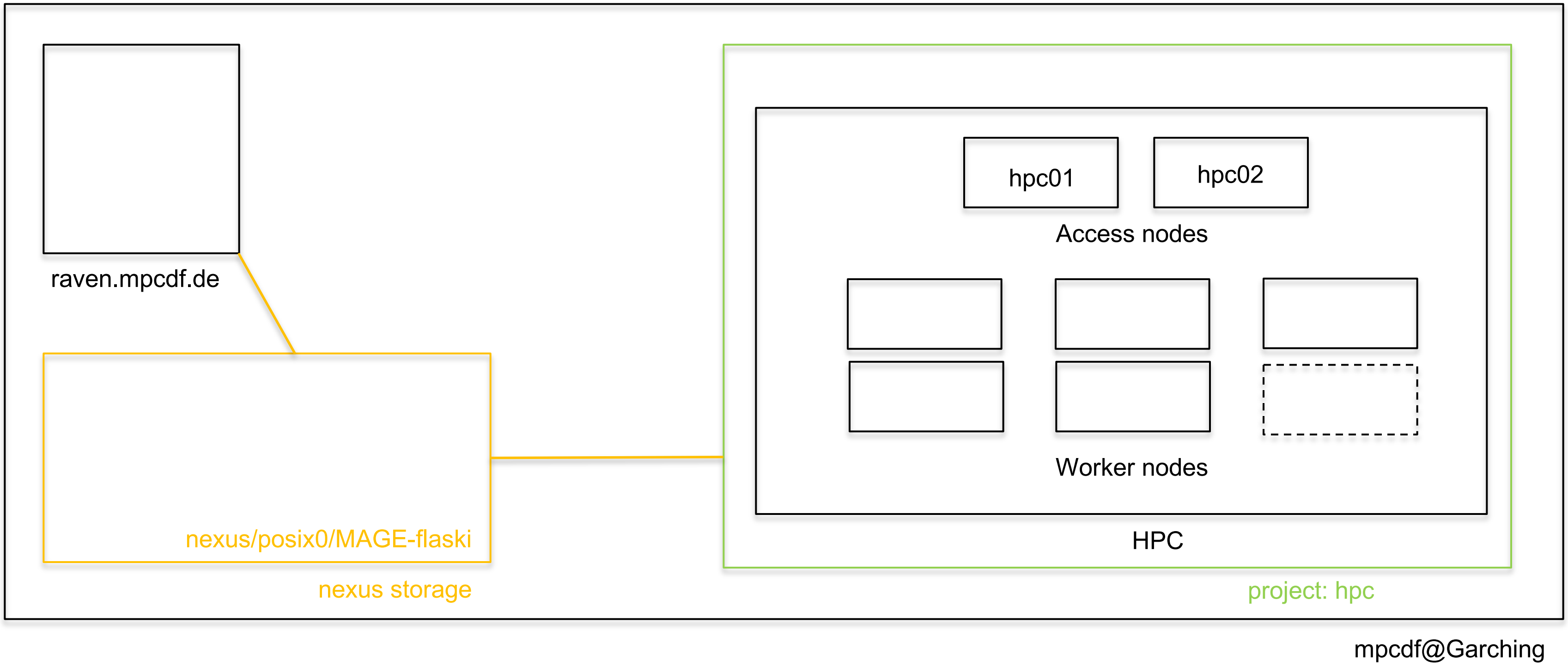
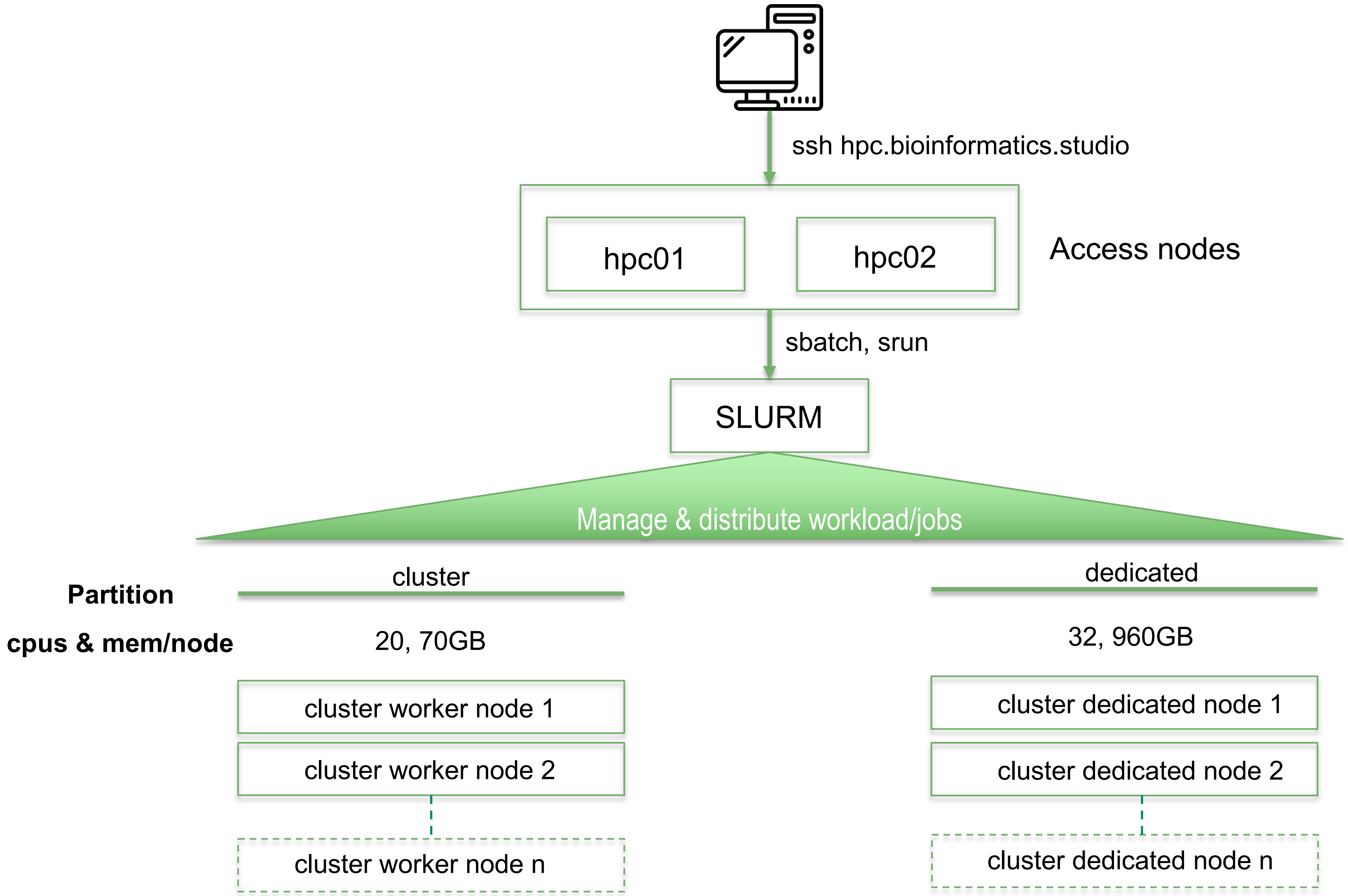
Introduction to hpc.bioinformatics.studio

Cloud Infrastructure



Workflow Architecture



ssh hpc.bioinformatics.studio

hpc01

hpc02

Access nodes

sbatch, srun

SLURM

Manage & distribute workload/jobs

Partition	cluster	dedicated
cpus & mem/node	20, 70GB	32, 960GB

cluster worker node 1

cluster worker node 2

cluster worker node n

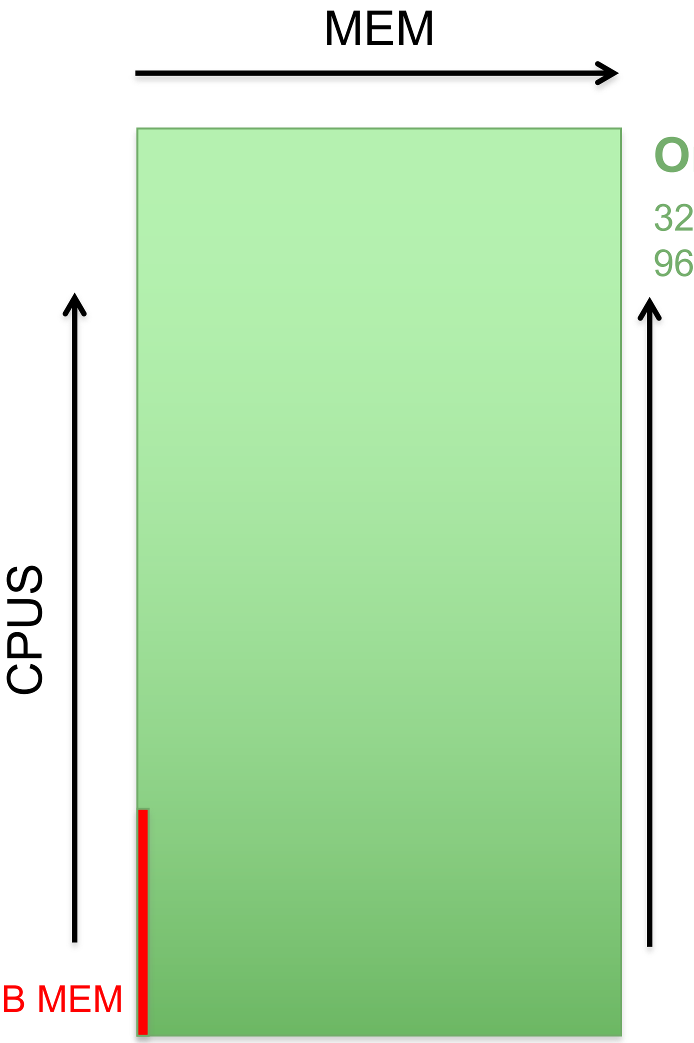
cluster dedicated node 1

cluster dedicated node 2

cluster dedicated node n

*** icons collected from https://www.freepik.com/

Why a HPC cluster?



One HPC node:

32 CPUS
960 GB MEM

MAC mini: 8 cpus, 16 GB MEM

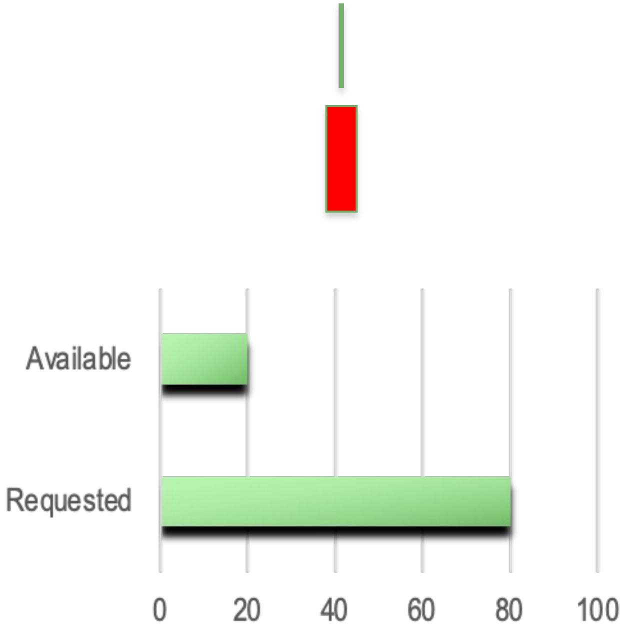
Why a HPC cluster?

MAC mini

1 user

4 raw data files

20 cpus / raw file

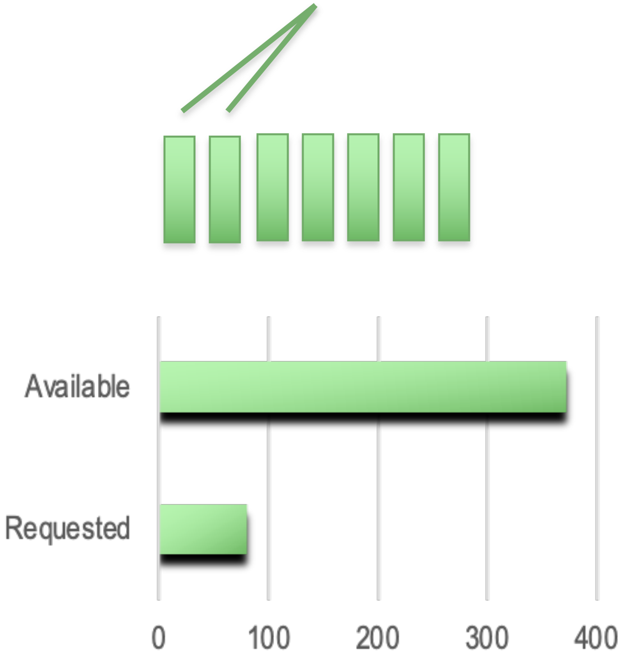


HPC CLUSTER

1 user

4 raw data files

20 cpus / raw file



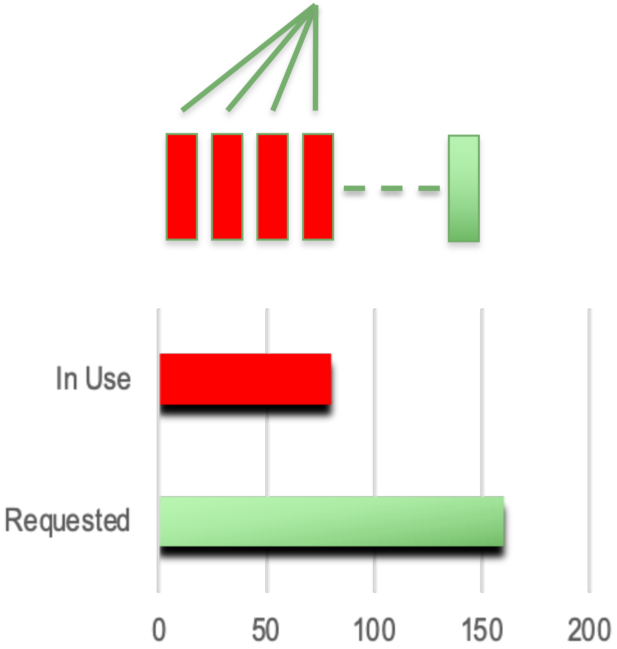
*** The resources shown here are to provide an overview, the numbers are not exact as the hpc.bioinformatics.studio

Why SLURM?

NO slurm

8 users

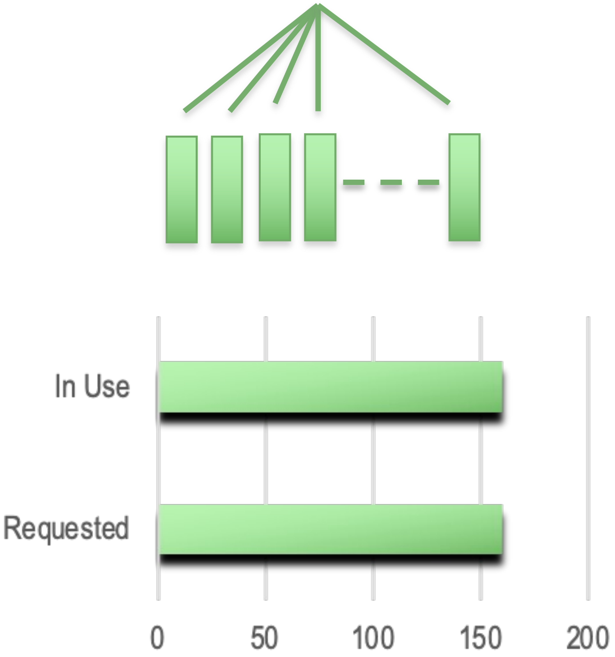
20 cpus/user



with slurm

8 users

20 cpus/user



How SLURM?

NO slurm

```
> bwa mem sample1.fastq
```

with slurm

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

How SLURM?

NO slurm

```
> bwa mem –T 18 sample1.fastq
```

with slurm

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

(5 days and 24 hours = 6 days

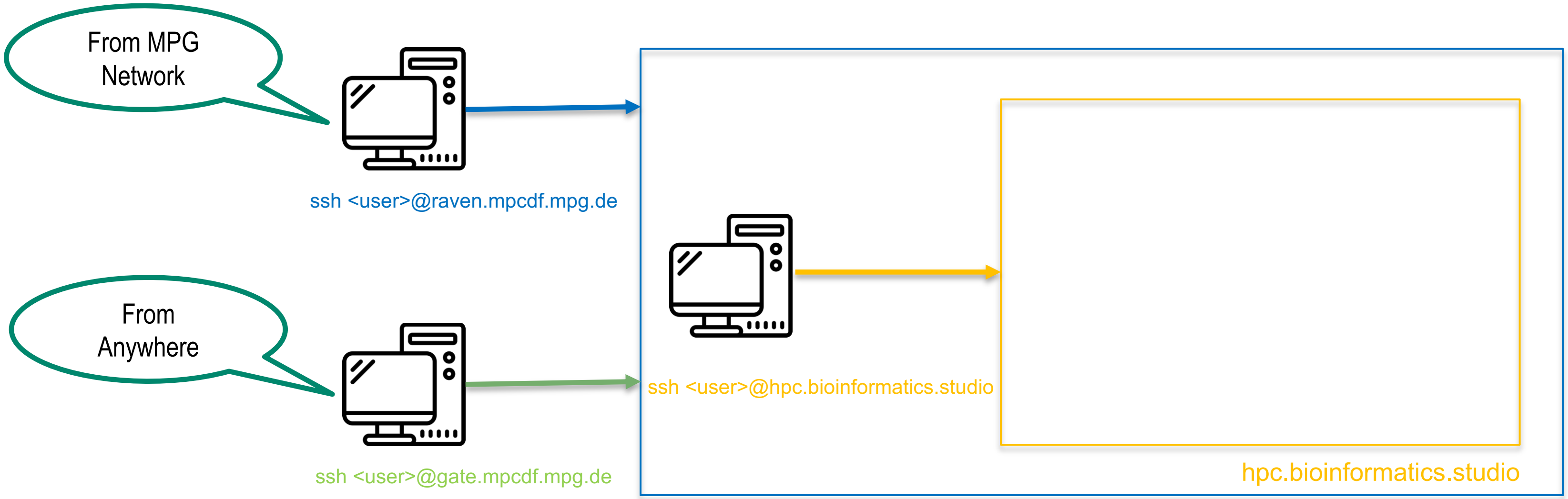
alternative: 144:00:00;

maximum = 14 days)

Getting Started

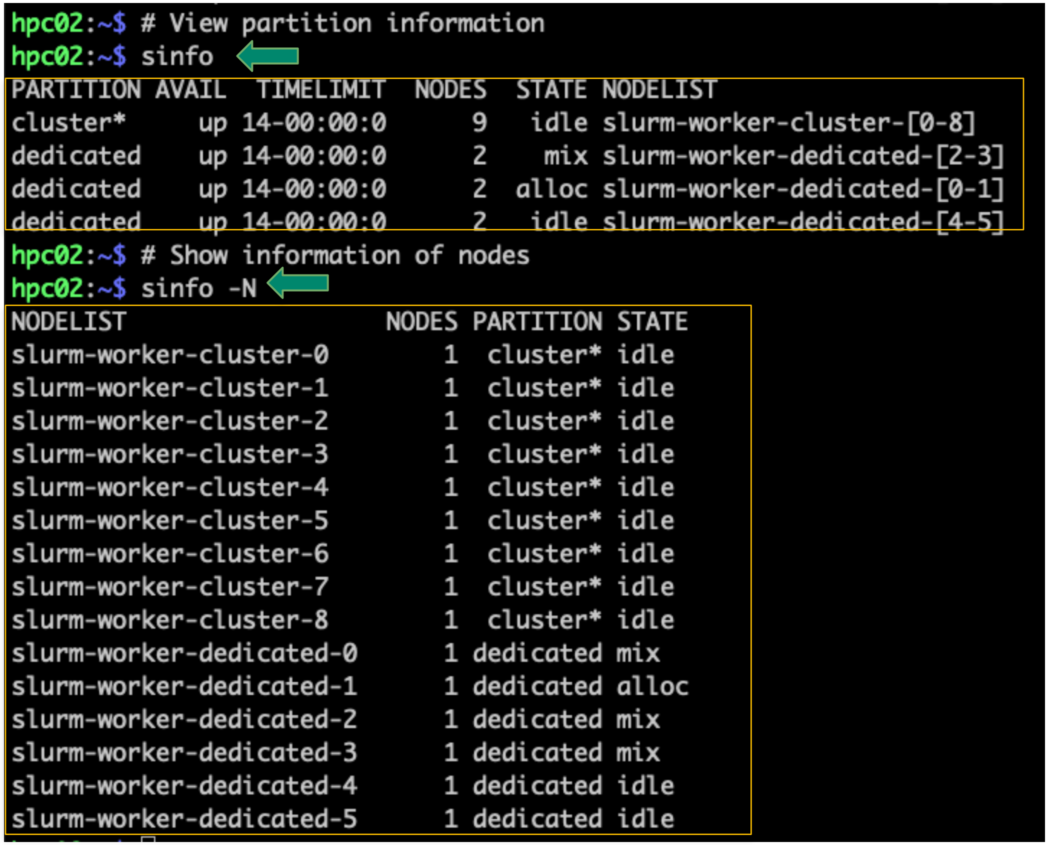
Prerequisite

- A user account at MPCDF (MPCDF Registration)
- A hpc.bioinformatics.studio account (contact: bioinformatics@age.mpg.de)


From MPG Network
From Anywhere
ssh <user>@raven.mpcdf.mpg.de
ssh <user>@gate.mpcdf.mpg.de
ssh <user>@hpc.bioinformatics.studio
hpc.bioinformatics.studio

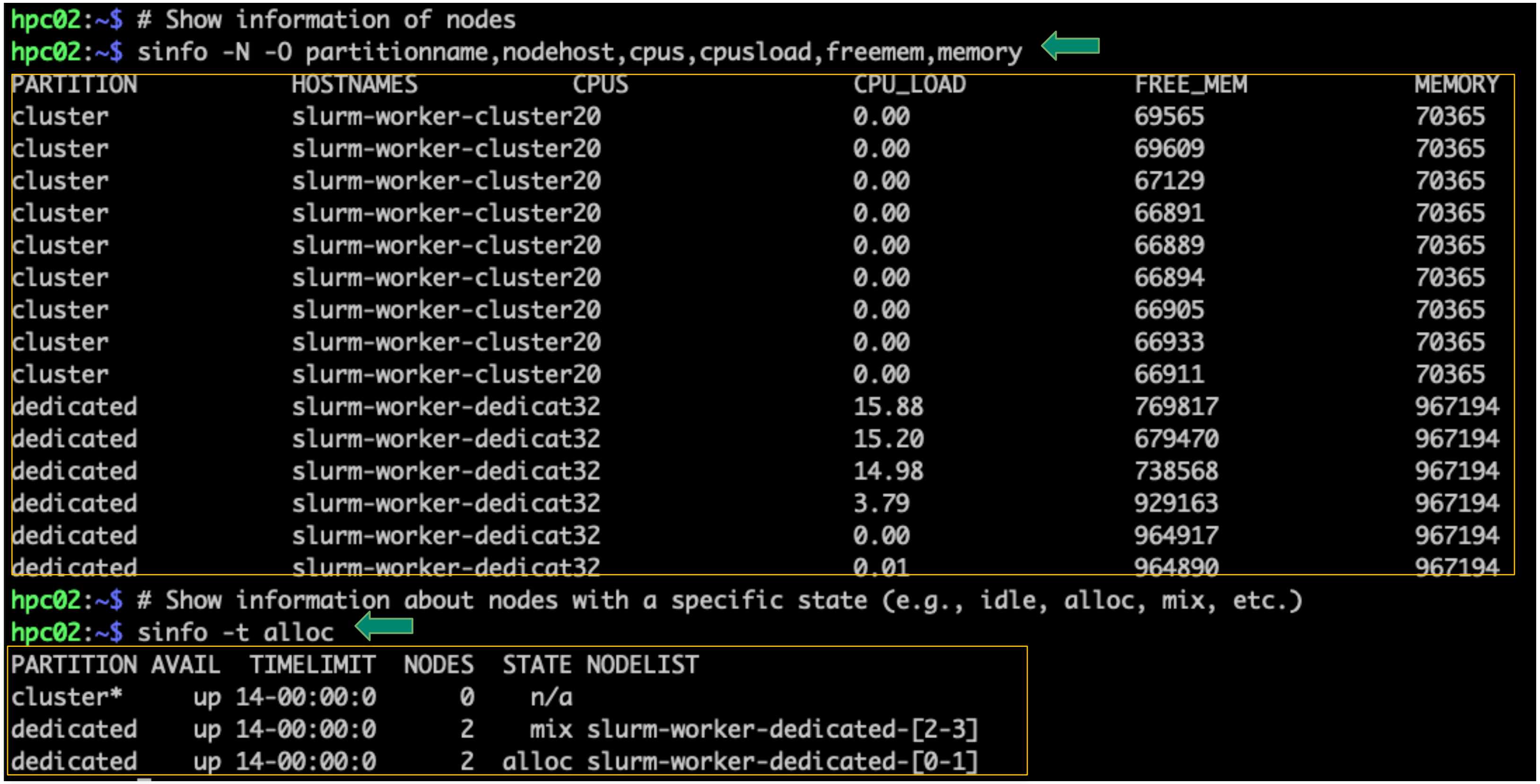
*** icons collected from https://www.freepik.com/

SLURM Commands: cluster info



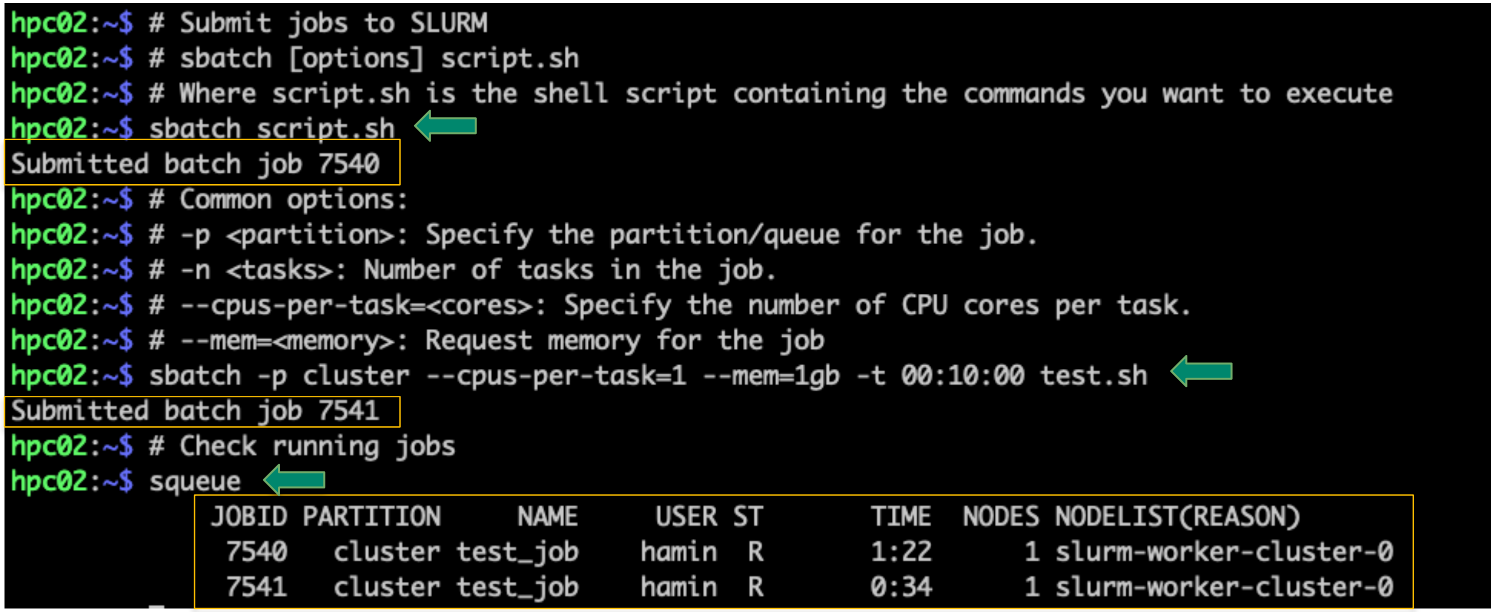
```
hpc02:~$ # View partition information
hpc02:~$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
cluster*     up 14-00:00:0      9   idle slurm-worker-cluster-[0-8]
dedicated    up 14-00:00:0      2    mix slurm-worker-dedicated-[2-3]
dedicated    up 14-00:00:0      2  alloc slurm-worker-dedicated-[0-1]
dedicated    up 14-00:00:0      2   idle slurm-worker-dedicated-[4-5]
hpc02:~$ # Show information of nodes
hpc02:~$ sinfo -N
NODELIST                   NODES PARTITION STATE
slurm-worker-cluster-0         1   cluster* idle
slurm-worker-cluster-1         1   cluster* idle
slurm-worker-cluster-2         1   cluster* idle
slurm-worker-cluster-3         1   cluster* idle
slurm-worker-cluster-4         1   cluster* idle
slurm-worker-cluster-5         1   cluster* idle
slurm-worker-cluster-6         1   cluster* idle
slurm-worker-cluster-7         1   cluster* idle
slurm-worker-cluster-8         1   cluster* idle
slurm-worker-dedicated-0       1 dedicated mix
slurm-worker-dedicated-1       1 dedicated alloc
slurm-worker-dedicated-2       1 dedicated mix
slurm-worker-dedicated-3       1 dedicated mix
slurm-worker-dedicated-4       1 dedicated idle
slurm-worker-dedicated-5       1 dedicated idle
```

SLURM Commands: cluster info



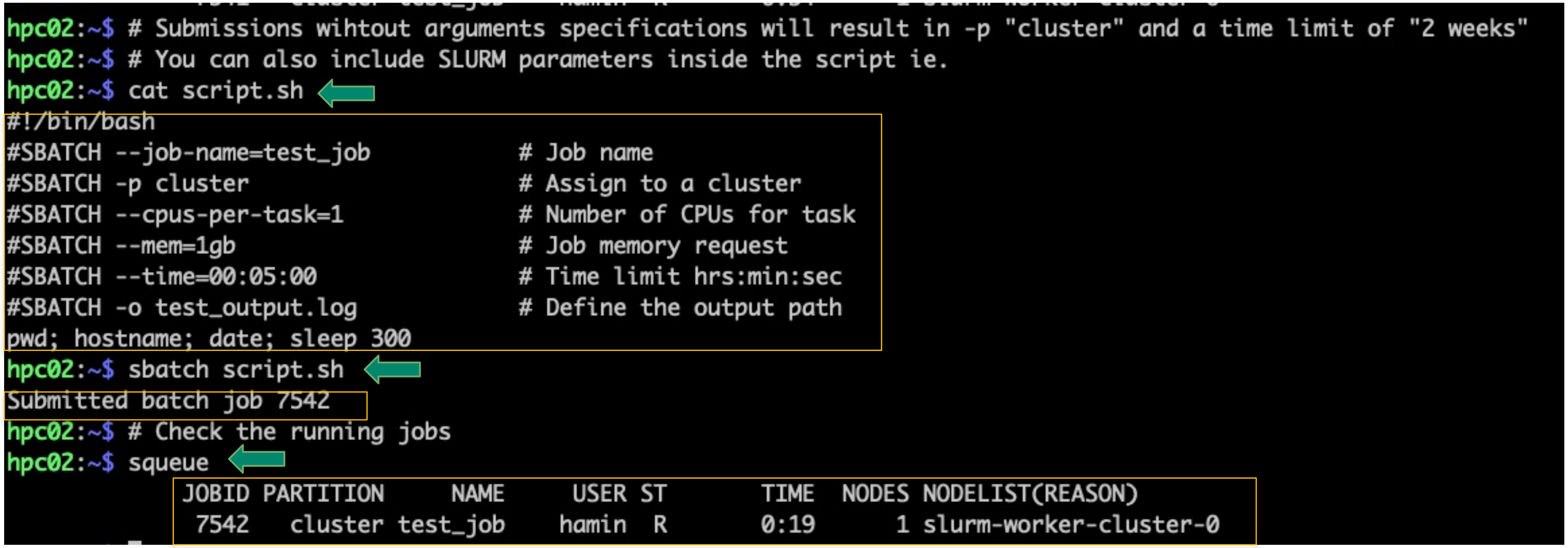
```
hpc02:~$ # Show information of nodes
hpc02:~$ sinfo -N -O partitionname,nodehost,cpus,cpusload,freemem,memory
PARTITION           HOSTNAMES           CPUS                CPU_LOAD            FREE_MEM            MEMORY
cluster             slurm-worker-cluster20                  0.00                69565               70365
cluster             slurm-worker-cluster20                  0.00                69609               70365
cluster             slurm-worker-cluster20                  0.00                67129               70365
cluster             slurm-worker-cluster20                  0.00                66891               70365
cluster             slurm-worker-cluster20                  0.00                66889               70365
cluster             slurm-worker-cluster20                  0.00                66894               70365
cluster             slurm-worker-cluster20                  0.00                66905               70365
cluster             slurm-worker-cluster20                  0.00                66933               70365
cluster             slurm-worker-cluster20                  0.00                66911               70365
dedicated           slurm-worker-dedicat32                  15.88               769817              967194
dedicated           slurm-worker-dedicat32                  15.20               679470              967194
dedicated           slurm-worker-dedicat32                  14.98               738568              967194
dedicated           slurm-worker-dedicat32                  3.79                929163              967194
dedicated           slurm-worker-dedicat32                  0.00                964917              967194
dedicated           slurm-worker-dedicat32                  0.01                964890              967194
hpc02:~$ # Show information about nodes with a specific state (e.g., idle, alloc, mix, etc.)
hpc02:~$ sinfo -t alloc
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
cluster*     up 14-00:00:0      0    n/a
dedicated    up 14-00:00:0      2    mix slurm-worker-dedicated-[2-3]
dedicated    up 14-00:00:0      2  alloc slurm-worker-dedicated-[0-1]
```

SLURM Commands: submitting jobs



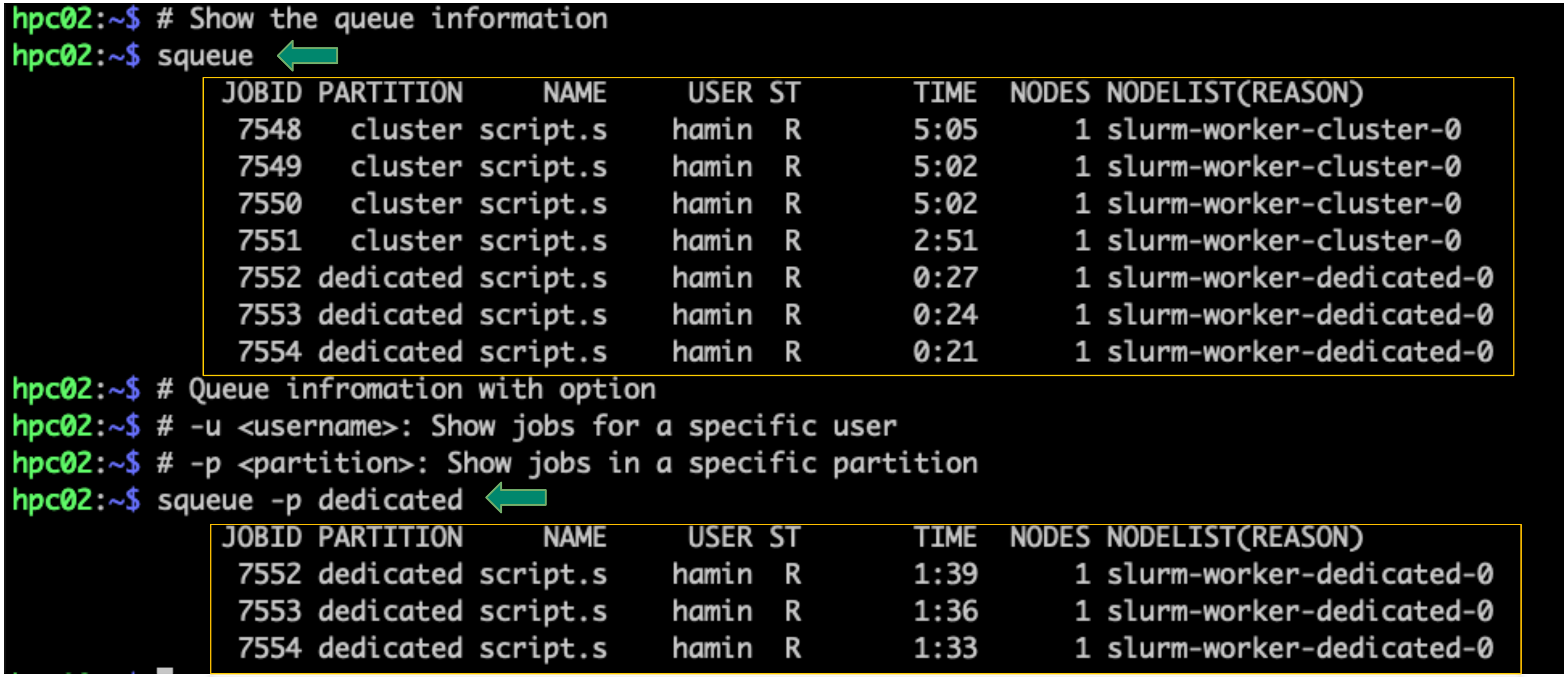
```
hpc02:~$ # Submit jobs to SLURM
hpc02:~$ # sbatch [options] script.sh
hpc02:~$ # Where script.sh is the shell script containing the commands you want to execute
hpc02:~$ sbatch script.sh
Submitted batch job 7540
hpc02:~$ # Common options:
hpc02:~$ # -p <partition>: Specify the partition/queue for the job.
hpc02:~$ # -n <tasks>: Number of tasks in the job.
hpc02:~$ # --cpus-per-task=<cores>: Specify the number of CPU cores per task.
hpc02:~$ # --mem=<memory>: Request memory for the job
hpc02:~$ sbatch -p cluster --cpus-per-task=1 --mem=1gb -t 00:10:00 test.sh
Submitted batch job 7541
hpc02:~$ # Check running jobs
hpc02:~$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
              7540   cluster test_job    hamin  R       1:22      1 slurm-worker-cluster-0
              7541   cluster test_job    hamin  R       0:34      1 slurm-worker-cluster-0
```

SLURM Commands: submitting jobs



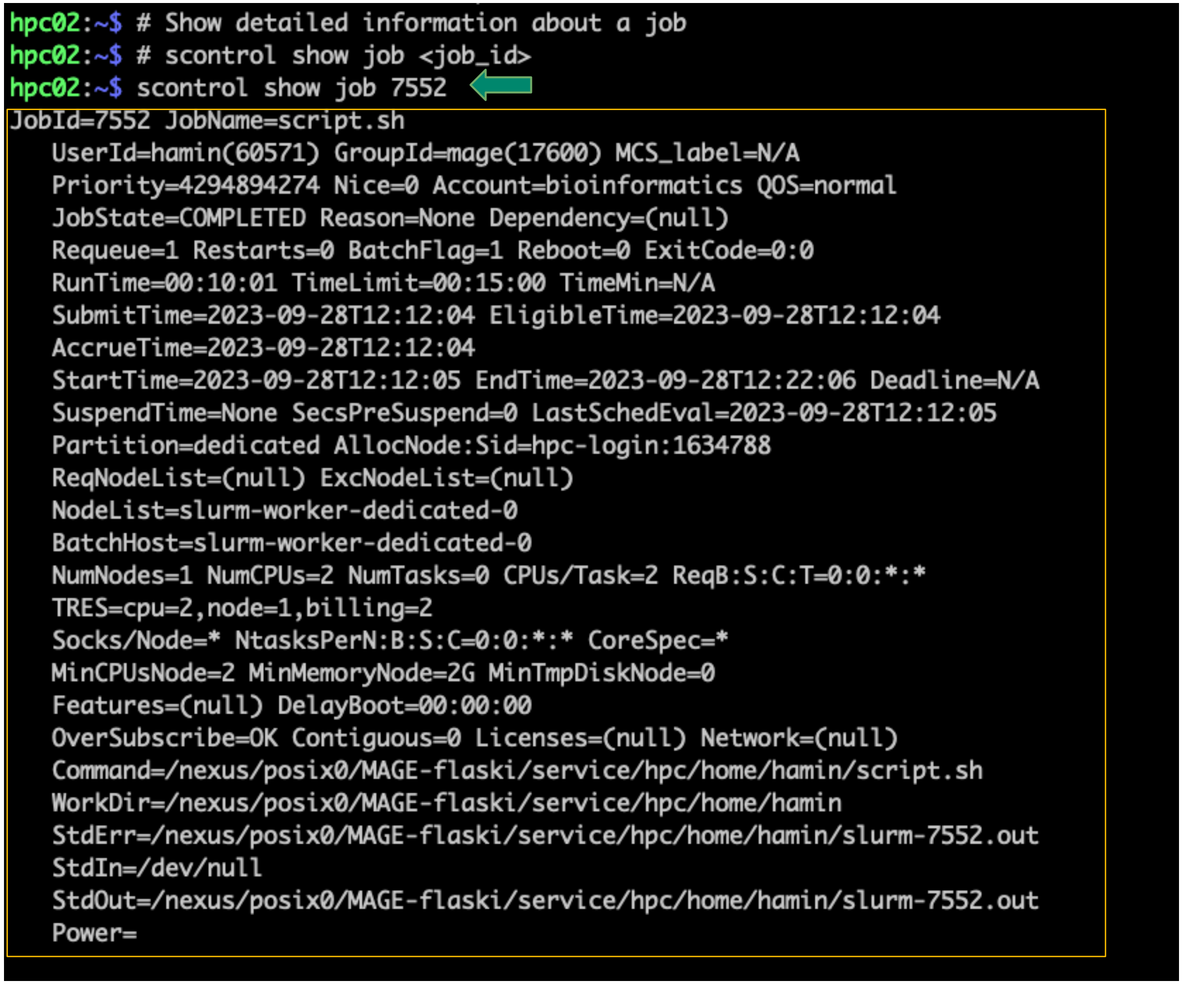
```
hpc02:~$ # Submissions wihtout arguments specifications will result in -p "cluster" and a time limit of "2 weeks"
hpc02:~$ # You can also include SLURM parameters inside the script ie.
hpc02:~$ cat script.sh
#!/bin/bash
#SBATCH --job-name=test_job          # Job name
#SBATCH -p cluster                   # Assign to a cluster
#SBATCH --cpus-per-task=1            # Number of CPUs for task
#SBATCH --mem=1gb                    # Job memory request
#SBATCH --time=00:05:00              # Time limit hrs:min:sec
#SBATCH -o test_output.log           # Define the output path
pwd; hostname; date; sleep 300
hpc02:~$ sbatch script.sh
Submitted batch job 7542
hpc02:~$ # Check the running jobs
hpc02:~$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
              7542   cluster test_job    hamin  R       0:19      1 slurm-worker-cluster-0
```

SLURM Commands: checking queue status



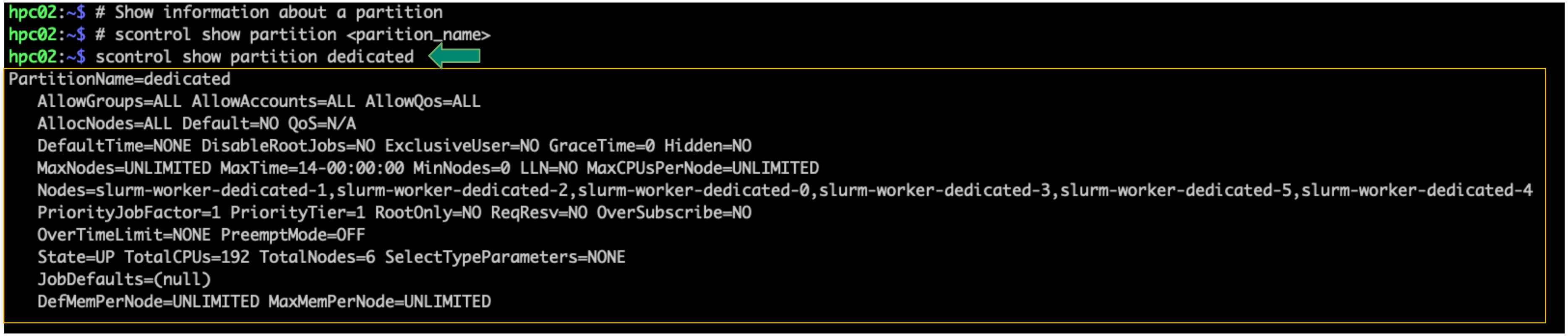
```
hpc02:~$ # Show the queue information
hpc02:~$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
              7548   cluster script.s    hamin  R       5:05      1 slurm-worker-cluster-0
              7549   cluster script.s    hamin  R       5:02      1 slurm-worker-cluster-0
              7550   cluster script.s    hamin  R       5:02      1 slurm-worker-cluster-0
              7551   cluster script.s    hamin  R       2:51      1 slurm-worker-cluster-0
              7552 dedicated script.s    hamin  R       0:27      1 slurm-worker-dedicated-0
              7553 dedicated script.s    hamin  R       0:24      1 slurm-worker-dedicated-0
              7554 dedicated script.s    hamin  R       0:21      1 slurm-worker-dedicated-0
hpc02:~$ # Queue infromation with option
hpc02:~$ # -u <username>: Show jobs for a specific user
hpc02:~$ # -p <partition>: Show jobs in a specific partition
hpc02:~$ squeue -p dedicated
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
              7552 dedicated script.s    hamin  R       1:39      1 slurm-worker-dedicated-0
              7553 dedicated script.s    hamin  R       1:36      1 slurm-worker-dedicated-0
              7554 dedicated script.s    hamin  R       1:33      1 slurm-worker-dedicated-0
```

SLURM Commands: controlling jobs



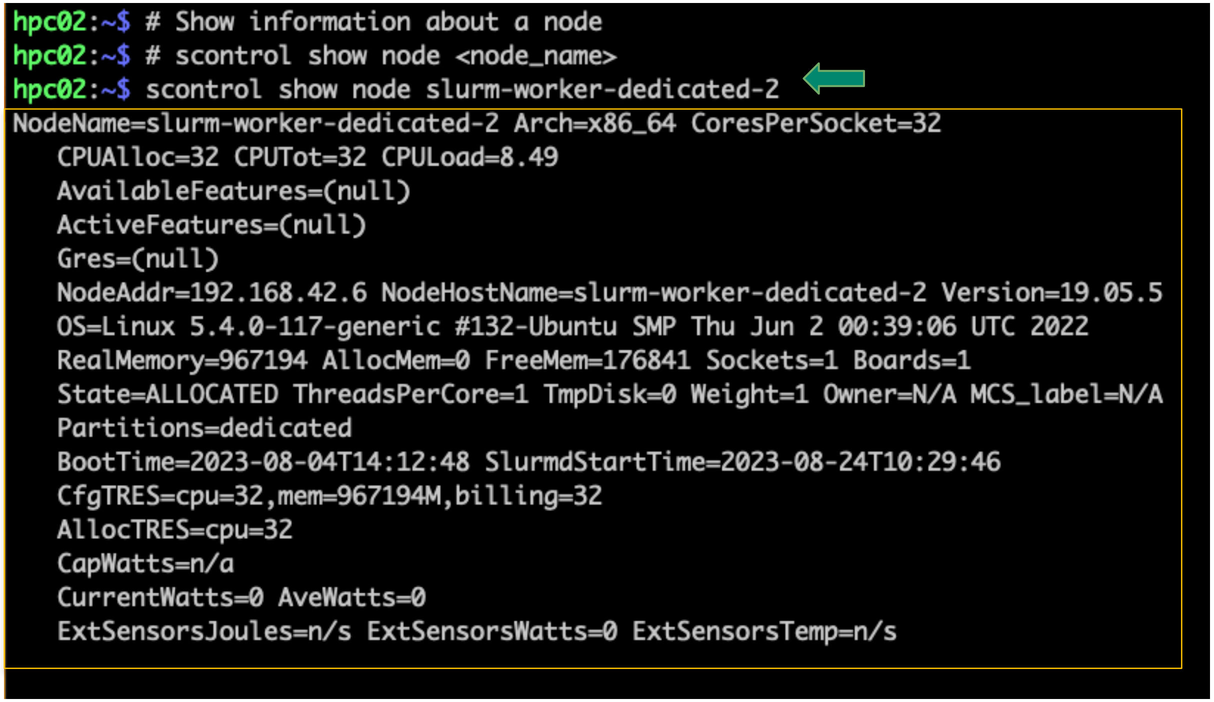
```
hpc02:~$ # Show detailed information about a job
hpc02:~$ # scontrol show job <job_id>
hpc02:~$ scontrol show job 7552
JobId=7552 JobName=script.sh
   UserId=hamin(60571) GroupId=mage(17600) MCS_label=N/A
   Priority=4294894274 Nice=0 Account=bioinformatics QOS=normal
   JobState=COMPLETED Reason=None Dependency=(null)
   Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
   RunTime=00:10:01 TimeLimit=00:15:00 TimeMin=N/A
   SubmitTime=2023-09-28T12:12:04 EligibleTime=2023-09-28T12:12:04
   AccrueTime=2023-09-28T12:12:04
   StartTime=2023-09-28T12:12:05 EndTime=2023-09-28T12:22:06 Deadline=N/A
   SuspendTime=None SecsPreSuspend=0 LastSchedEval=2023-09-28T12:12:05
   Partition=dedicated AllocNode:Sid=hpc-login:1634788
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=slurm-worker-dedicated-0
   BatchHost=slurm-worker-dedicated-0
   NumNodes=1 NumCPUs=2 NumTasks=0 CPUs/Task=2 ReqB:S:C:T=0:0:*:*
   TRES=cpu=2,node=1,billing=2
   Socks/Node=* NtasksPerN:B:S:C=0:0:*:* CoreSpec=*
   MinCPUsNode=2 MinMemoryNode=2G MinTmpDiskNode=0
   Features=(null) DelayBoot=00:00:00
   OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)
   Command=/nexus/posix0/MAGE-flaski/service/hpc/home/hamin/script.sh
   WorkDir=/nexus/posix0/MAGE-flaski/service/hpc/home/hamin
   StdErr=/nexus/posix0/MAGE-flaski/service/hpc/home/hamin/slurm-7552.out
   StdIn=/dev/null
   StdOut=/nexus/posix0/MAGE-flaski/service/hpc/home/hamin/slurm-7552.out
   Power=
```

SLURM Commands: controlling jobs



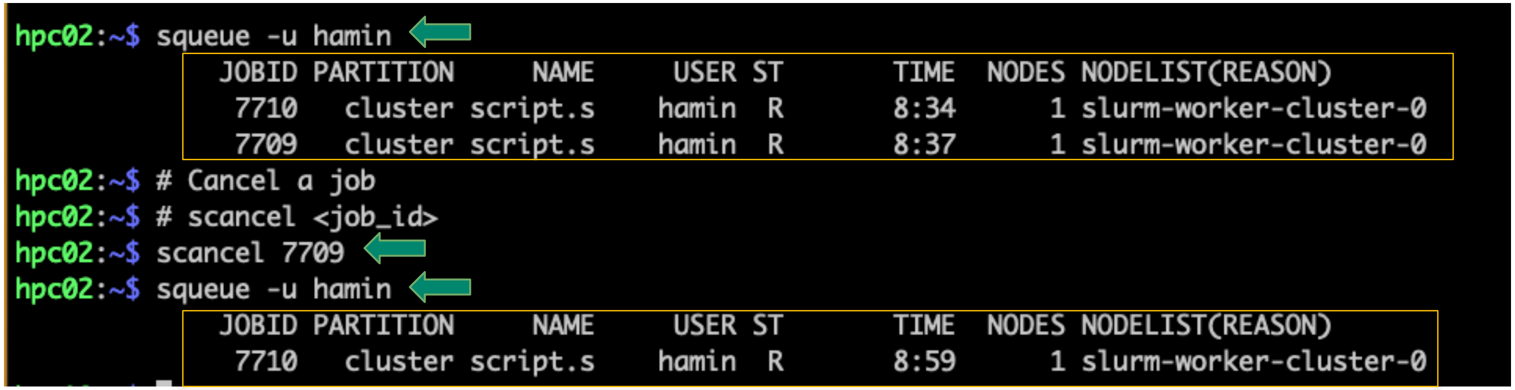
```
hpc02:~$ # Show information about a partition
hpc02:~$ # scontrol show partition <parition_name>
hpc02:~$ scontrol show partition dedicated
PartitionName=dedicated
   AllowGroups=ALL AllowAccounts=ALL AllowQos=ALL
   AllocNodes=ALL Default=NO QoS=N/A
   DefaultTime=NONE DisableRootJobs=NO ExclusiveUser=NO GraceTime=0 Hidden=NO
   MaxNodes=UNLIMITED MaxTime=14-00:00:00 MinNodes=0 LLN=NO MaxCPUsPerNode=UNLIMITED
   Nodes=slurm-worker-dedicated-1,slurm-worker-dedicated-2,slurm-worker-dedicated-0,slurm-worker-dedicated-3,slurm-worker-dedicated-5,slurm-worker-dedicated-4
   PriorityJobFactor=1 PriorityTier=1 RootOnly=NO ReqResv=NO OverSubscribe=NO
   OverTimeLimit=NONE PreemptMode=OFF
   State=UP TotalCPUs=192 TotalNodes=6 SelectTypeParameters=NONE
   JobDefaults=(null)
   DefMemPerNode=UNLIMITED MaxMemPerNode=UNLIMITED
```

SLURM Commands: controlling jobs



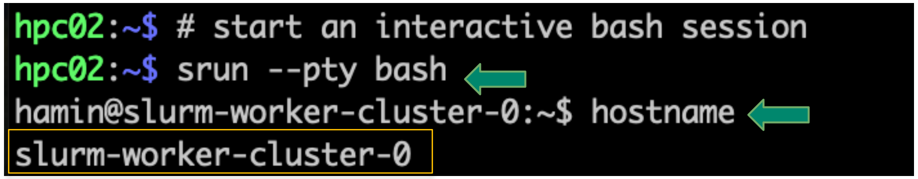
```
hpc02:~$ # Show information about a node
hpc02:~$ # scontrol show node <node_name>
hpc02:~$ scontrol show node slurm-worker-dedicated-2
NodeName=slurm-worker-dedicated-2 Arch=x86_64 CoresPerSocket=32
   CPUAlloc=32 CPUTot=32 CPULoad=8.49
   AvailableFeatures=(null)
   ActiveFeatures=(null)
   Gres=(null)
   NodeAddr=192.168.42.6 NodeHostName=slurm-worker-dedicated-2 Version=19.05.5
   OS=Linux 5.4.0-117-generic #132-Ubuntu SMP Thu Jun 2 00:39:06 UTC 2022
   RealMemory=967194 AllocMem=0 FreeMem=176841 Sockets=1 Boards=1
   State=ALLOCATED ThreadsPerCore=1 TmpDisk=0 Weight=1 Owner=N/A MCS_label=N/A
   Partitions=dedicated
   BootTime=2023-08-04T14:12:48 SlurmdStartTime=2023-08-24T10:29:46
   CfgTRES=cpu=32,mem=967194M,billing=32
   AllocTRES=cpu=32
   CapWatts=n/a
   CurrentWatts=0 AveWatts=0
   ExtSensorsJoules=n/s ExtSensorsWatts=0 ExtSensorsTemp=n/s
```

SLURM Commands: cancel a job

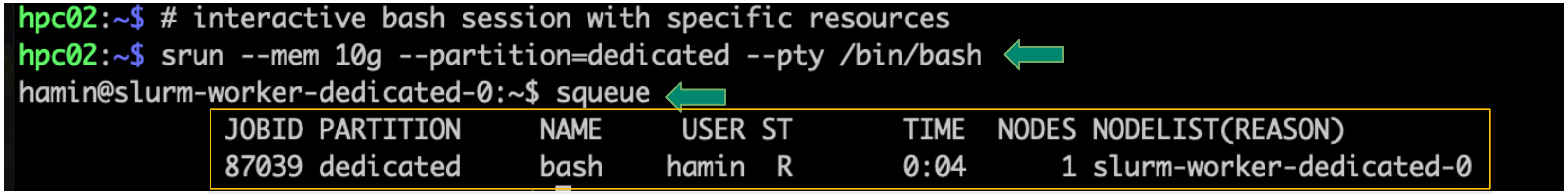


```
hpc02:~$ squeue -u hamin
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
              7710   cluster script.s    hamin  R       8:34      1 slurm-worker-cluster-0
              7709   cluster script.s    hamin  R       8:37      1 slurm-worker-cluster-0
hpc02:~$ # Cancel a job
hpc02:~$ # scancel <job_id>
hpc02:~$ scancel 7709
hpc02:~$ squeue -u hamin
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
              7710   cluster script.s    hamin  R       8:59      1 slurm-worker-cluster-0
```

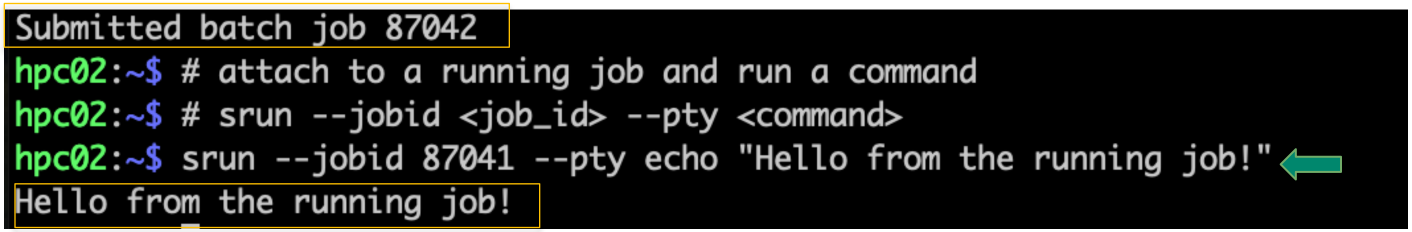
SLURM Commands: interactive session



```
hpc02:~$ # start an interactive bash session
hpc02:~$ srun --pty bash
hamin@slurm-worker-cluster-0:~$ hostname
slurm-worker-cluster-0
```

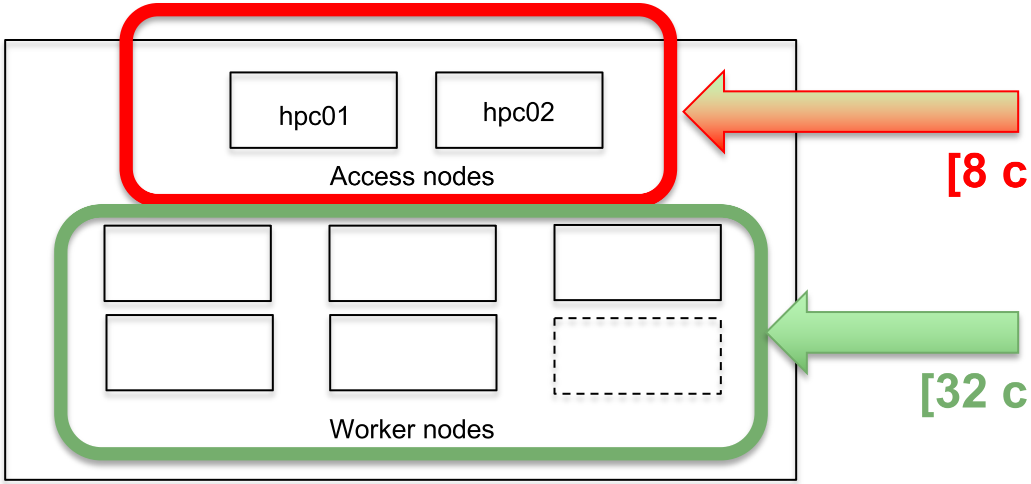


```
hpc02:~$ # interactive bash session with specific resources
hpc02:~$ srun --mem 10g --partition=dedicated --pty /bin/bash
hamin@slurm-worker-dedicated-0:~$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             87039 dedicated     bash    hamin  R       0:04      1 slurm-worker-dedicated-0
```



```
Submitted batch job 87042
hpc02:~$ # attach to a running job and run a command
hpc02:~$ # srun --jobid <job_id> --pty <command>
hpc02:~$ srun --jobid 87041 --pty echo "Hello from the running job!"
Hello from the running job!
```

Effective Use: access nodes are not for computation



Not for Computation
(low on resources)
[8 cpus, 25GB mem per node]

For Computation
(high on resources)
[32 cpus, 960GB mem per node]

sbatch <script> : runs on worker nodes

bash <script> : runs on aceess nodes

Effective Use: prevent overloading the cluster

```
#!/bin/bash
# Limit the number of simultaneously running jobs
cd ~/project/raw_data
for f in $(ls *.fastq);
  do  rm ~/project/slurm_logs/${f}.*.out

  # wait if the running jobs exceed the limit
  while [  `squeue -u username | wc -l` -gt "500" ];
    do echo "sleeping"; sleep 300
  done

  sbatch --cpus-per-task=4 --mem=8gb --time=5-24 \
  -p cluster -o ~/project/slurm_logs/${f}.%j.out ~/project/tmp/${f}.sh << EOF
  #!/bin/bash
  # necessary operations
  EOF

done
exit
```

Use Case

If you need to run a large number of jobs
(a job for each file)

Effective Use: resource assignment

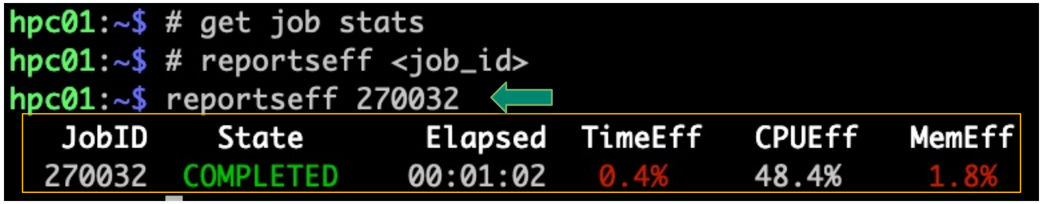
Over assignments of resources (e.g. number of CPUs: *--cpus-per-task*, memory: --mem) occupies unnecessary space or computational power

Think about it!

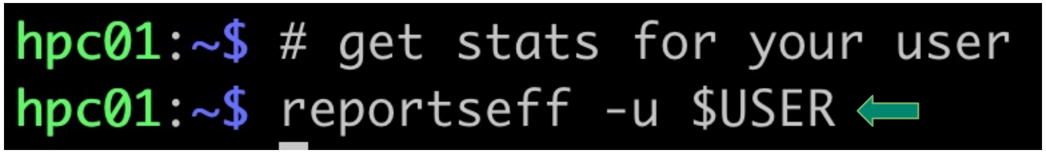
A MAC mini holds: 8 cpus, 16 GB mem

Your job may not need the resources you are allocating!

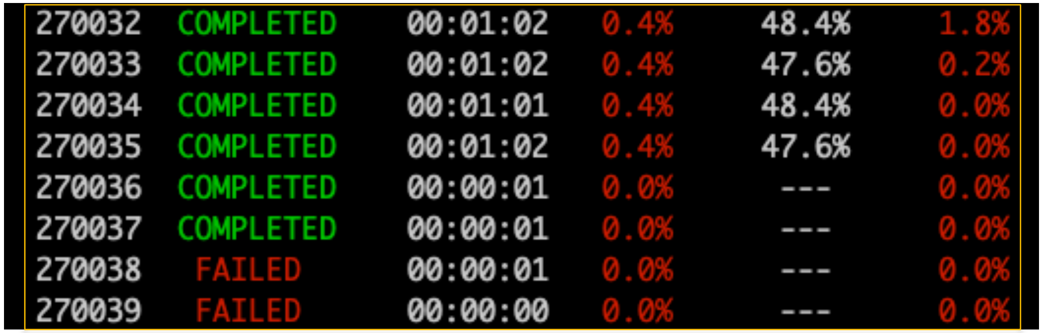
Effective Use: get job stats



```
hpc01:~$ # get job stats
hpc01:~$ # reportseff <job_id>
hpc01:~$ reportseff 270032
    JobID      State          Elapsed  TimeEff   CPUEff   MemEff
   270032   COMPLETED        00:01:02   0.4%     48.4%     1.8%
```



```
hpc01:~$ # get stats for your user
hpc01:~$ reportseff -u $USER
```



```
 270032  COMPLETED    00:01:02  0.4%    48.4%    1.8%
 270033  COMPLETED    00:01:02  0.4%    47.6%    0.2%
 270034  COMPLETED    00:01:01  0.4%    48.4%    0.0%
 270035  COMPLETED    00:01:02  0.4%    47.6%    0.0%
 270036  COMPLETED    00:00:01  0.0%     ---     0.0%
 270037  COMPLETED    00:00:01  0.0%     ---     0.0%
 270038   FAILED      00:00:01  0.0%     ---     0.0%
 270039   FAILED      00:00:00  0.0%     ---     0.0%
```

Can also get resource usage of running process with:
srun --jobid <job_id> --pty htop --user=$USER

SLURM Concepts: at a glance

An open-source workload manager and job scheduler

Manages and schedules tasks across a cluster of computers

Job: Unit of work submitted to SLURM for execution

Partitions: Groups of nodes with similar characteristics

Nodes: Individual computers in the cluster that execute jobs

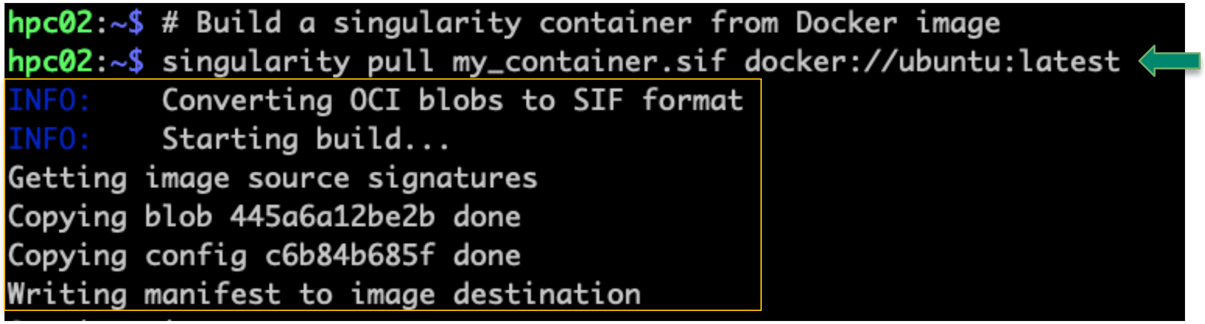
Resources: Includes CPU cores, memory, and other hardware resources

Singularity/Apptainer

Why Singularity?

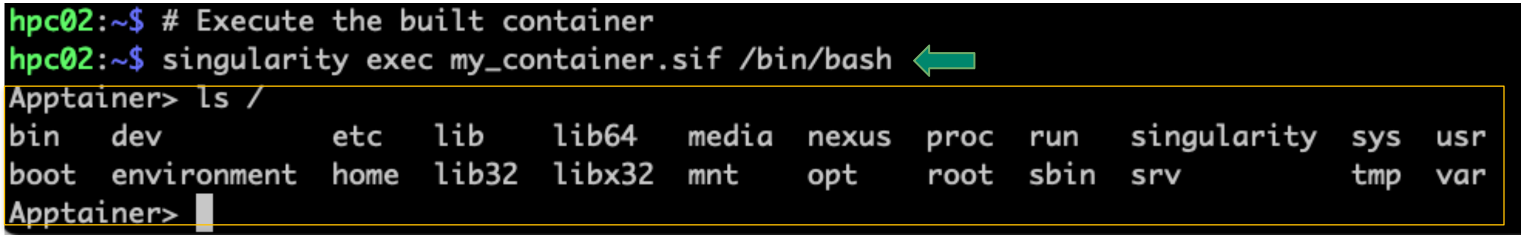
- Container engine for HPC
- No root privilege required
- Reproducible, portable, distributable container
- Easy conversion from docker to singularity container

Singularity: example

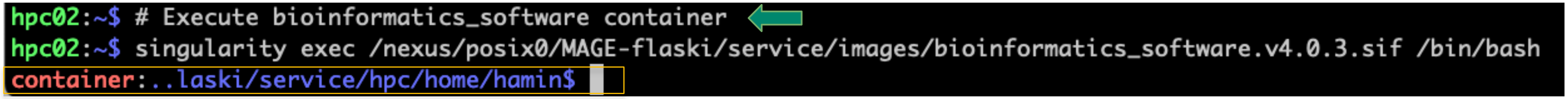


```
hpc02:~$ # Build a singularity container from Docker image
hpc02:~$ singularity pull my_container.sif docker://ubuntu:latest
INFO:    Converting OCI blobs to SIF format
INFO:    Starting build...
Getting image source signatures
Copying blob 445a6a12be2b done
Copying config c6b84b685f done
Writing manifest to image destination
```

* alternates: singularity run <image>, singularity shell <image>, singularity build <image_name> <image>



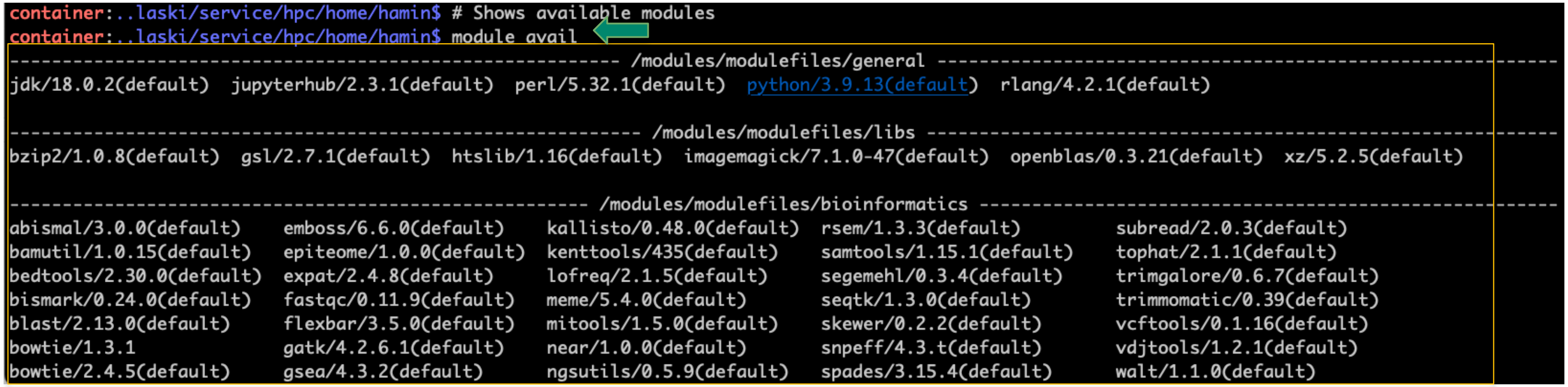
```
hpc02:~$ # Execute the built container
hpc02:~$ singularity exec my_container.sif /bin/bash
Apptainer> ls /
bin   dev          etc   lib    lib64   media  nexus  proc  run   singularity  sys  usr
boot  environment  home  lib32  libx32  mnt    opt    root  sbin  srv          tmp  var
Apptainer>
```



```
hpc02:~$ # Execute bioinformatics_software container
hpc02:~$ singularity exec /nexus/posix0/MAGE-flaski/service/images/bioinformatics_software.v4.0.3.sif /bin/bash
container:..laski/service/hpc/home/hamin$
```

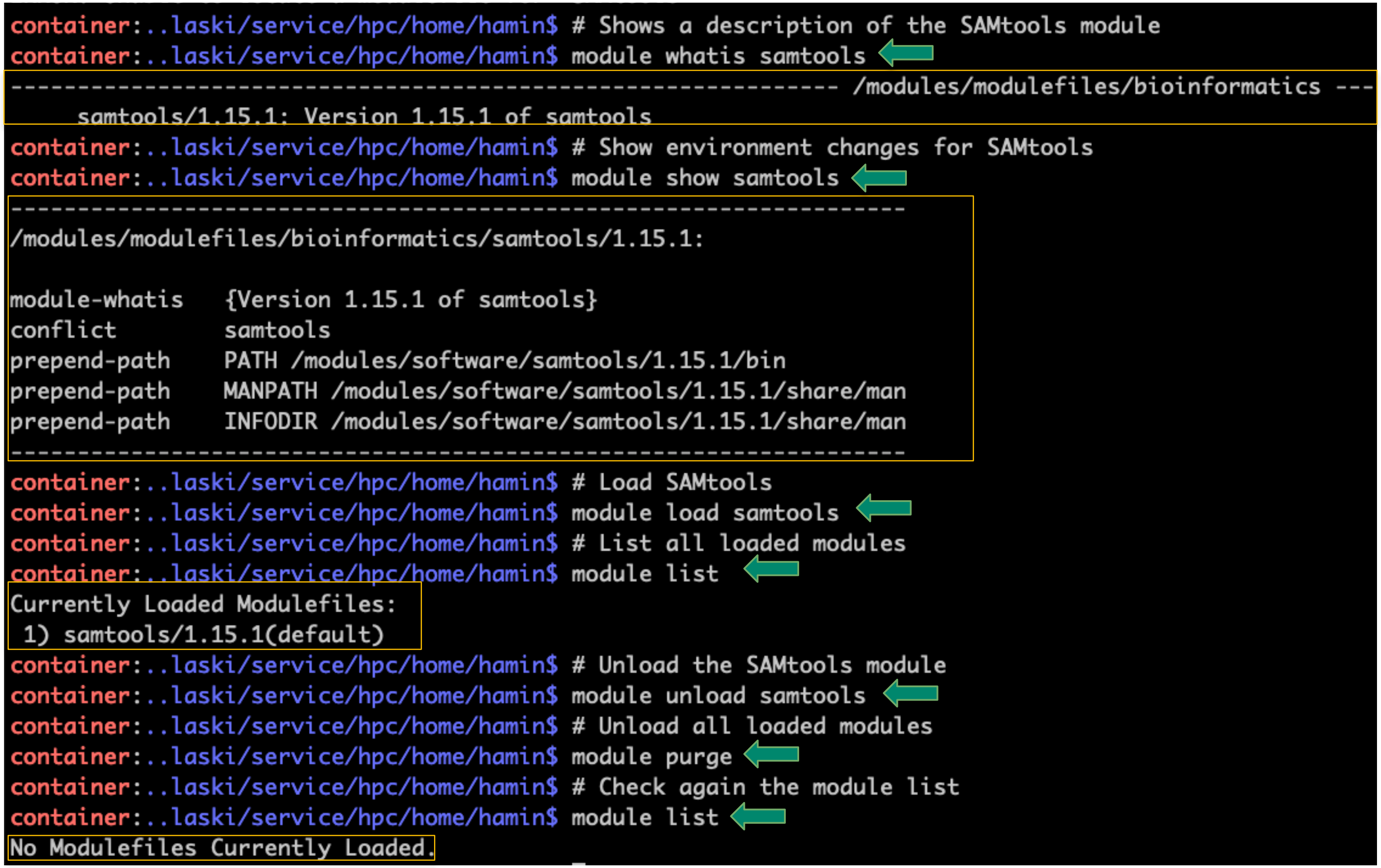
The Modules System

- Our mpgagebioinformatics/bioinformatics_software make use of the modules system to load and unload required software
- The modules system loads software (version of choice) and changes environment variables (eg. LD_LIBRARY_PATH)



```
container:..laski/service/hpc/home/hamin$ # Shows available modules
container:..laski/service/hpc/home/hamin$ module avail
---------------------------------------------------------- /modules/modulefiles/general -----------------------------------------------------------
jdk/18.0.2(default)  jupyterhub/2.3.1(default)  perl/5.32.1(default)  python/3.9.13(default)  rlang/4.2.1(default)

------------------------------------------------------------ /modules/modulefiles/libs ------------------------------------------------------------
bzip2/1.0.8(default)  gsl/2.7.1(default)  htslib/1.16(default)  imagemagick/7.1.0-47(default)  openblas/0.3.21(default)  xz/5.2.5(default)

------------------------------------------------------- /modules/modulefiles/bioinformatics -------------------------------------------------------
abismal/3.0.0(default)    emboss/6.6.0(default)    kallisto/0.48.0(default)  rsem/1.3.3(default)         subread/2.0.3(default)
bamutil/1.0.15(default)   epiteome/1.0.0(default)  kenttools/435(default)    samtools/1.15.1(default)    tophat/2.1.1(default)
bedtools/2.30.0(default)  expat/2.4.8(default)     lofreq/2.1.5(default)     segemehl/0.3.4(default)     trimgalore/0.6.7(default)
bismark/0.24.0(default)   fastqc/0.11.9(default)   meme/5.4.0(default)       seqtk/1.3.0(default)        trimmomatic/0.39(default)
blast/2.13.0(default)     flexbar/3.5.0(default)   mitools/1.5.0(default)    skewer/0.2.2(default)       vcftools/0.1.16(default)
bowtie/1.3.1              gatk/4.2.6.1(default)    near/1.0.0(default)       snpeff/4.3.t(default)       vdjtools/1.2.1(default)
bowtie/2.4.5(default)     gsea/4.3.2(default)      ngsutils/0.5.9(default)   spades/3.15.4(default)      walt/1.1.0(default)
```

The Modules System



```
container:..laski/service/hpc/home/hamin$ # Shows a description of the SAMtools module
container:..laski/service/hpc/home/hamin$ module whatis samtools
------------------------------------------------------------ /modules/modulefiles/bioinformatics ---
     samtools/1.15.1: Version 1.15.1 of samtools
container:..laski/service/hpc/home/hamin$ # Show environment changes for SAMtools
container:..laski/service/hpc/home/hamin$ module show samtools
-------------------------------------------------------------------
/modules/modulefiles/bioinformatics/samtools/1.15.1:

module-whatis   {Version 1.15.1 of samtools}
conflict        samtools
prepend-path    PATH /modules/software/samtools/1.15.1/bin
prepend-path    MANPATH /modules/software/samtools/1.15.1/share/man
prepend-path    INFODIR /modules/software/samtools/1.15.1/share/man
-------------------------------------------------------------------
container:..laski/service/hpc/home/hamin$ # Load SAMtools
container:..laski/service/hpc/home/hamin$ module load samtools
container:..laski/service/hpc/home/hamin$ # List all loaded modules
container:..laski/service/hpc/home/hamin$ module list
Currently Loaded Modulefiles:
 1) samtools/1.15.1(default)
container:..laski/service/hpc/home/hamin$ # Unload the SAMtools module
container:..laski/service/hpc/home/hamin$ module unload samtools
container:..laski/service/hpc/home/hamin$ # Unload all loaded modules
container:..laski/service/hpc/home/hamin$ module purge
container:..laski/service/hpc/home/hamin$ # Check again the module list
container:..laski/service/hpc/home/hamin$ module list
No Modulefiles Currently Loaded.
```

RAVEN & hpc.bioinformatics.studio

Where to Run Your Jobs?

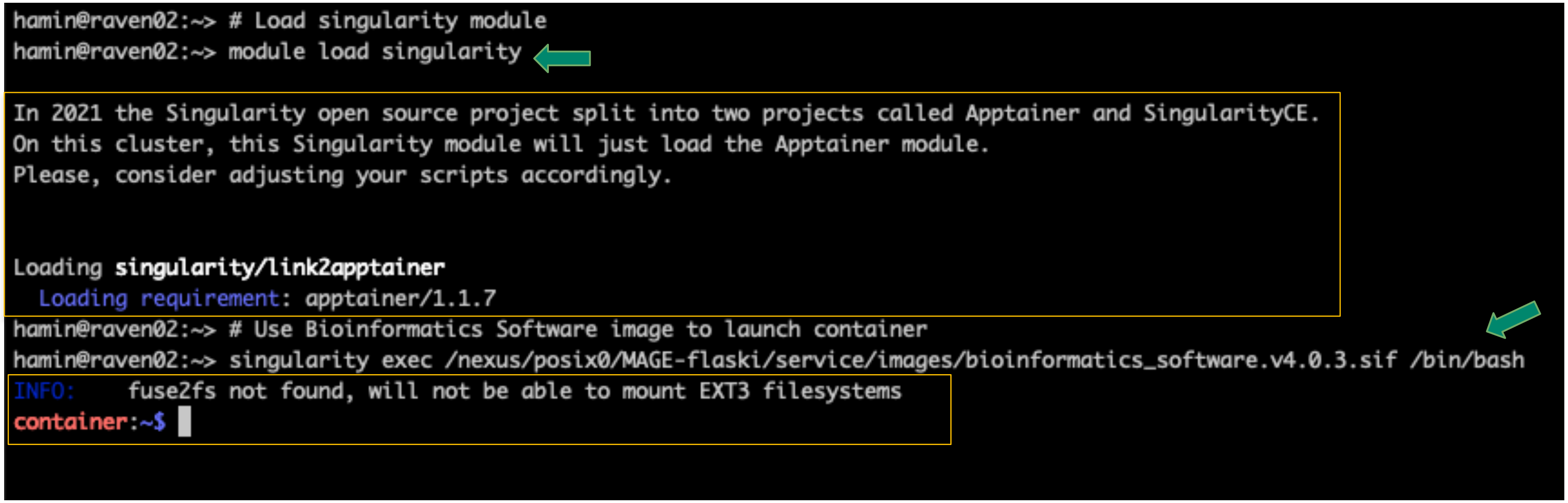
You can run your slurm jobs in both Raven & hpc.bioinformatics.studio

RAVEN	hpc.bioinformatics.studio
• For all MPI institutes • More resources • More users • Less memory access per job • Less time-limit	• For MPG users only • Less resources • Less users • Higher memory access per job • Higher time-limit (14 days)

Use Bioinformatics Containers

Useful Bioinformatics software containers are available to use in:
/nexus/posix0/MAGE-flaski/service/images/

Raven

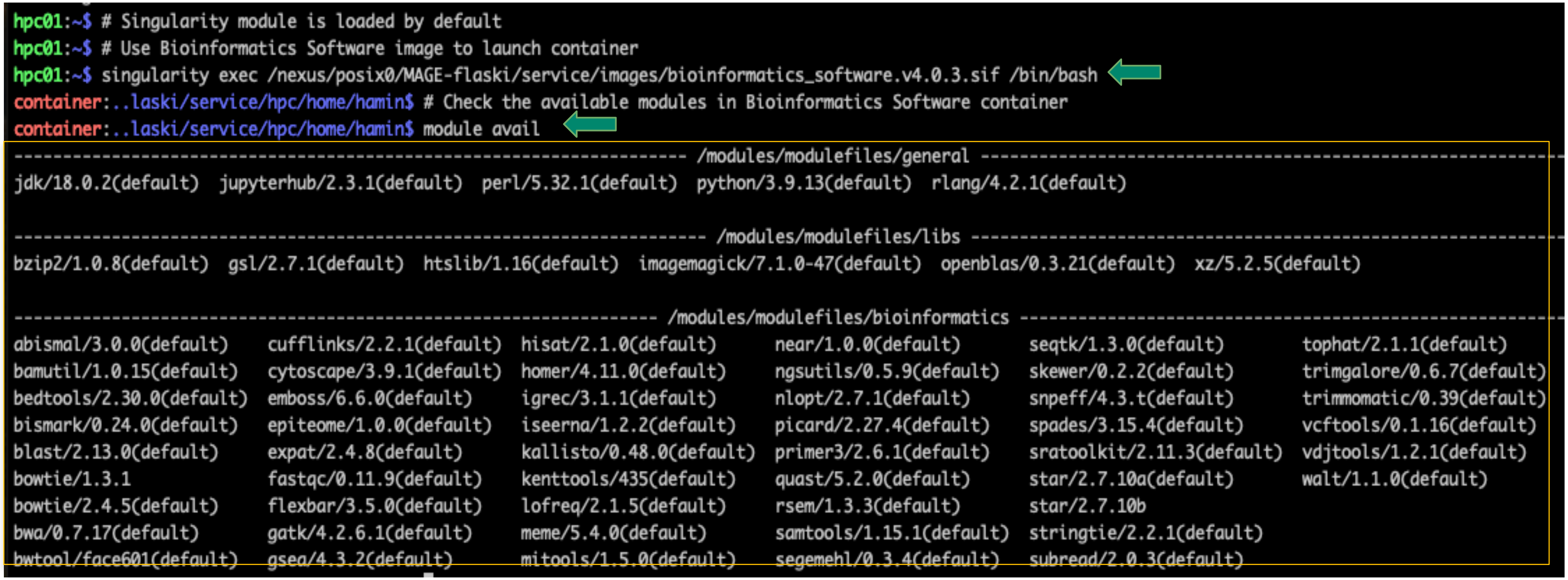


```
hamin@raven02:~> # Load singularity module
hamin@raven02:~> module load singularity

In 2021 the Singularity open source project split into two projects called Apptainer and SingularityCE.
On this cluster, this Singularity module will just load the Apptainer module.
Please, consider adjusting your scripts accordingly.


Loading singularity/link2apptainer
  Loading requirement: apptainer/1.1.7
hamin@raven02:~> # Use Bioinformatics Software image to launch container
hamin@raven02:~> singularity exec /nexus/posix0/MAGE-flaski/service/images/bioinformatics_software.v4.0.3.sif /bin/bash
INFO:    fuse2fs not found, will not be able to mount EXT3 filesystems
container:~$ 
```

Use Bioinformatics Containers

Useful Bioinformatics software containers are available to use in:
/nexus/posix0/MAGE-flaski/service/images/

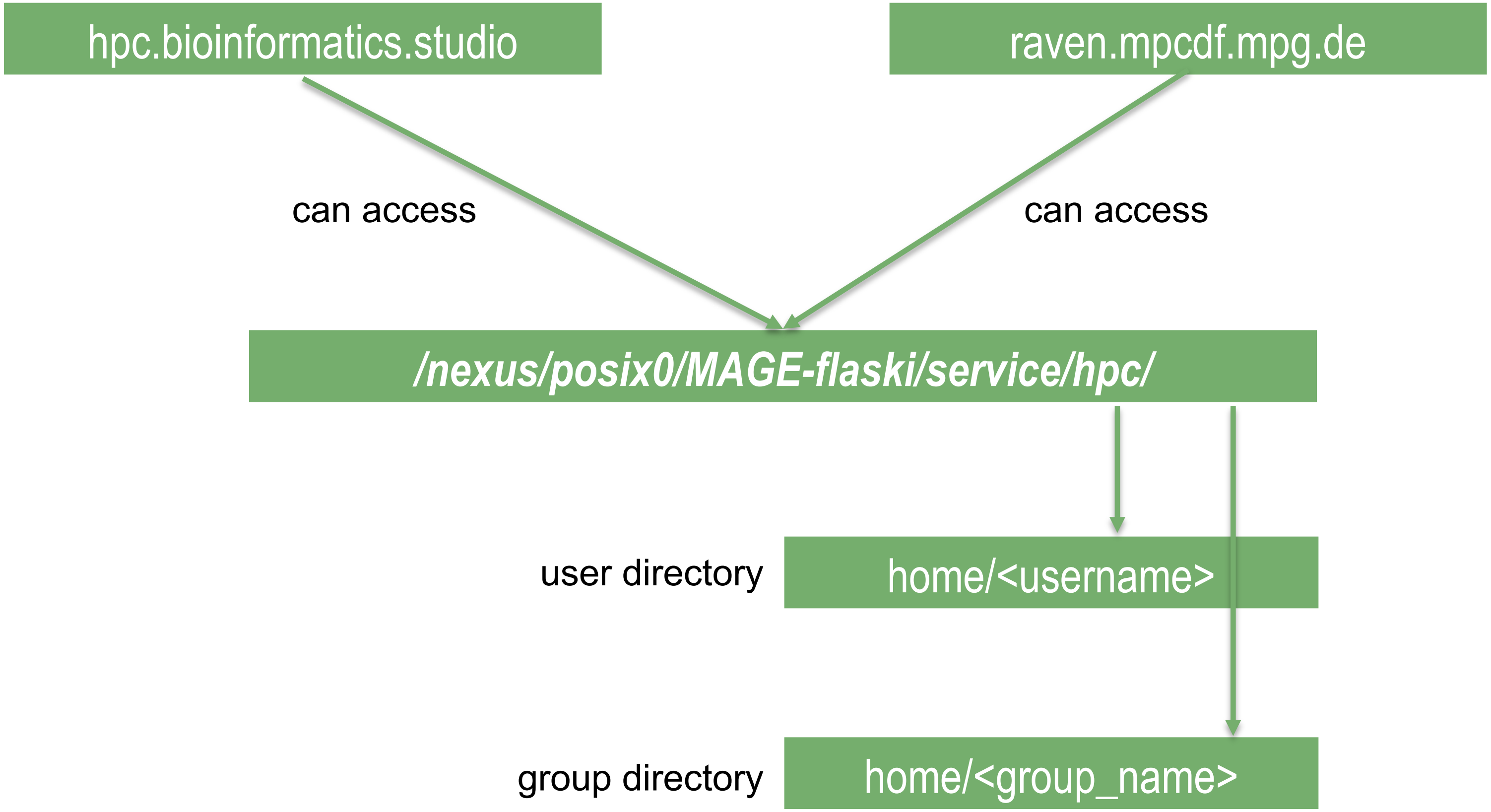
hpc.bioinformatics.studio



```
hpc01:~$ # Singularity module is loaded by default
hpc01:~$ # Use Bioinformatics Software image to launch container
hpc01:~$ singularity exec /nexus/posix0/MAGE-flaski/service/images/bioinformatics_software.v4.0.3.sif /bin/bash
container:..laski/service/hpc/home/hamin$ # Check the available modules in Bioinformatics Software container
container:..laski/service/hpc/home/hamin$ module avail
--------------------------------------------------------------------- /modules/modulefiles/general ------------------------------------------------------------
jdk/18.0.2(default)  jupyterhub/2.3.1(default)  perl/5.32.1(default)  python/3.9.13(default)  rlang/4.2.1(default)

----------------------------------------------------------------------- /modules/modulefiles/libs --------------------------------------------------------------
bzip2/1.0.8(default)  gsl/2.7.1(default)  htslib/1.16(default)  imagemagick/7.1.0-47(default)  openblas/0.3.21(default)  xz/5.2.5(default)

------------------------------------------------------------------ /modules/modulefiles/bioinformatics ---------------------------------------------------------
abismal/3.0.0(default)    cufflinks/2.2.1(default)  hisat/2.1.0(default)      near/1.0.0(default)       seqtk/1.3.0(default)        tophat/2.1.1(default)
bamutil/1.0.15(default)   cytoscape/3.9.1(default)  homer/4.11.0(default)     ngsutils/0.5.9(default)   skewer/0.2.2(default)       trimgalore/0.6.7(default)
bedtools/2.30.0(default)  emboss/6.6.0(default)     igrec/3.1.1(default)      nlopt/2.7.1(default)      snpeff/4.3.t(default)       trimmomatic/0.39(default)
bismark/0.24.0(default)   epiteome/1.0.0(default)   iseerna/1.2.2(default)    picard/2.27.4(default)    spades/3.15.4(default)      vcftools/0.1.16(default)
blast/2.13.0(default)     expat/2.4.8(default)      kallisto/0.48.0(default)  primer3/2.6.1(default)    sratoolkit/2.11.3(default)  vdjtools/1.2.1(default)
bowtie/1.3.1              fastqc/0.11.9(default)    kenttools/435(default)    quast/5.2.0(default)      star/2.7.10a(default)       walt/1.1.0(default)
bowtie/2.4.5(default)     flexbar/3.5.0(default)    lofreq/2.1.5(default)     rsem/1.3.3(default)       star/2.7.10b
bwa/0.7.17(default)       gatk/4.2.6.1(default)     meme/5.4.0(default)       samtools/1.15.1(default)  stringtie/2.2.1(default)
bwtool/face601(default)   gsea/4.3.2(default)       mitools/1.5.0(default)    segemehl/0.3.4(default)   subread/2.0.3(default)
```

Data Handling

Data Access



hpc.bioinformatics.studio

raven.mpcdf.mpg.de

can access

can access

/nexus/posix0/MAGE-flaski/service/hpc/

user directory

home/<username>

group directory

home/<group_name>

Data Limit

user directory

home/<username>

Data limit: *100 GB per user*
Close to threshold (80 GB+): *warning email*
Cross limit (100 GB+): *notify to limit size*
Failed to limit: *data cleaned up*

User not logged in for 3 months: *tar data & deactivate user*

group directory

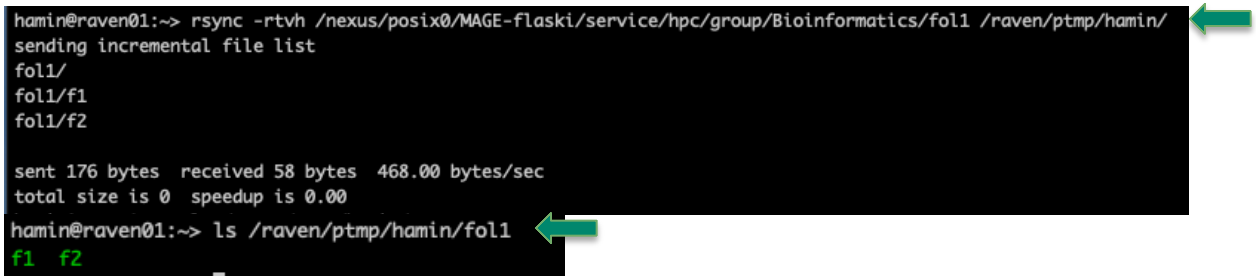
home/<group_name>

File not accessed in 6 weeks: *delete file*

Backup Data

From *raven.mpcdf.mpg.de* transfer data to */raven/ptmp*

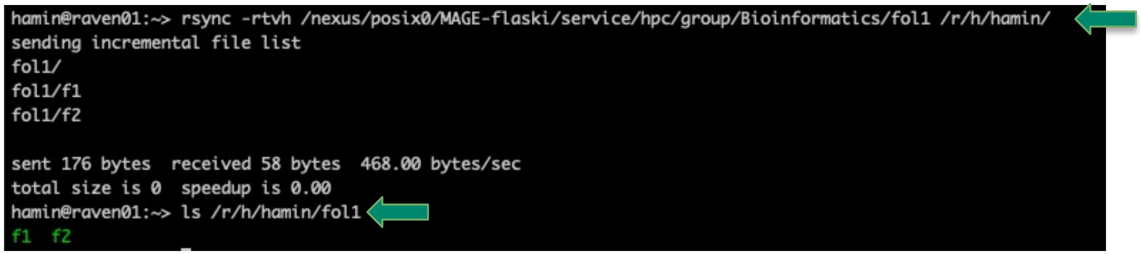
```
rsync -rtvh /nexus/posix0/MAGE-flaski/service/hpc/group/<group>/<folder> /raven/ptmp/<user>/
```



```
hamin@raven01:~> rsync -rtvh /nexus/posix0/MAGE-flaski/service/hpc/group/Bioinformatics/fol1 /raven/ptmp/hamin/
sending incremental file list
fol1/
fol1/f1
fol1/f2

sent 176 bytes  received 58 bytes  468.00 bytes/sec
total size is 0  speedup is 0.00
hamin@raven01:~> ls /raven/ptmp/hamin/fol1
f1  f2
```

Or to archive file system */r*

```
rsync -rtvh /nexus/posix0/MAGE-flaski/service/hpc/group/<group>/<folder> /r/<username first letter>/<user>/
```

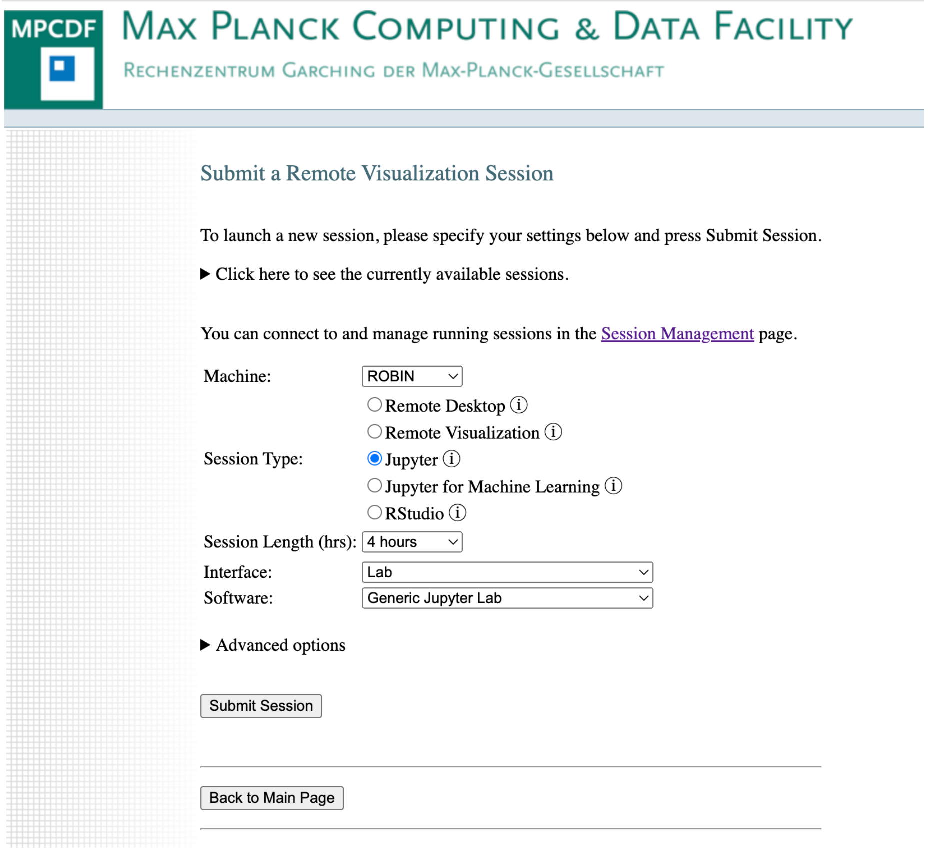


```
hamin@raven01:~> rsync -rtvh /nexus/posix0/MAGE-flaski/service/hpc/group/Bioinformatics/fol1 /r/h/hamin/
sending incremental file list
fol1/
fol1/f1
fol1/f2

sent 176 bytes  received 58 bytes  468.00 bytes/sec
total size is 0  speedup is 0.00
hamin@raven01:~> ls /r/h/hamin/fol1
f1  f2
```

Remote Visualization Services

Run from RAVEN

Documentation to get started: https://docs.mpcdf.mpg.de/doc/visualization/index.html
Start a tool/session: https://rvs.mpcdf.mpg.de/



MPCDF
MAX PLANCK COMPUTING & DATA FACILITY
RECHENZENTRUM GARCHING DER MAX-PLANCK-GESELLSCHAFT

Submit a Remote Visualization Session

To launch a new session, please specify your settings below and press Submit Session.

▶ Click here to see the currently available sessions.

You can connect to and manage running sessions in the Session Management page.

Machine: ROBIN

Session Type:
○ Remote Desktop ⓘ
○ Remote Visualization ⓘ
● Jupyter ⓘ
○ Jupyter for Machine Learning ⓘ
○ RStudio ⓘ

Session Length (hrs): 4 hours

Interface: Lab

Software: Generic Jupyter Lab

▶ Advanced options

Run from hpc.bioinformatics.studio

Documentation to get started:
https://github.com/mpg-age-bioinformatics/cluster_first_steps/tree/master/visual_tools

** follow the 3 steps described there to launch a service interface*

Available Scripts to Run Services

posit-jupyter: Jupyter Lab from Posit

jupyternb: Jupyter Notebook from Posit

vscode: Visual Studio Code

rstudio: Rstudio from the Rocker Project

Thank You!

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

Support: bioinformatics@age.mpg.de

Website: https://bioinformatics.age.mpg.de/