Clusters

Academic Enhancement Team

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Clusters

Outline

- What is a cluster?
- How to get started?
- Interacting with Linux (tmux)
- What software do you need?
- How to run jobs on a cluster.

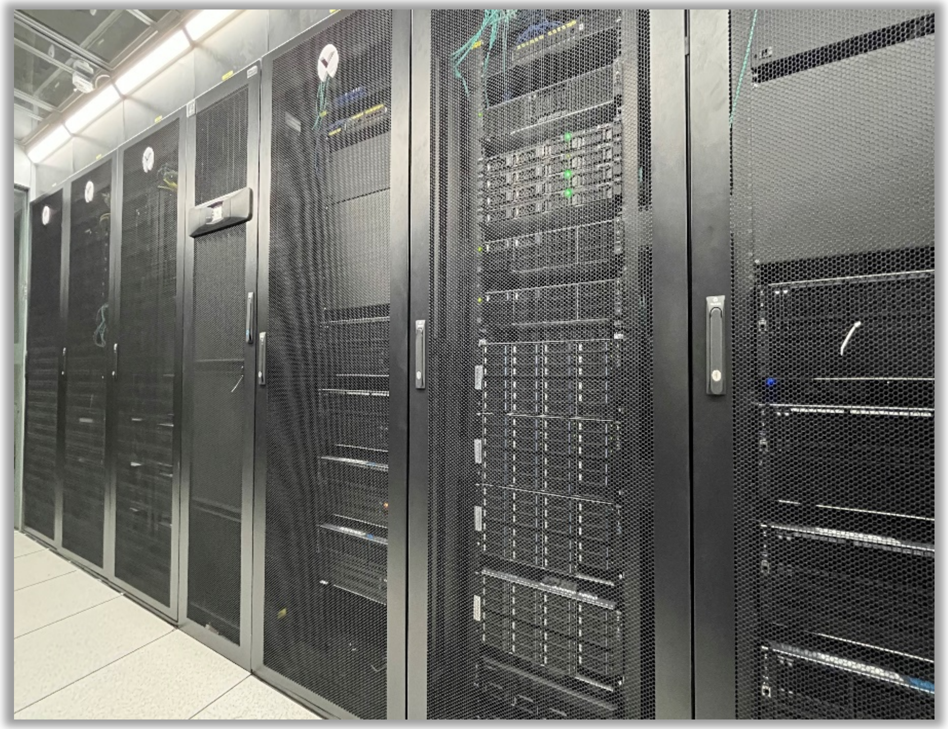
Clusters

What is a cluster?

What is a cluster?

An Cluster is a system composed of **multiple servers** connected by a **high-speed network**, working together to process a large amount of computational tasks.

- **Storage System**: Consists of a range of devices for storing and managing vast amounts of data, ensuring that all computing nodes can quickly access the required information.
- **Scheduling System**: Used to manage and allocate computing tasks and cluster resources, ensuring efficient task operation.
- **Software Tools and Programming Libraries**: These tools and libraries provide users with the ability to write programs (including Shell scripts) that can be executed across multiple nodes, fully utilizing the computational power of the entire cluster.



https://hpc.xjtlu.edu.cn

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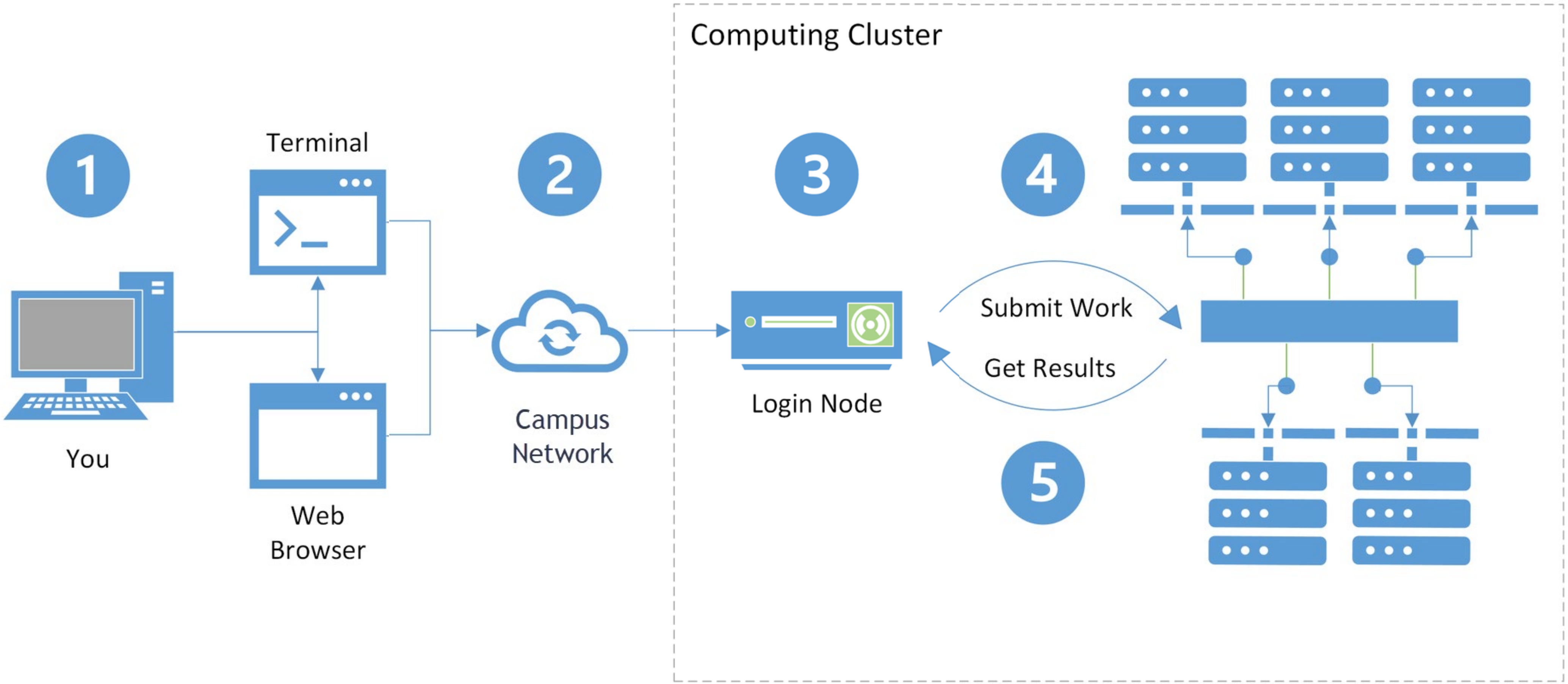
How to get started?

How to get started?



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Interacting with Linux

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Interacting with Linux: tmux

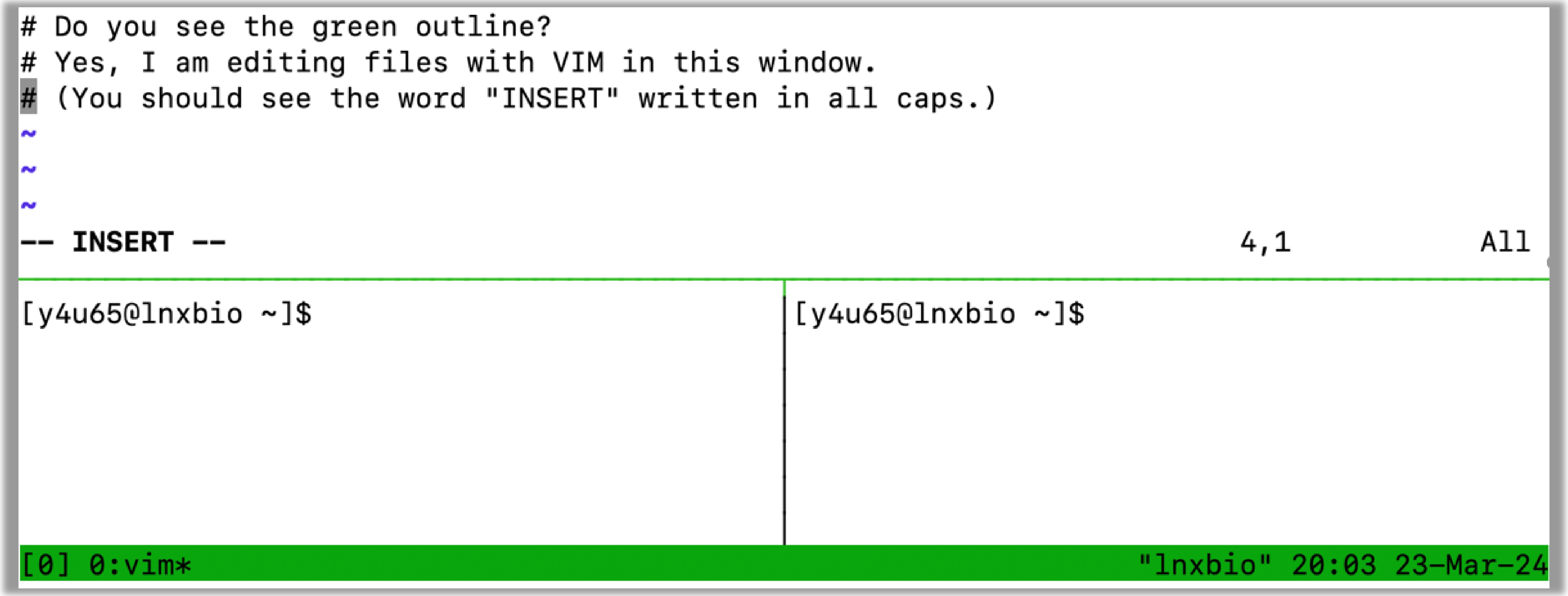
Tmux is a tool that allows you to manage multiple tasks within a single window.

- **Multitasking is simplified:** you can view files, write code, and monitor the status of other running programs simultaneously.

- **Work continues uninterrupted:** even if your computer shuts down or the network disconnects, your work persists. Upon reconnection, it's easy to resume where you left off.

- **Task switching is effortless:** supporting multiple windows and shortcut key navigation.

Interacting with Linux: tmux



```
# Do you see the green outline?
# Yes, I am editing files with VIM in this window.
# (You should see the word "INSERT" written in all caps.)
~
~
~
-- INSERT --                                          4,1           All
```

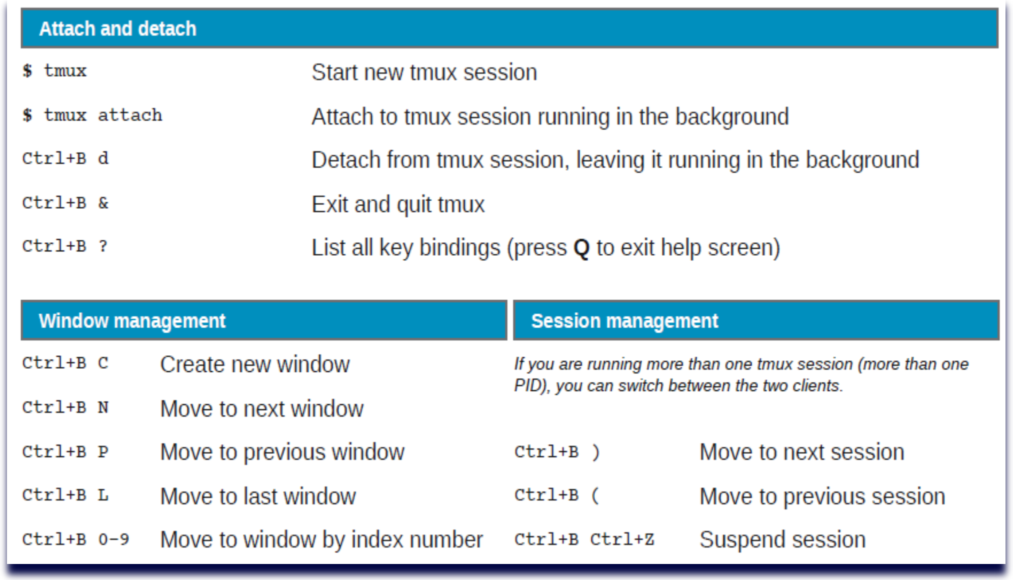
```
[y4u65@lnxbio ~]$
```

```
[y4u65@lnxbio ~]$
```

```
[0] 0:vim*                                    "lnxbio" 20:03 23-Mar-24
```

tmux XJTLU | HIGH PERFORMANCE COMPUTING

Interacting with Linux: tmux



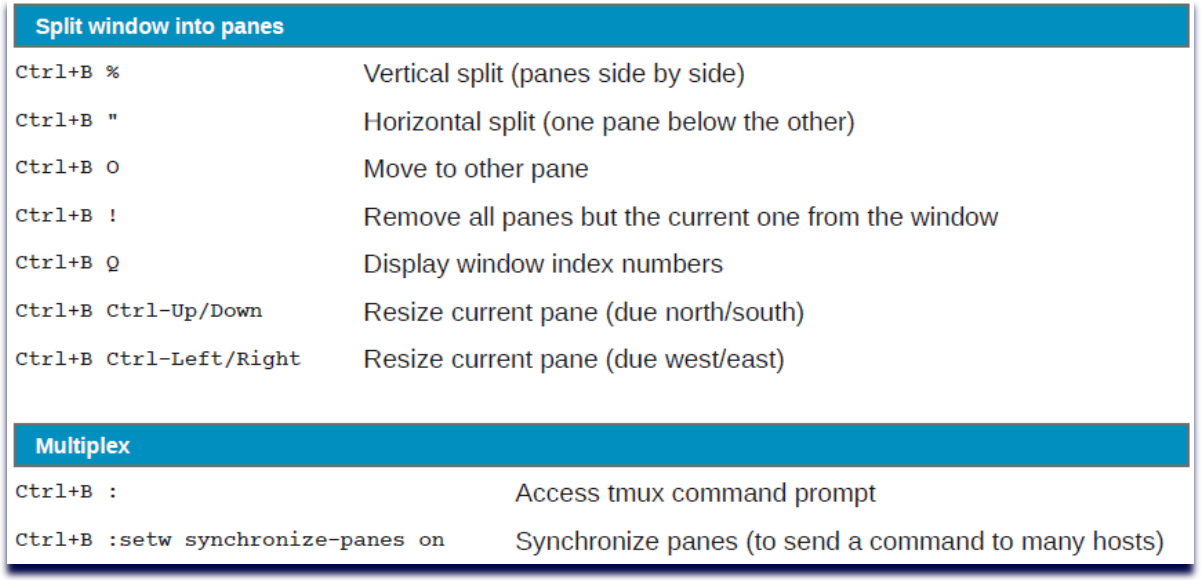
Attach and detach	
`$ tmux`	Start new tmux session
`$ tmux attach`	Attach to tmux session running in the background
`Ctrl+B d`	Detach from tmux session, leaving it running in the background
`Ctrl+B &`	Exit and quit tmux
`Ctrl+B ?`	List all key bindings (press **Q** to exit help screen)

Window management	
`Ctrl+B C`	Create new window
`Ctrl+B N`	Move to next window
`Ctrl+B P`	Move to previous window
`Ctrl+B L`	Move to last window
`Ctrl+B 0-9`	Move to window by index number

Session management

If you are running more than one tmux session (more than one PID), you can switch between the two clients.

`Ctrl+B )`	Move to next session
`Ctrl+B (`	Move to previous session
`Ctrl+B Ctrl+Z`	Suspend session



Split window into panes	
`Ctrl+B %`	Vertical split (panes side by side)
`Ctrl+B "`	Horizontal split (one pane below the other)
`Ctrl+B O`	Move to other pane
`Ctrl+B !`	Remove all panes but the current one from the window
`Ctrl+B Q`	Display window index numbers
`Ctrl+B Ctrl-Up/Down`	Resize current pane (due north/south)
`Ctrl+B Ctrl-Left/Right`	Resize current pane (due west/east)

Multiplex	
`Ctrl+B :`	Access tmux command prompt
`Ctrl+B :setw synchronize-panes on`	Synchronize panes (to send a command to many hosts)

Clusters

What software do you need?

What software do you need: Lmod and Spack

- **Lmod** is a program to manage the user environment under Linux.
- Use the ***module*** command of the Lmod to browse, find or load installed software.

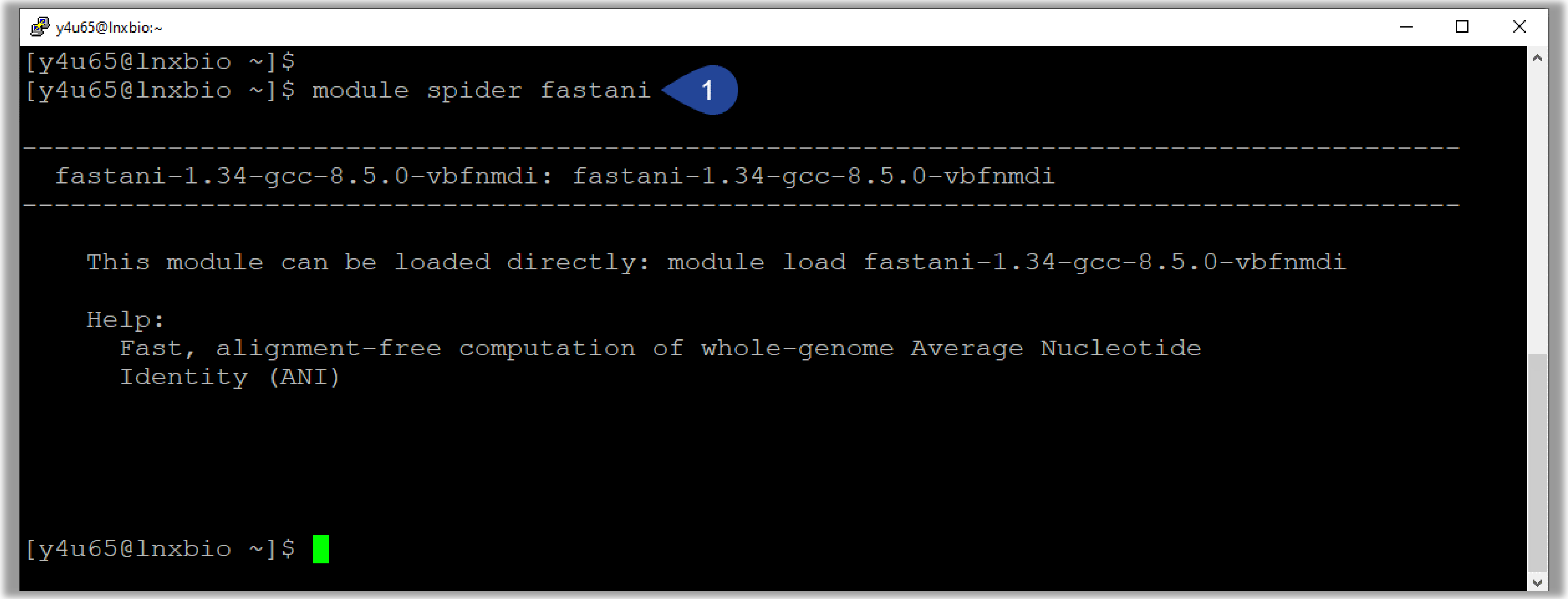
- **Spack** is a package manager for supercomputers, Linux, and macOS.
- **Administrators** generally use it to install software.

What software do you need: Lmod

QUICK START	
Tip: Use the module command of the Lmod to browse, find or load installed software.	
List available modules	module avail
Finds all modules that have “spider” in their name.	module spider fastani
Load fastani-1.34-gcc-8.5.0-vbfnmdi	module load fastani-1.34-gcc-8.5.0-vbfnmdi
List loaded modules	module list
unload all modules	module purge

What software do you need: Lmod

`module spider fastani`



```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ module spider fastani

-----------------------------------------------------------------------------------------
  fastani-1.34-gcc-8.5.0-vbfnmdi: fastani-1.34-gcc-8.5.0-vbfnmdi
-----------------------------------------------------------------------------------------

    This module can be loaded directly: module load fastani-1.34-gcc-8.5.0-vbfnmdi

    Help:
      Fast, alignment-free computation of whole-genome Average Nucleotide
      Identity (ANI)




[y4u65@lnxbio ~]$
```

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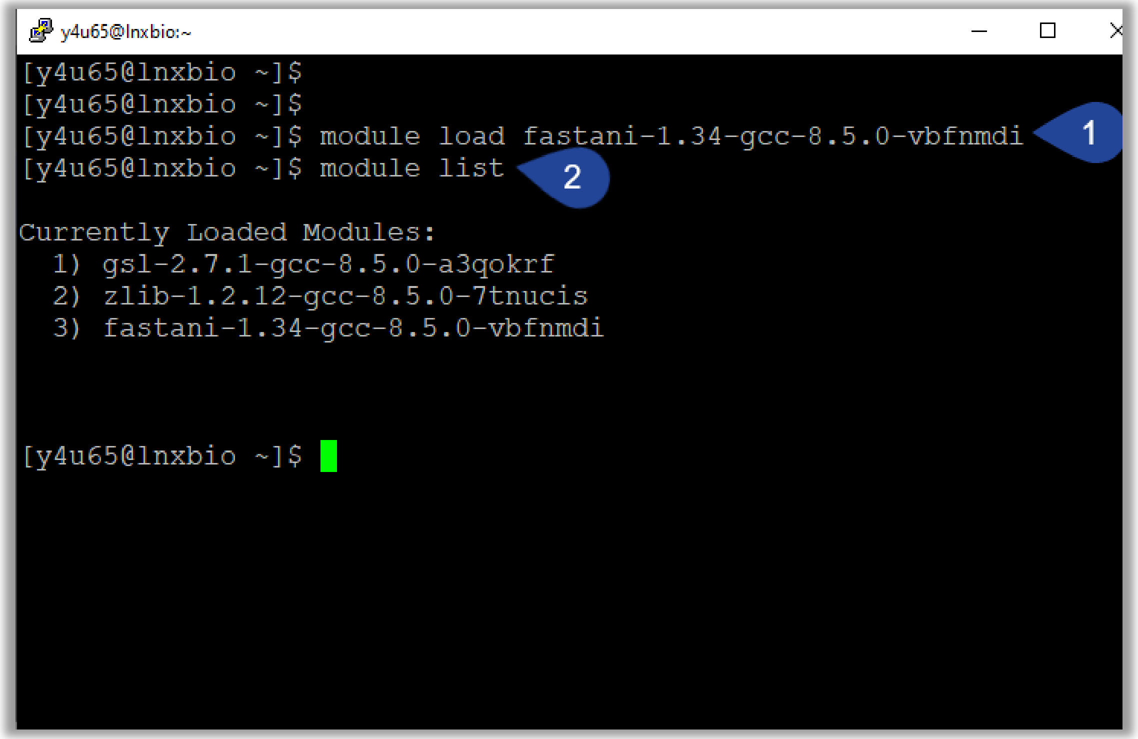
What software do you need: Lmod

module load fastani-1.34-gcc-8.5.0-vbfnmdi

fastANI -h

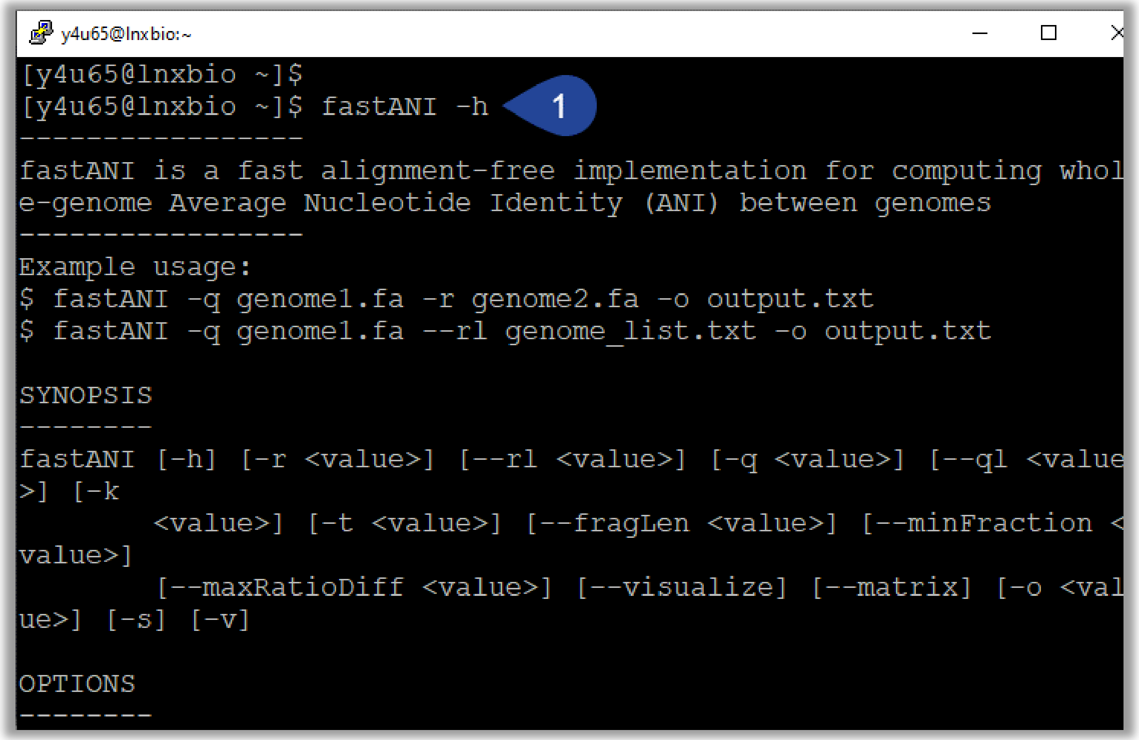


```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ module load fastani-1.34-gcc-8.5.0-vbfnmdi
[y4u65@lnxbio ~]$ module list

Currently Loaded Modules:
  1) gsl-2.7.1-gcc-8.5.0-a3qokrf
  2) zlib-1.2.12-gcc-8.5.0-7tnucis
  3) fastani-1.34-gcc-8.5.0-vbfnmdi



[y4u65@lnxbio ~]$ 
```



```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ fastANI -h
-----------------
fastANI is a fast alignment-free implementation for computing whol
e-genome Average Nucleotide Identity (ANI) between genomes
-----------------
Example usage:
$ fastANI -q genome1.fa -r genome2.fa -o output.txt
$ fastANI -q genome1.fa --rl genome_list.txt -o output.txt

SYNOPSIS
--------
fastANI [-h] [-r <value>] [--rl <value>] [-q <value>] [--ql <value
>] [-k
        <value>] [-t <value>] [--fragLen <value>] [--minFraction <
value>]
        [--maxRatioDiff <value>] [--visualize] [--matrix] [-o <val
ue>] [-s] [-v]

OPTIONS
--------
```

Tip: The installed software name may differ from the actual software name. The Tab key can display complete information when loading a command.

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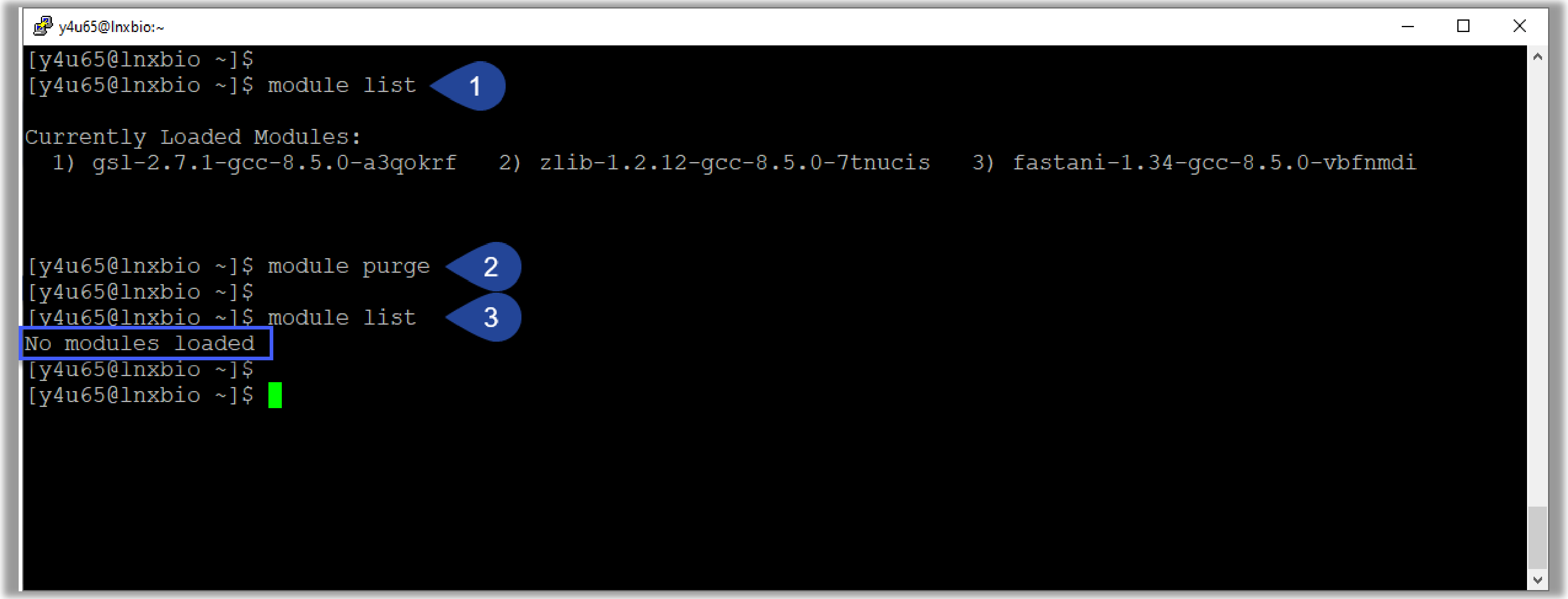
What software do you need: Lmod

module purge



```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ module list

Currently Loaded Modules:
  1) gsl-2.7.1-gcc-8.5.0-a3qokrf   2) zlib-1.2.12-gcc-8.5.0-7tnucis   3) fastani-1.34-gcc-8.5.0-vbfnmdi



[y4u65@lnxbio ~]$ module purge
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ module list
No modules loaded
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$
```

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What software do you need: Lmod

Question

1) Use the "module" command to query software starting with "metaw". What's the full name you found?

2) Use "module" to load "metawrap" and try to query its help information.

3) Which option of "module" can query all software?

Didn't find the software you need?
https://esupport.xjtlu.edu.cn
Note: provide your account name.

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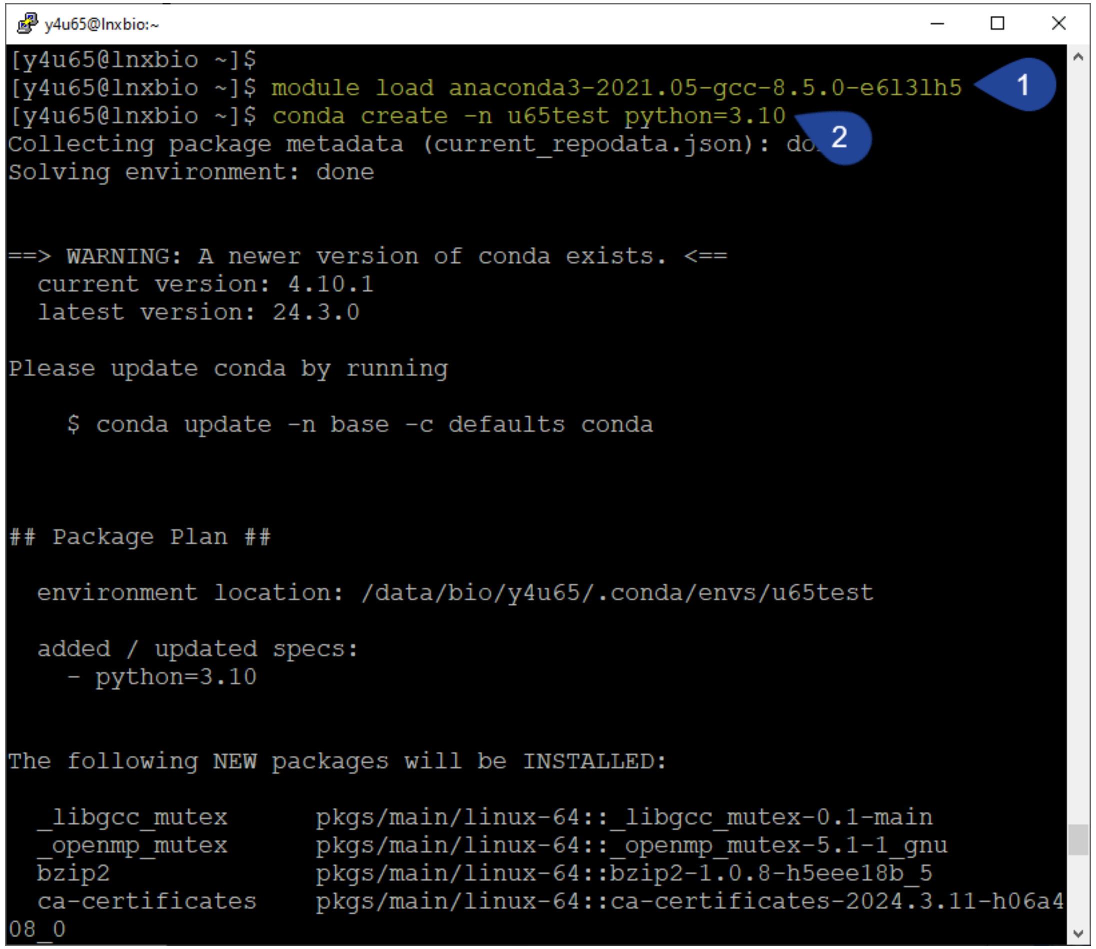
What software do you need: anaconda

- **Anaconda** is an open-source Python distribution containing many scientific computing and data analysis libraries.
- **Anaconda's** design is primarily optimized for single-user environments, so you may encounter limitations when sharing libraries and environments in a multi-user cluster, as it is not designed for this use case.
- Use the **conda** command of the anaconda to browse, find or load installed software.

What software do you need: anaconda

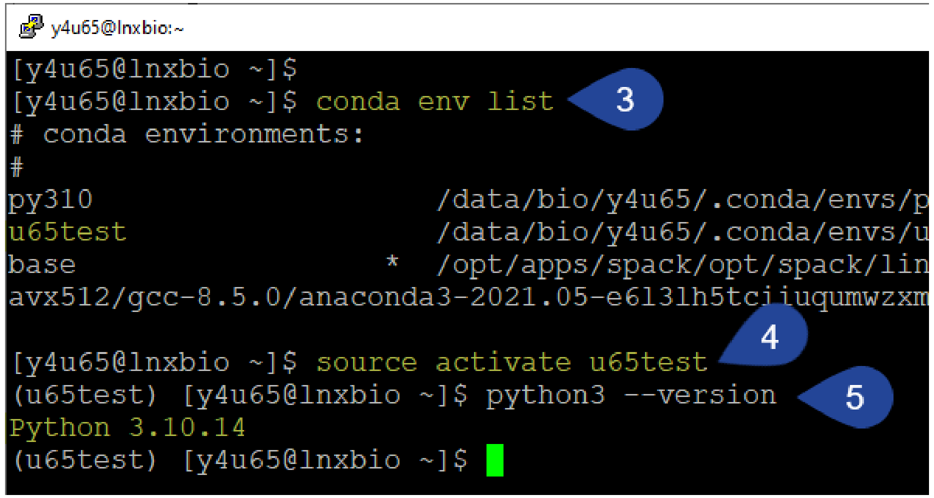
QUICK START	
Tip: It is recommended to create a new environment for any new project or workflow.	
get help for any command	conda COMMAND --help
list all environments and locations	conda env list
create environment with Python version	conda create -n ENVNAME python=3.10
conda remove -n ENVNAME --all	conda remove -n ENVNAME --all
install packages in environment	conda install -n ENVNAME PKG1 PKG2
remove package from environment	conda uninstall PKGNAME -n ENVNAME
Activate the virtual environment env	source activate ENVNAME
Deactivate the virtual environment	conda deactivate
install specific version of package	conda install PKGNAME=3.1.4
list installed packages	conda list
uninstall package	conda uninstall PKGNAME
remove all unused files	conda clean --all

What software do you need: anaconda



```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ module load anaconda3-2021.05-gcc-8.5.0-e613lh5
[y4u65@lnxbio ~]$ conda create -n u65test python=3.10
Collecting package metadata (current_repodata.json): do
Solving environment: done


==> WARNING: A newer version of conda exists. <==
  current version: 4.10.1
  latest version: 24.3.0

Please update conda by running

    $ conda update -n base -c defaults conda



## Package Plan ##

  environment location: /data/bio/y4u65/.conda/envs/u65test

  added / updated specs:
    - python=3.10


The following NEW packages will be INSTALLED:

  _libgcc_mutex      pkgs/main/linux-64::_libgcc_mutex-0.1-main
  _openmp_mutex      pkgs/main/linux-64::_openmp_mutex-5.1-1_gnu
  bzip2              pkgs/main/linux-64::bzip2-1.0.8-h5eee18b_5
  ca-certificates    pkgs/main/linux-64::ca-certificates-2024.3.11-h06a4
08_0
```

This example demonstrates how to use the conda command to create a virtual environment named "*u65test*" and use Python version "*3.10*".



```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ conda env list
# conda environments:
#
py310                    /data/bio/y4u65/.conda/envs/p
u65test                  /data/bio/y4u65/.conda/envs/u
base                  *  /opt/apps/spack/opt/spack/lin
avx512/gcc-8.5.0/anaconda3-2021.05-e613lh5tcjiuqumwzxm

[y4u65@lnxbio ~]$ source activate u65test
(u65test) [y4u65@lnxbio ~]$ python3 --version
Python 3.10.14
(u65test) [y4u65@lnxbio ~]$
```

Note: Before using the conda command, anaconda needs to be loaded first.

ANACONDA

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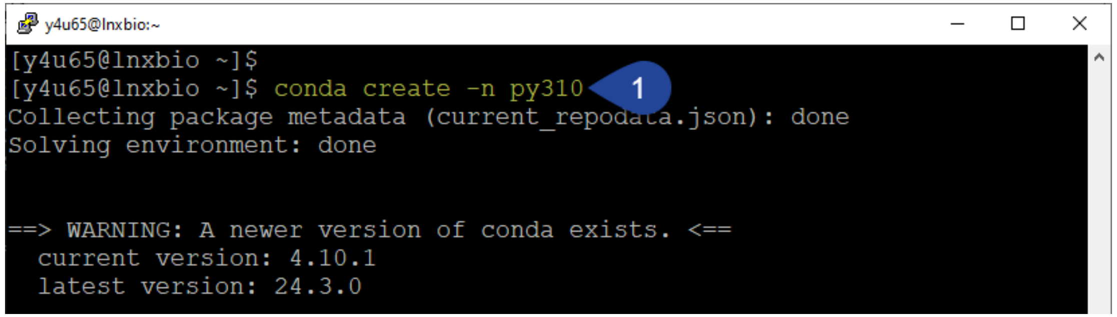
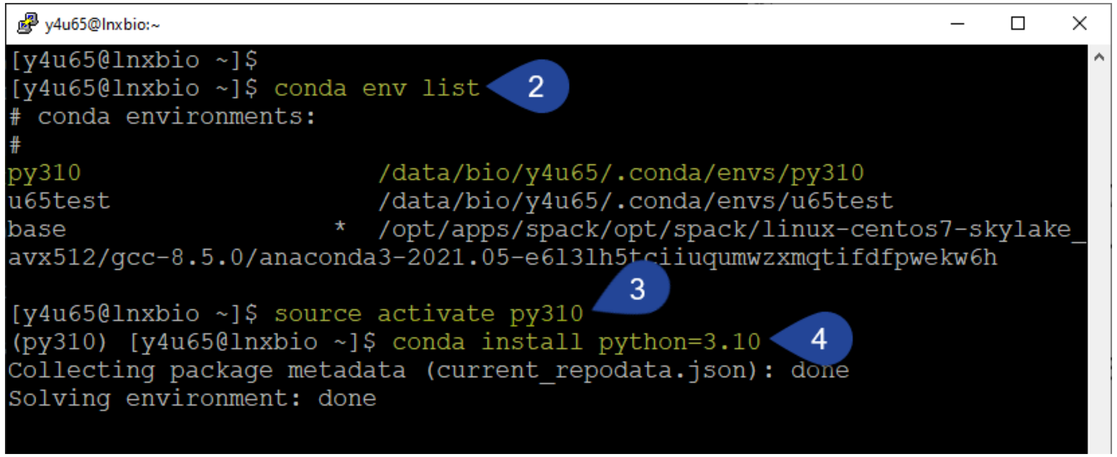
What software do you need: anaconda

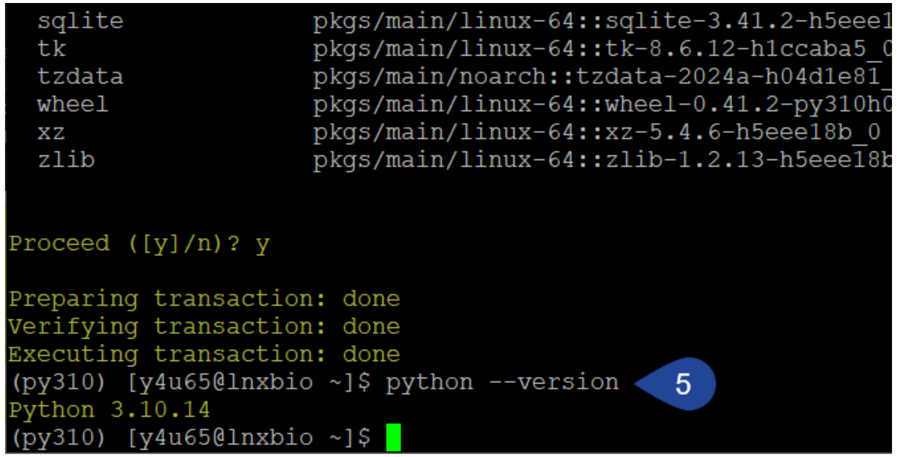


```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ conda create -n py310
Collecting package metadata (current_repodata.json): done
Solving environment: done


==> WARNING: A newer version of conda exists. <==
  current version: 4.10.1
  latest version: 24.3.0
```

This example demonstrates how to use the conda command to create a virtual environment named “py310" and install Python version "3.10" in this virtual environment.



```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ conda env list
# conda environments:
#
py310                    /data/bio/y4u65/.conda/envs/py310
u65test                  /data/bio/y4u65/.conda/envs/u65test
base                  *  /opt/apps/spack/opt/spack/linux-centos7-skylake_
avx512/gcc-8.5.0/anaconda3-2021.05-e613lh5tciiuqumwzxmqtifdfpwekw6h

[y4u65@lnxbio ~]$ source activate py310
(py310) [y4u65@lnxbio ~]$ conda install python=3.10
Collecting package metadata (current_repodata.json): done
Solving environment: done
```



```
  sqlite             pkgs/main/linux-64::sqlite-3.41.2-h5eee1
  tk                 pkgs/main/linux-64::tk-8.6.12-h1ccaba5_0
  tzdata             pkgs/main/noarch::tzdata-2024a-h04d1e81_
  wheel              pkgs/main/linux-64::wheel-0.41.2-py310h0
  xz                 pkgs/main/linux-64::xz-5.4.6-h5eee18b_0
  zlib               pkgs/main/linux-64::zlib-1.2.13-h5eee18b


Proceed ([y]/n)? y

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
(py310) [y4u65@lnxbio ~]$ python --version
Python 3.10.14
(py310) [y4u65@lnxbio ~]$
```

Note: *Before using the conda command, anaconda needs to be loaded first.*

What software do you need

Questions

1) Create a virtual environment named "*pyp310*" and install Python 3.10.

2) Use conda to create a virtual environment named “*pypy310*", activate it, and install Python 3.10.

Clusters

How to run jobs on a cluster

How to run jobs on a cluster: slurm

Slurm is based on resource allocation and designed for clusters to provide efficient job scheduling and management.

Streamline your research endeavors with slurm workload manager

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How to run jobs on a cluster: slurm

Must do before practice

- Apply for resources: Use the command srun to apply for eight core computing resources.

```
srun -n 8 -N 1 --pty /bin/bash
```

- End the exercise: Enter exit to release the requested computing resources.

```
exit
```

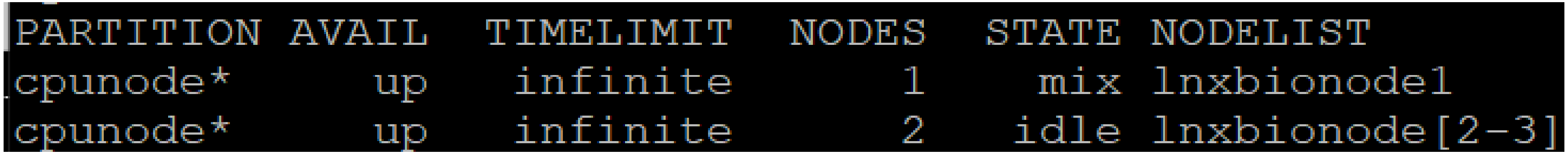
How to run jobs on a cluster: slurm

QUICK START		
Commands	Syntax	Purpose
sinfo	sinfo	Used to view partition and node information.
srun	srun -n 8 *metawrap -h*	Used to run a job (job step) on the resources allocated with sbatch or salloc
sbatch	sbatch *run.slurm*	Submit a job script filename
squeue	squeue -u $USER	Show job queue for user
scancel	scancel *4444*	Delete job 4444
sacct	sacct	Used to view accounting data for jobs and job steps in the job accounting log.

How to run jobs on a cluster: sinfo

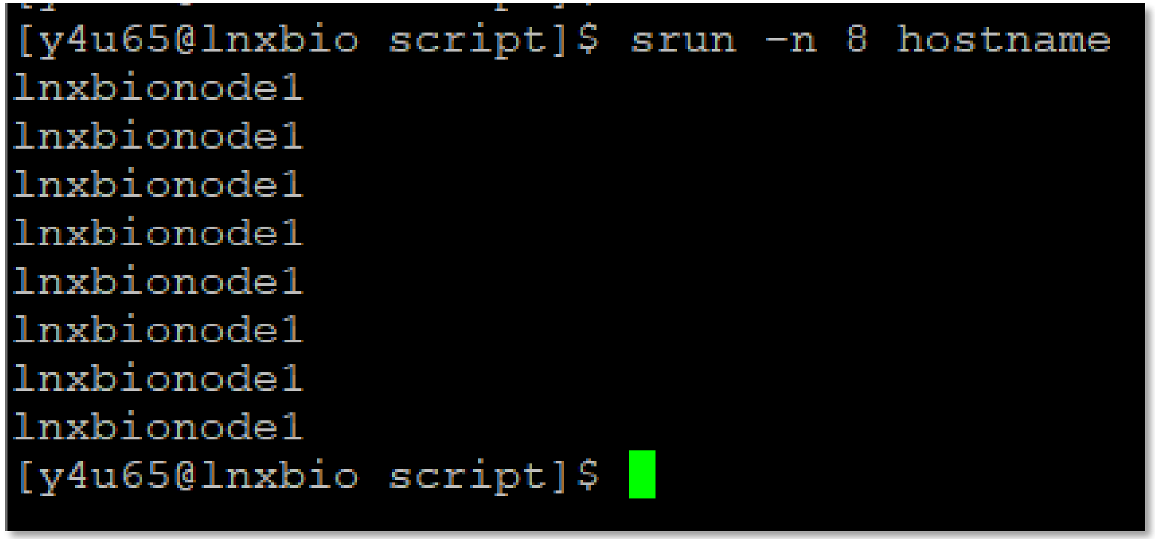
sinfo: Used to view partition and node information.

Slurm partitions are logical subdivisions of a cluster’s resources. They enable efficient resource allocation, accommodating different job types, priorities, and user/group restrictions within a shared computing environment. Partitions ensure sensitive research data is only processed and stored within designated and controlled environments. These isolations help prevent unauthorized access and reduce the risk of data leaks and tampering.



```
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
cpunode*     up   infinite      1    mix lnxbionode1
cpunode*     up   infinite      2   idle lnxbionode[2-3]
```

How to run jobs on a cluster: srun



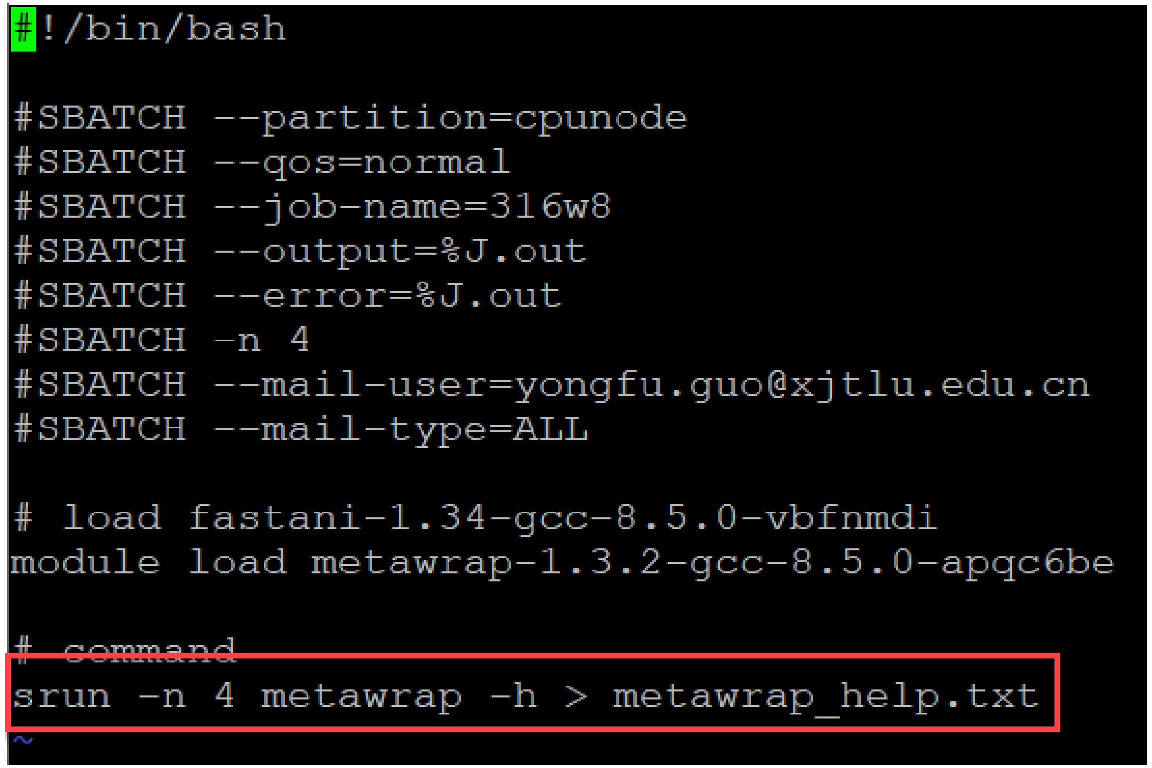
```
[y4u65@lnxbio script]$ srun -n 8 hostname
lnxbionode1
lnxbionode1
lnxbionode1
lnxbionode1
lnxbionode1
lnxbionode1
lnxbionode1
lnxbionode1
[y4u65@lnxbio script]$ 
```

srun

The srun command is an integral part of the Slurm scheduling system. It "knows" the configuration of the machine and recognizes the environmental variables set by the scheduler, such as cores per nodes.

Typically, the srun command is used with a command like *metawrap* in a slurm script.

How to run jobs on a cluster: sbatch

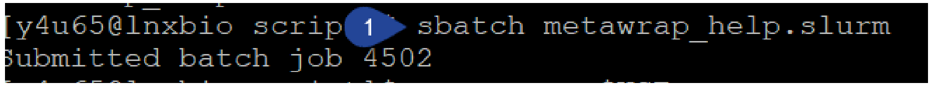


```
#!/bin/bash

#SBATCH --partition=cpunode
#SBATCH --qos=normal
#SBATCH --job-name=316w8
#SBATCH --output=%J.out
#SBATCH --error=%J.out
#SBATCH -n 4
#SBATCH --mail-user=yongfu.guo@xjtlu.edu.cn
#SBATCH --mail-type=ALL

# load fastani-1.34-gcc-8.5.0-vbfnmdi
module load metawrap-1.3.2-gcc-8.5.0-apqc6be

# command
srun -n 4 metawrap -h > metawrap_help.txt
~
```

Script name: metawrap_help.slurm

sbatch

Batch jobs are run by submitting a job script to the scheduler with the sbatch command. The job script contains the commands to set up your environment and run your application.



```
]y4u65@lnxbio scrip     sbatch metawrap_help.slurm
ubmitted batch job 4502
```

srun

Batch jobs are run by submitting a job script to the scheduler with the sbatch command.

How to run jobs on a cluster: slurm script

Tip:

- Every Slurm job script needs to start with #!/bin/bash, which indicates that the Bash shell is used to execute the script.
- We must start with "#SBATCH" and use spaces to differentiate the options. For example, when filling in the partition options, use the --partition option to specify the partition name the job will run on.

```
#SBATCH --partition=cpunode
```

- Please ensure that before submitting the Slurm job, your script has included commands to load all required software modules; for example, add module load metawrap-1.3.2-gcc-8.5.0-apqc6be to load a specific module version.

How to run jobs on a cluster: script example

```
#SBATCH --partition=cpunode
#SBATCH --qos=normal
#SBATCH --job-name=316w8
#SBATCH --output=%J.out
#SBATCH --error=%J.out
#SBATCH -n 8
#SBATCH --mail-user=mouzheng.xu@xjtlu.edu.cn
#SBATCH --mail-type=ALL
```

sbatch options

```
# load metawrap
module load metawrap-1.3.2-gcc-8.5.0-apqc6be
```

Load metawrap

```
# command
srun -N 1 -n 8 metawrap -h > metawrap_help.txt
```

Use the srun command to submit multiple files to metawrap for processing.

How to run jobs on a cluster: script example

Cheat sheet	
Options	**Purpose**
#SBATCH --partition=cpunode	Request a specific partition for the resource allocation
#SBATCH --qos=normal	Request a quality of service for the job. the limit of resources.
#SBATCH --job-name=316w8	Setting Job name
#SBATCH --output=%J.out	Setting output file name (%j will replace by jobid)
#SBATCH --error=%J.out	Setting error file name (%j will replace by jobid)
#SBATCH -n 8	Number of tasks
#SBATCH --mail-user=mouzheng.xu@xjtlu.edu.cn	User to receive email notification of state changes as defined by --mail-type.
#SBATCH --mail-type=ALL	Notify the user by email when certain event types occur. Valid type values are NONE, BEGIN, END, FAIL, REQUEUE, ALL
module load metawrap-1.3.2-gcc-8.5.0-apqc6be	load metawrap-1.3.2-gcc-8.5.0-apqc6be module
srun -N 1 -n 8 metawrap -h > metawrap_help.txt	he srun command is used to initiate the job, with -N 1 specifying the use of one node, and -n 8 indicating the utilization of eight tasks.

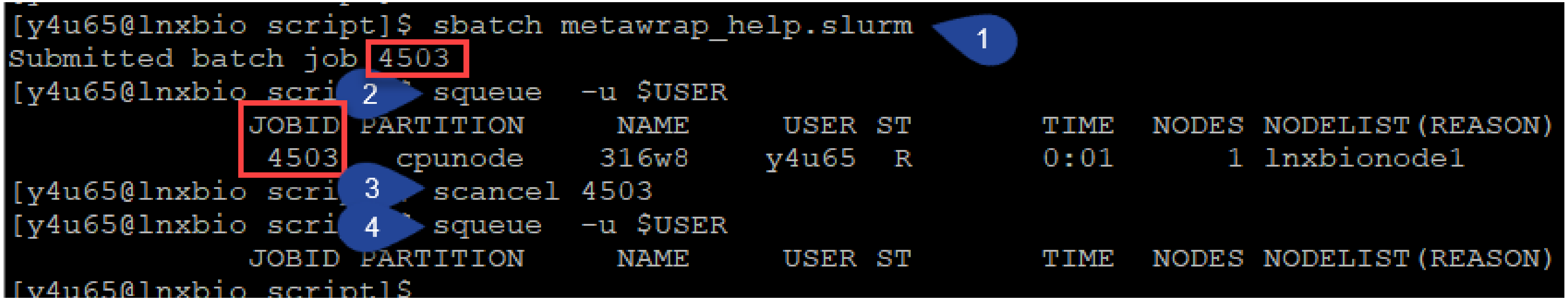
How to run jobs on a cluster: squeue and scancel

squeue: Show the state of jobs.
squeue -u: See your jobs running or waiting to run.

scancel: Cancel a pending or running job on the cluster**.**

squeue -u $USER

scancel 4503

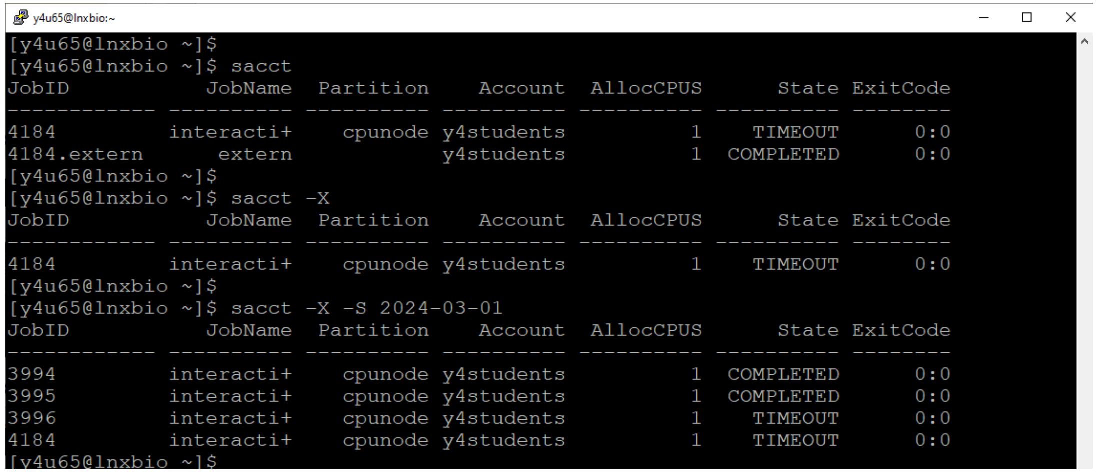


```
[y4u65@lnxbio script]$ sbatch metawrap_help.slurm
Submitted batch job 4503
[y4u65@lnxbio scri         squeue  -u $USER
            JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             4503   cpunode    316w8    y4u65  R       0:01      1 lnxbionode1
[y4u65@lnxbio scri         scancel 4503
[y4u65@lnxbio scri         squeue  -u $USER
            JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
[y4u65@lnxbio script]$
```

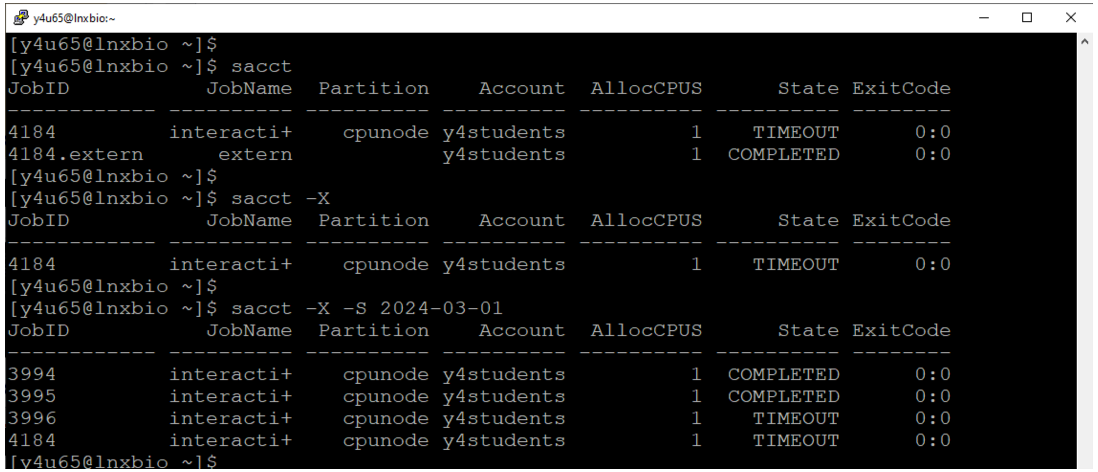
How to run jobs on a cluster: sacct

sacct: Use sacct to view accounting information about jobs AND job steps.

sacct -X -S 2024-03-01



```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ sacct
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
4184         interacti+    cpunode y4students          1    TIMEOUT      0:0
4184.extern      extern            y4students          1  COMPLETED      0:0
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ sacct -X
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
4184         interacti+    cpunode y4students          1    TIMEOUT      0:0
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ sacct -X -S 2024-03-01
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
3994         interacti+    cpunode y4students          1  COMPLETED      0:0
3995         interacti+    cpunode y4students          1  COMPLETED      0:0
3996         interacti+    cpunode y4students          1    TIMEOUT      0:0
4184         interacti+    cpunode y4students          1    TIMEOUT      0:0
[y4u65@lnxbio ~]$
```



```
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ sacct
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
4184         interacti+    cpunode y4students          1    TIMEOUT      0:0
4184.extern      extern            y4students          1  COMPLETED      0:0
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ sacct -X
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
4184         interacti+    cpunode y4students          1    TIMEOUT      0:0
[y4u65@lnxbio ~]$
[y4u65@lnxbio ~]$ sacct -X -S 2024-03-01
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
3994         interacti+    cpunode y4students          1  COMPLETED      0:0
3995         interacti+    cpunode y4students          1  COMPLETED      0:0
3996         interacti+    cpunode y4students          1    TIMEOUT      0:0
4184         interacti+    cpunode y4students          1    TIMEOUT      0:0
[y4u65@lnxbio ~]$
```

Use sacct -e to print a list of fields that can be specified with the --format option.

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How to run jobs on a cluster

Questions

Try to use “srun” and “sbatch” these two ways to output the result of "metawrap -h" into a text file.

THANK YOU

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