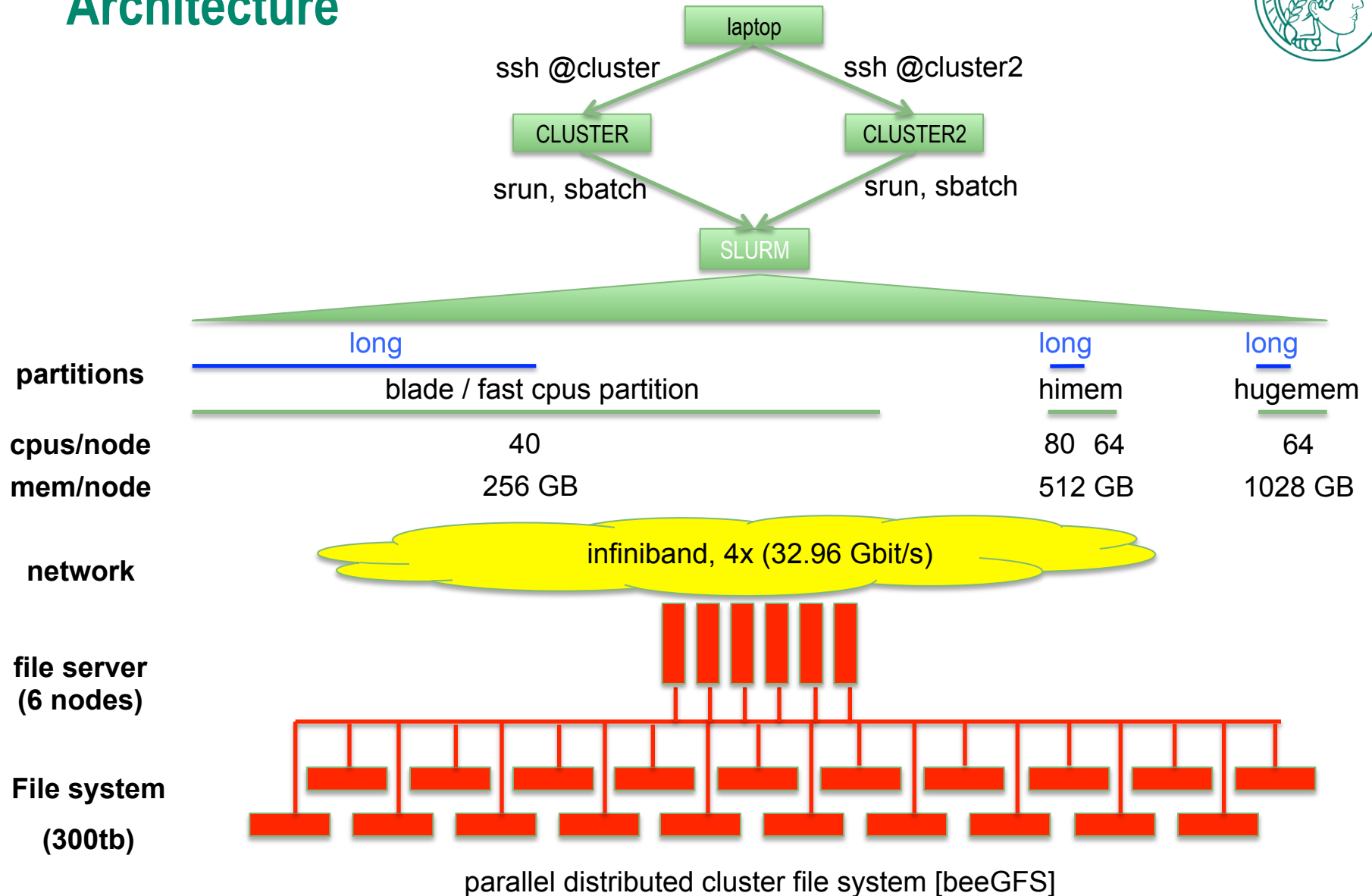


# High Performance Computing

and the Simple Linux Utility for Resource Management (SLURM)

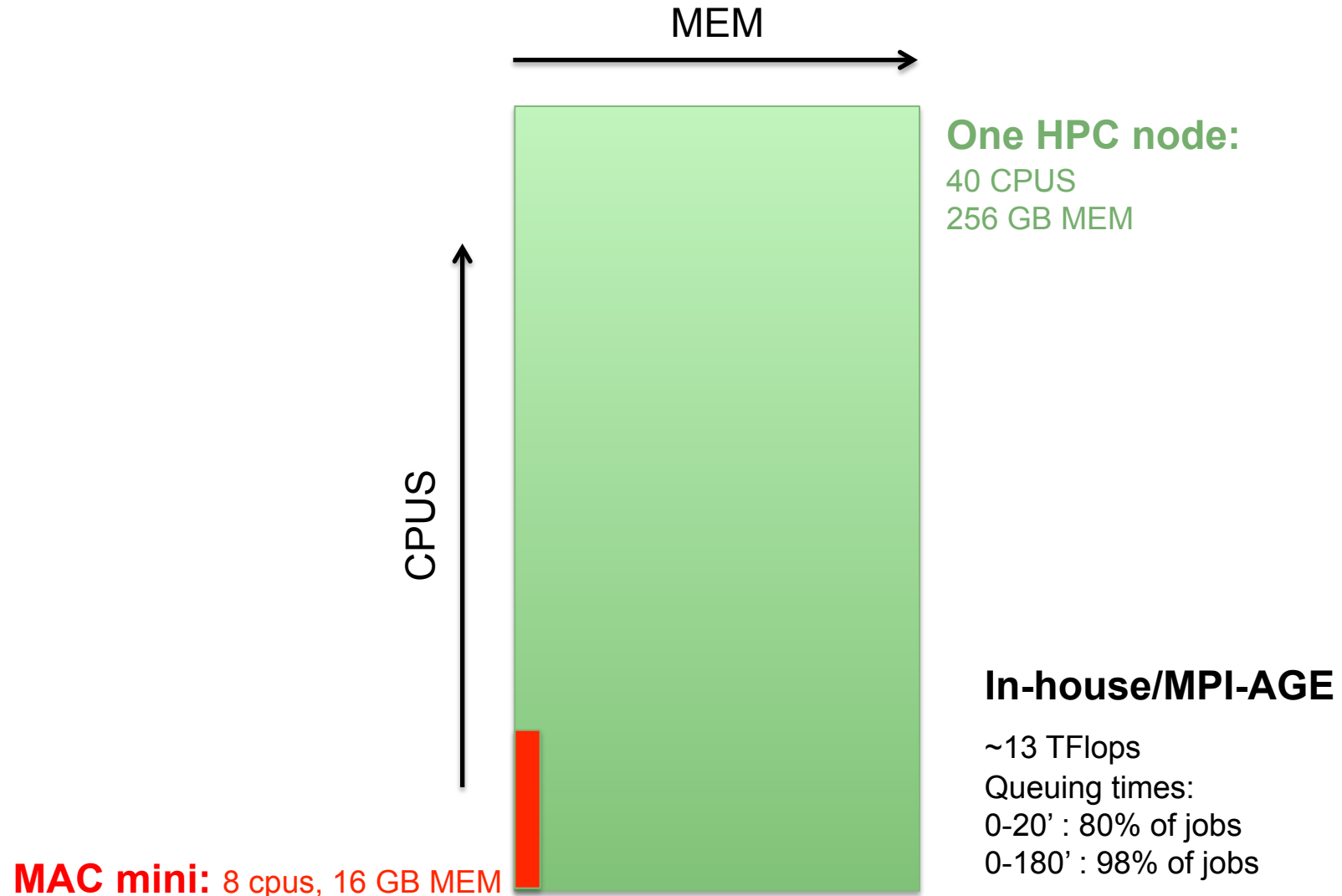


# Architecture





# Why a HPC cluster?





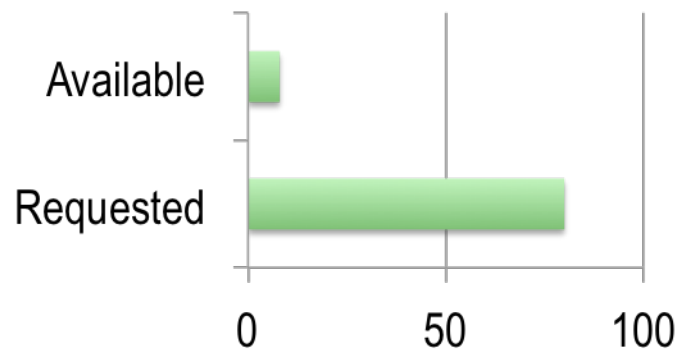
# Why a HPC cluster?

## MAC mini

1 user

4 raw data files

20 cpus / raw file

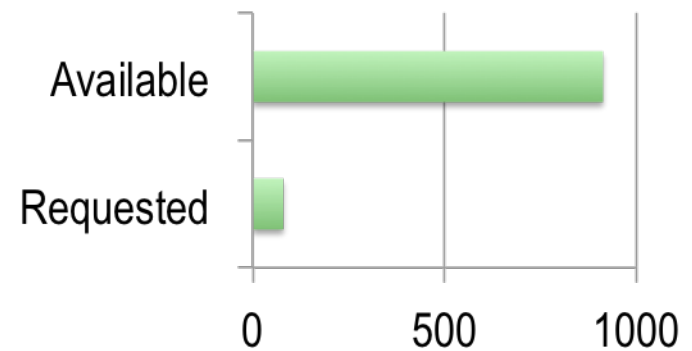
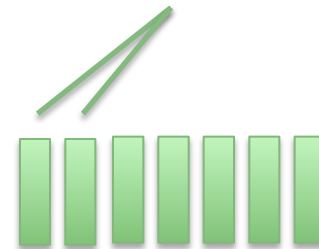


## HPC CLUSTER

1 user

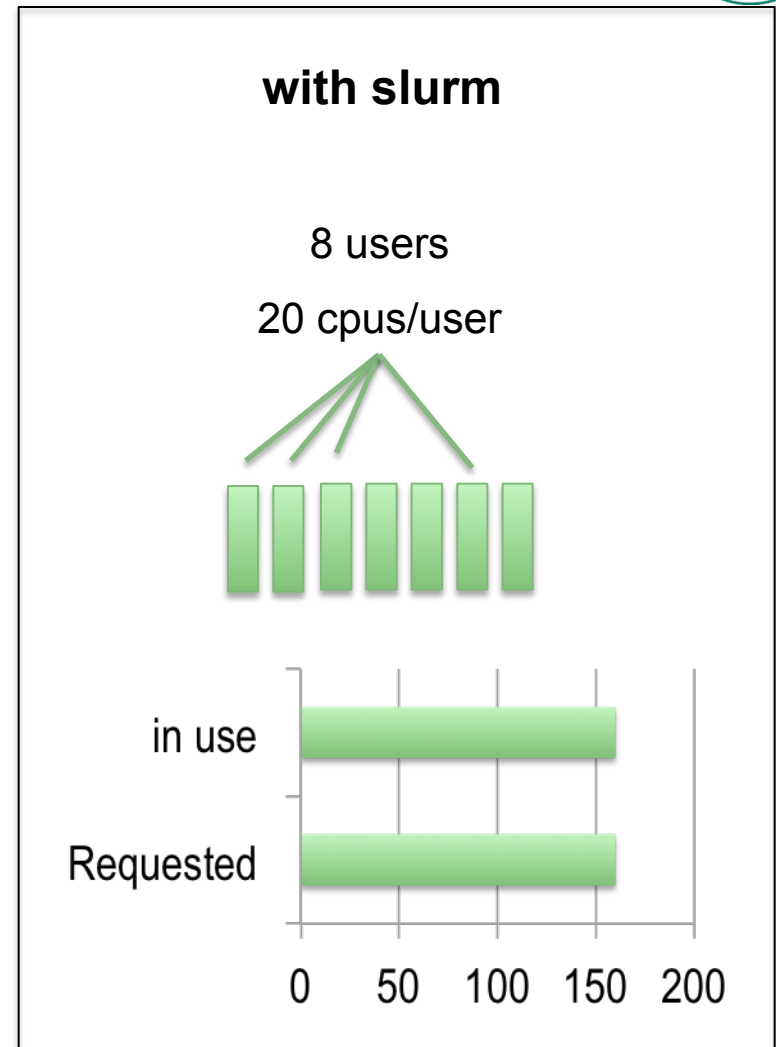
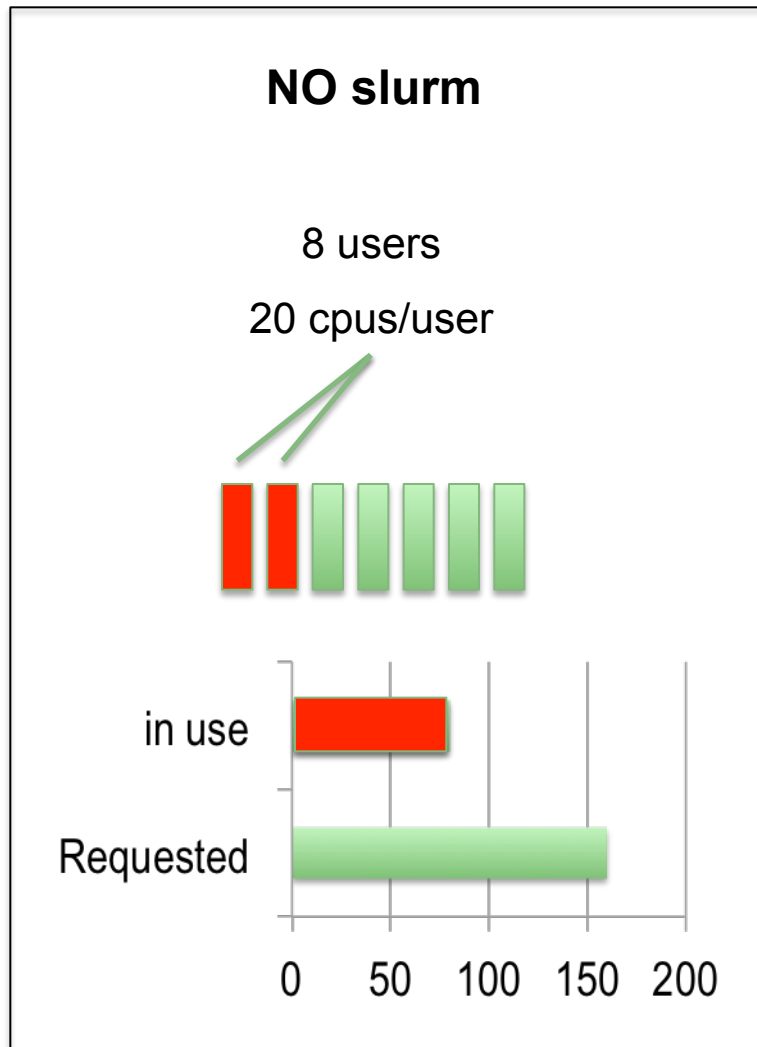
4 raw data files

20 cpus / raw file





# Why SLURM?



# 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
for f in $(ls *.fastq); do echo "#!/bin/bash
cd ~/project/raw_data
bwa mem -T 18 ${f}
rm ~/project/tmp/${f}.sh
" > ~/project/tmp/${f}.sh
chmod 755 ~/project/tmp/${f}.sh
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
done; exit
```

# go to folder containing files  
# for each file, echo a script  
# that goes to folder  
# executes job on file and  
# once completed removes  
# temporary script  
# removes pre-existing logs  
# start batch job  
# keeps log with job number



## 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



JobID	Partition	UserID	Name	State	Time Running	Node Count	NodeList
▶ 165733	blade	JDoe	interactive_shell	RUNNING	7-20:41:54	1	node01
▶ 166640	blade	JDoe	interactive_shell	RUNNING	6-06:17:45	1	node01
▶ 166970	blade	JDoe	interactive_shell	RUNNING	5-00:24:27	1	node01
▶ 167097	blade	JDoe	interactive_shell	RUNNING	4-03:34:43	1	node01
▶ 167648	blade	JDoe	rsem-calculate-expression	RUNNING	3-01:49:49	1	node01
▶ 168275	blade	JDoe	interactive_shell	RUNNING	1-05:59:20	1	node01
▶ 168353	blade	JDoe	interactive_shell	RUNNING	09:05:15	1	node03
▶ 168504	himem	JDoe	go.sh	RUNNING	00:01:14	1	node03

- Full Info
- Signal
- Requeue
- Cancel
- Suspend/Resume
- Edit Job
- Partition
- Nodes
- Reservation

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](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](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

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