PARAM SANGANAK

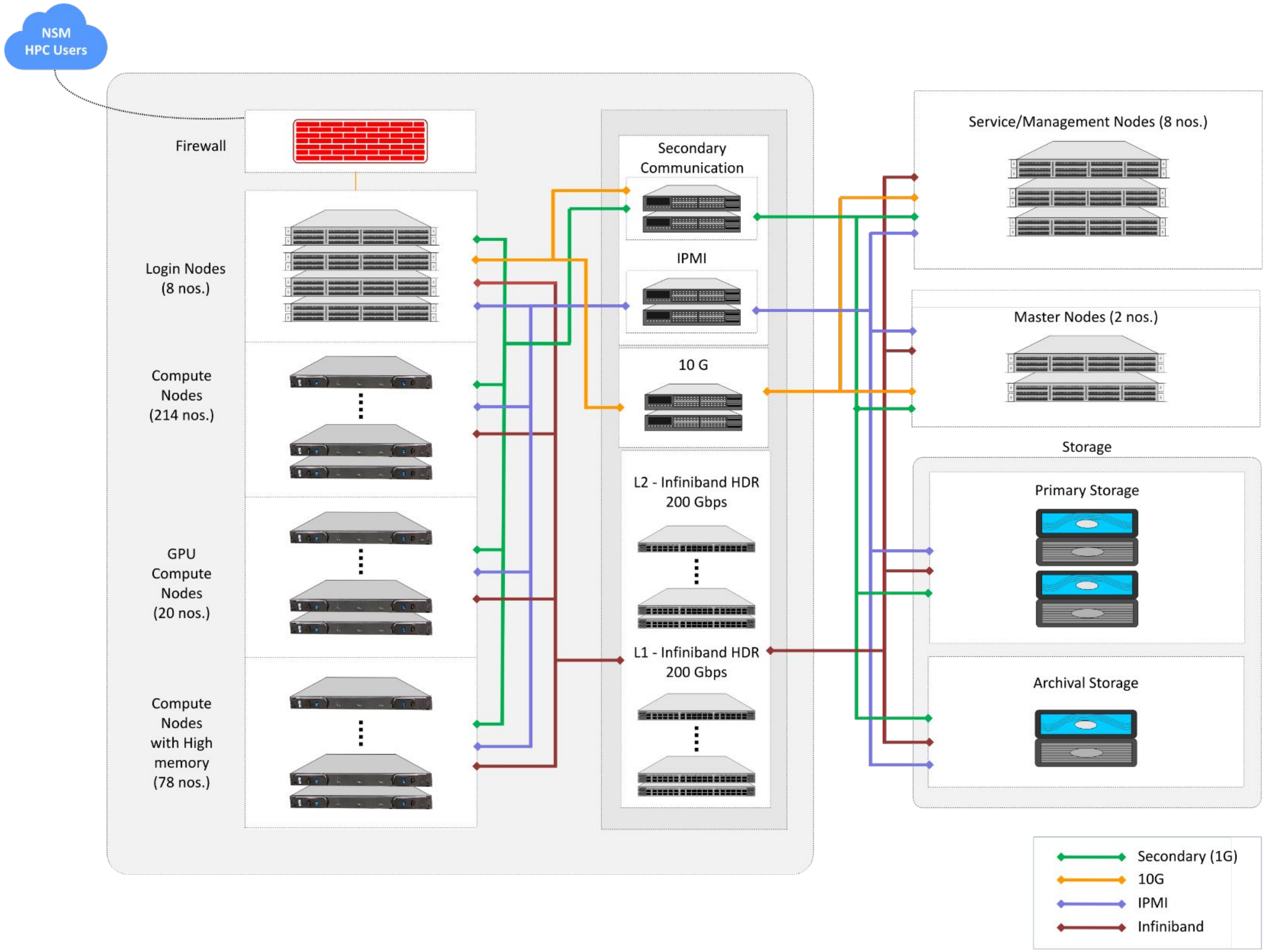
Agenda

- Declaration
- Software Stack
- Components of HPC
- PARAM-Sanganak Architecture
- Technical Specification of PARAM-Sanganak
- How to access Param-Sanganak.

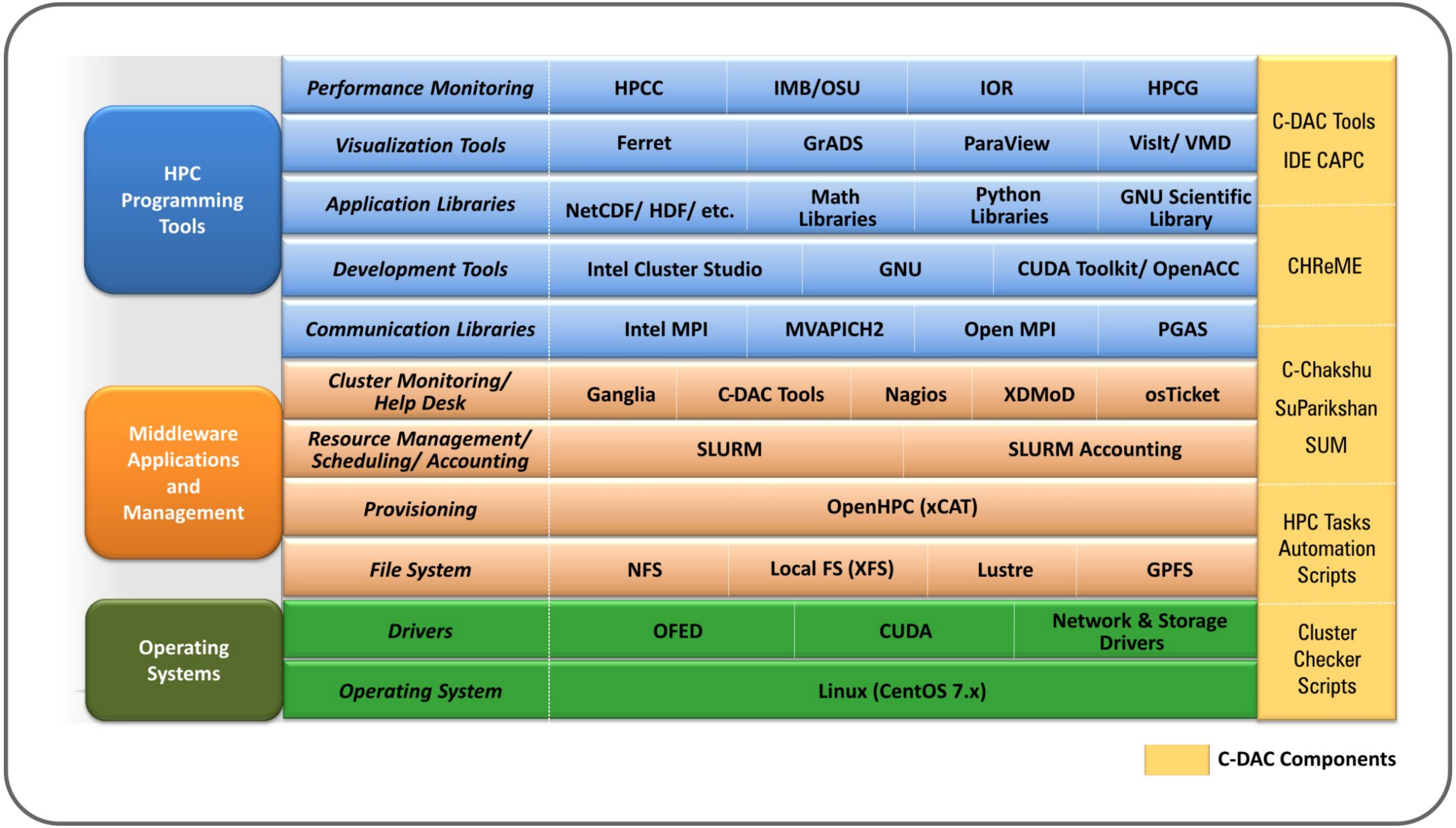
Declaration :PARAM Sanganak usage policies

1. The Resources provided to you on PARAM Sanganak facility should not be used for any commercial purpose i.e., it is restricted for the Hackathon purpose only.
2. Sharing your login credentials with some third person will revoke the responsibility of PARAM Sanganak administration committee for data theft and your account will also be disabled. The third person will also be held accountable for misusing the PARAM Sanganak facility.
3. It is strictly recommended that you should not run jobs on login node and any such incident reported will result in cancellation of the job and any repeat action will result in closure of your account.
4. You will be solely responsible for keeping your password strong and safe.
5. If found in any engagement or promotion of activities like hacking, reverse-engineering, violating intellectual property rights on or using the PARAM Sanganak facility, you will be barred from having account on any Supercomputer setup under the National Supercomputing Mission.
6. The facility is built with least downtime requirement; however, it depends on various factors like Hardware reliability, Power outage, network outage, scheduled maintenance due to which the facility could be unavailable completely/partially. Notification of all scheduled / unscheduled maintenance will be made known to the users via Website, Email, broadcast message, newsgroups etc.
7. This facility will not be used for any purpose connected with Chemical or Biological or Nuclear weapons or missiles capable of delivering such Weapons.

Architecture Diagram



Software Stack



HPC Programming Tools	*Performance Monitoring*	HPCC	IMB/OSU	IOR	HPCG	
	Visualization Tools	Ferret	GrADS	ParaView	VisIt/ VMD	
	Application Libraries	NetCDF/ HDF/ etc.	Math Libraries	Python Libraries	GNU Scientific Library	
	Development Tools	Intel Cluster Studio	GNU	CUDA Toolkit/ OpenACC		
	Communication Libraries	Intel MPI	MVAPICH2	Open MPI	PGAS	
Middleware Applications and Management	*Cluster Monitoring/ Help Desk*	Ganglia	C-DAC Tools	Nagios	XDMoD	osTicket
	Resource Management/ Scheduling/ Accounting	SLURM	SLURM Accounting			
	Provisioning	OpenHPC (xCAT)				
	File System	NFS	Local FS (XFS)	Lustre	GPFS	
Operating Systems	*Drivers*	OFED	CUDA	Network & Storage Drivers		
	Operating System	Linux (CentOS 7.x)				

C-DAC Tools
IDE CAPC

CHReME

C-Chakshu
SuParikshan
SUM

HPC Tasks Automation Scripts

Cluster Checker Scripts

🟨 C-DAC Components

System Configuration

System Specifications

Theoretical Peak Floating-point Performance Total (Rpeak)	1.67 PFLOPS
Base Specifications (Compute Nodes)	2 X Intel Xeon Cascadelake 8268, 24 Cores, 2.9 GHz, Processors per node, 192 GB Memory, 480 GB SSD
Master/Service/Login Nodes	20 nos.
CPU only Compute Nodes (Memory)	214 nos. (192GB)
GPU Compute Nodes (Memory)	20 (192 GB)
High Memory Compute Nodes	78 nos. (768GB)
Total Memory	104.832 TB
Interconnect	Primary: 100Gbps Mellanox Infiniband Interconnect network 100% non blocking, fat tree topology Secondary: 10G/1G Ethernet Network Management network: 1G Ethernet

CPU Only Compute Nodes

- 214 Nodes
- 10272 Cores
- Compute power of Rpeak 953.2 TFLOPS
- Each Node with
  - 2 X Intel Xeon Cascadelake 8268, 24 cores, 2.9 GHz, processors
  - 192 GB memory
  - 480 GB SSD

GPU Compute Nodes

- 20 Nodes
- 800 CPU Cores
- 204800 CUDA Cores
- Rpeak CPU 64 TFLOPS + GPU 312 TF
- Each Node with
  - 2 X Intel Xeon Skylake 6248, 20 cores, 2.5 GHz, processors
  - 192 GB Memory
  - 2 x NVIDIA V100 SXM2 GPU Cards
  - 480 GB SSD

High Memory Compute Nodes

- 78 Nodes
- 3744 Cores
- Compute power of Rpeak 347.33 TFLOPS
- Each Node with
  - 2 X Intel Xeon Cascadelake 8268, 24 cores, 2.9 GHz, processors
  - 768 GB Memory
  - 480 GB SSD

Accessing the cluster

Login Environment

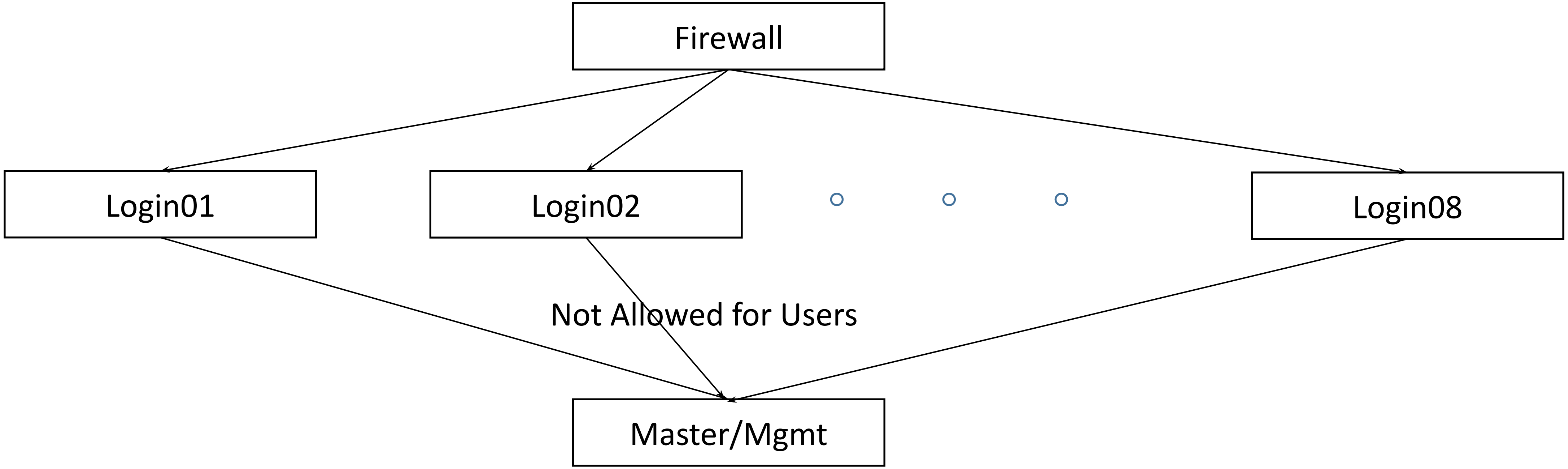
- The cluster can be accessed through 8 general login nodes.
- The login nodes is primary gateway to the rest of the cluster.
- User can perform all its functions on login node.
- All libraries, compilers, preinstalled applications, user installed application are available over login nodes.

Remote Login

- You may access login node through ssh.
- Using SSH in Windows (Putty,Moab-xterm,etc).
- Using SSH in Linux via terminal (ssh –p 4422 example user@paramsanganak.iitk.ac.in).

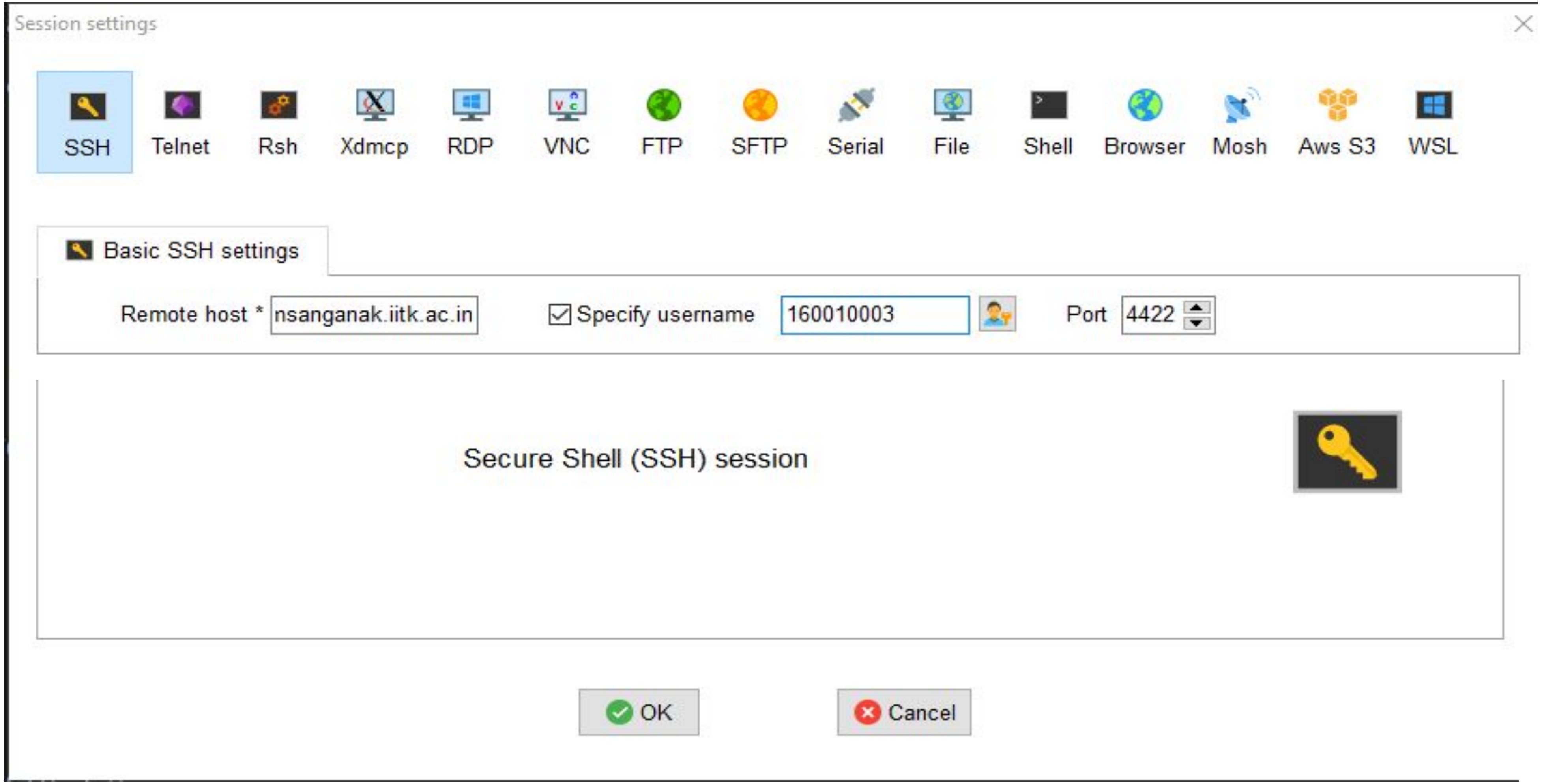
Access Policy

- **Access to Login nodes are in Round-Robin Mode.**
- **Users are not allowed to access Master/Management Nodes**



How to login

MobaXterm :



Remote host * nsanganak.iitk.ac.in

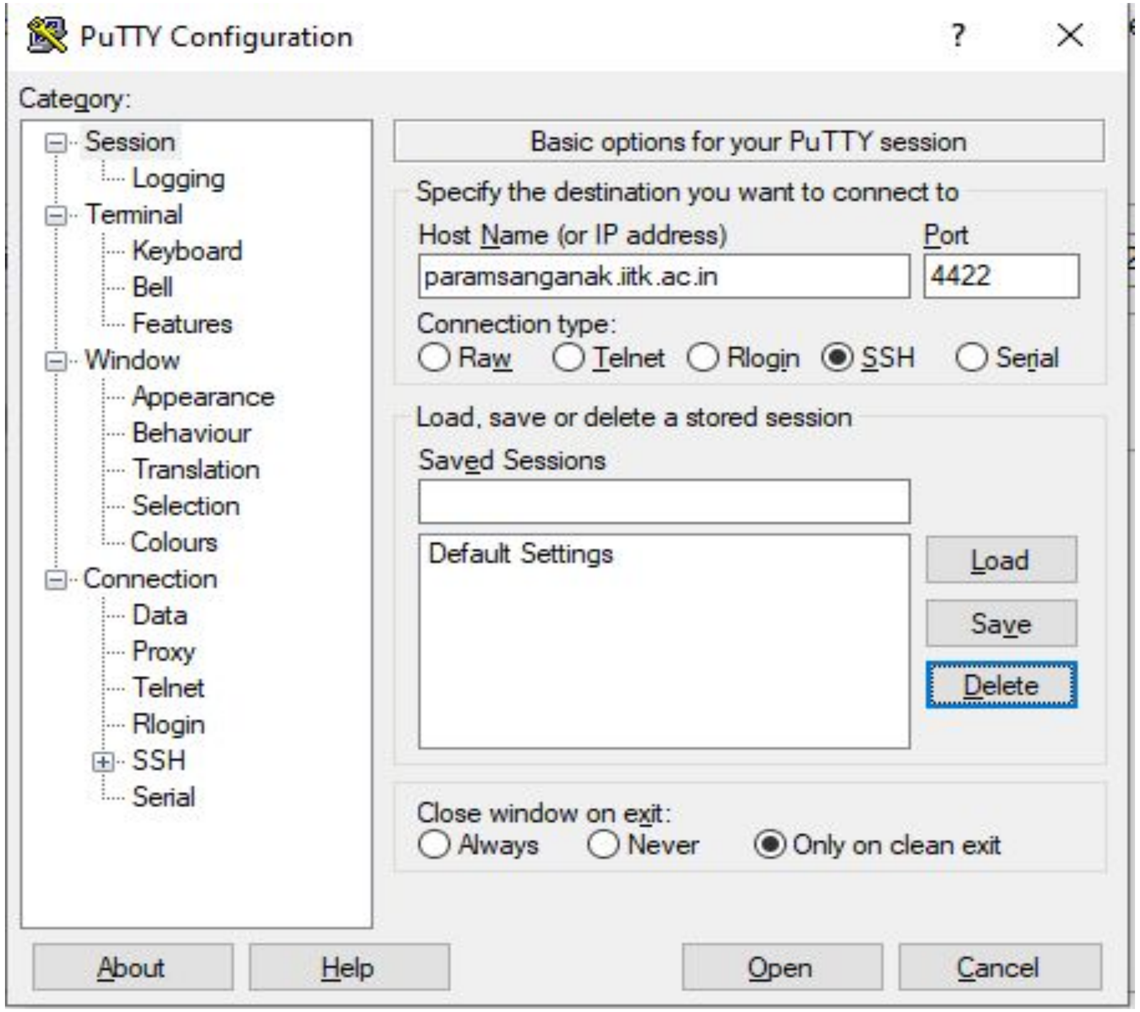
☑ Specify username 160010003

Port 4422

Secure Shell (SSH) session

How to login

PuTTY:



PuTTY Configuration

Category:

- Session
  - Logging
- Terminal
  - Keyboard
  - Bell
  - Features
- Window
  - Appearance
  - Behaviour
  - Translation
  - Selection
  - Colours
- Connection
  - Data
  - Proxy
  - Telnet
  - Rlogin
  - SSH
  - Serial

Basic options for your PuTTY session

Specify the destination you want to connect to

Host Name (or IP address): paramsanganak.iitk.ac.in

Port: 4422

Connection type: ○ Raw ○ Telnet ○ Rlogin ● SSH ○ Serial

Load, save or delete a stored session

Saved Sessions

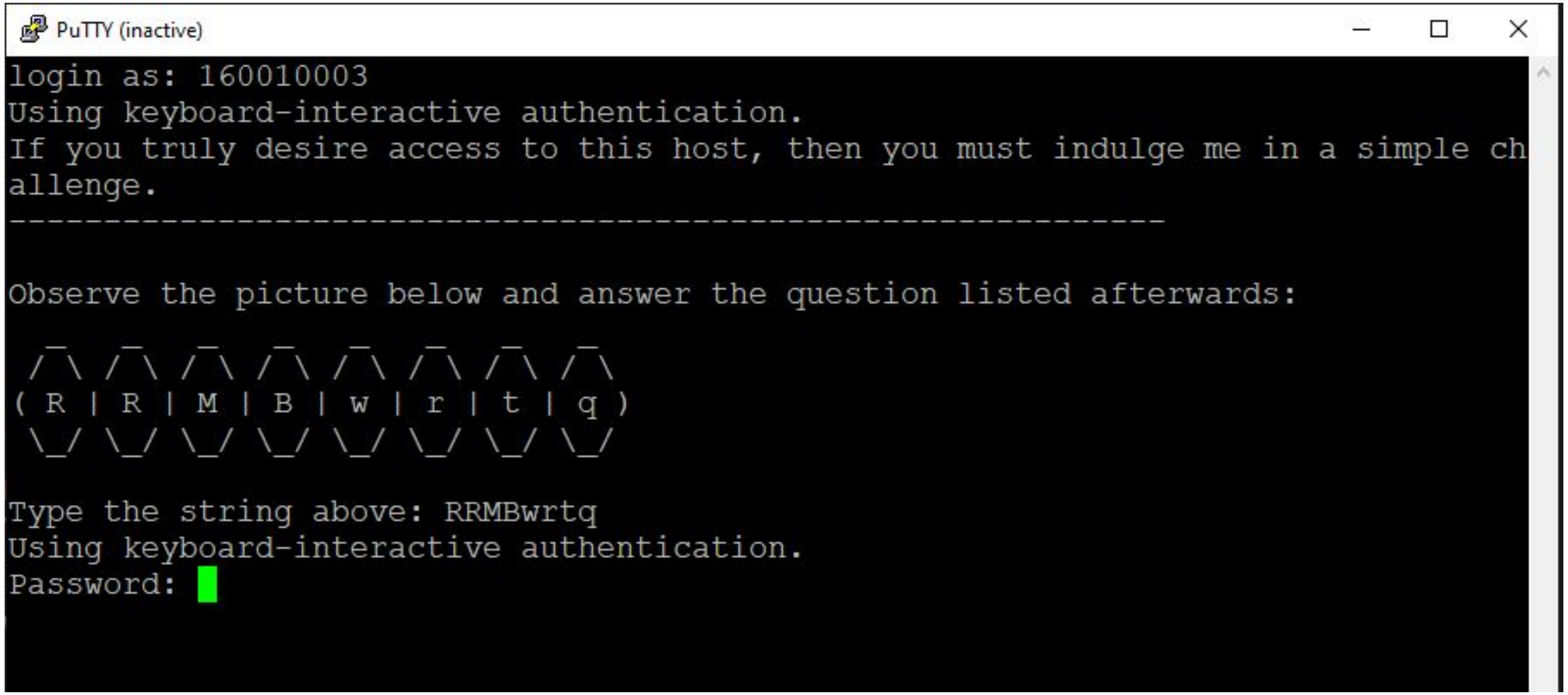
Default Settings

Close window on exit: ○ Always ○ Never ● Only on clean exit

How to login

Command: ssh (Linux users)

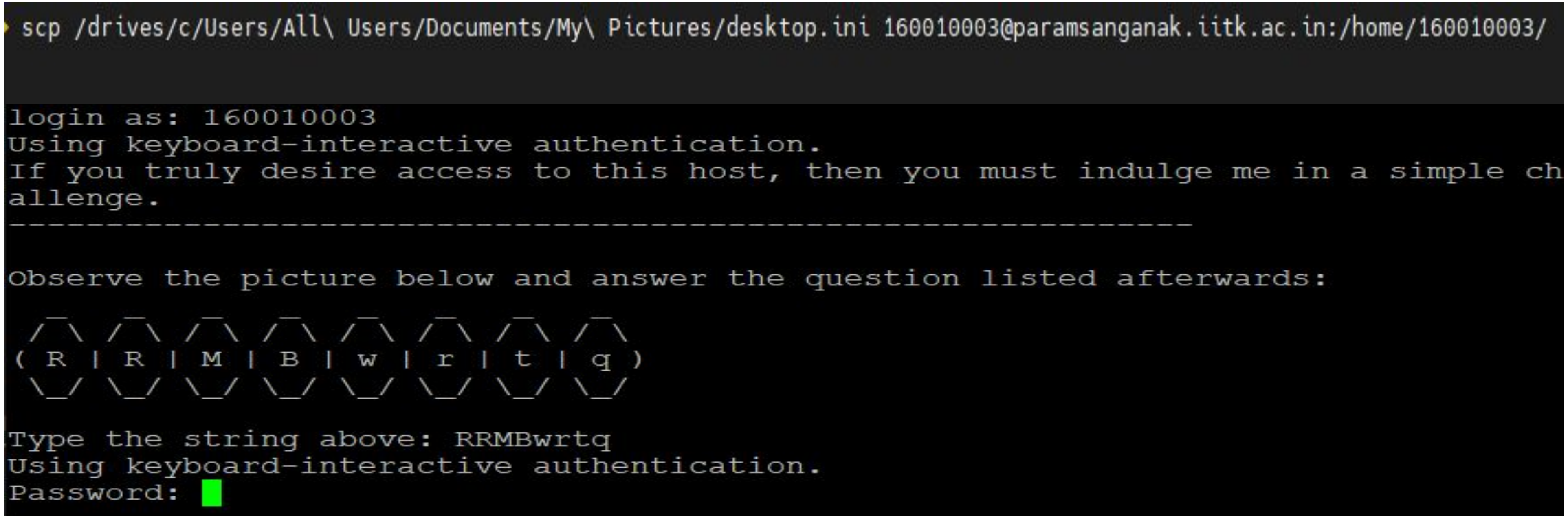
```
$ ssh <username>@paramsanganak.iitk.ac.in -p 4422
```



```
login as: 160010003
Using keyboard-interactive authentication.
If you truly desire access to this host, then you must indulge me in a simple ch
allenge.
-------------------------------------------------------------

Observe the picture below and answer the question listed afterwards:

  _   _   _   _   _   _   _   _
 / \ / \ / \ / \ / \ / \ / \ / \
( R | R | M | B | w | r | t | q )
 \_/ \_/ \_/ \_/ \_/ \_/ \_/ \_/

Type the string above: RRMBwrtq
Using keyboard-interactive authentication.
Password: █
```

Copy files

Command: scp for linux users

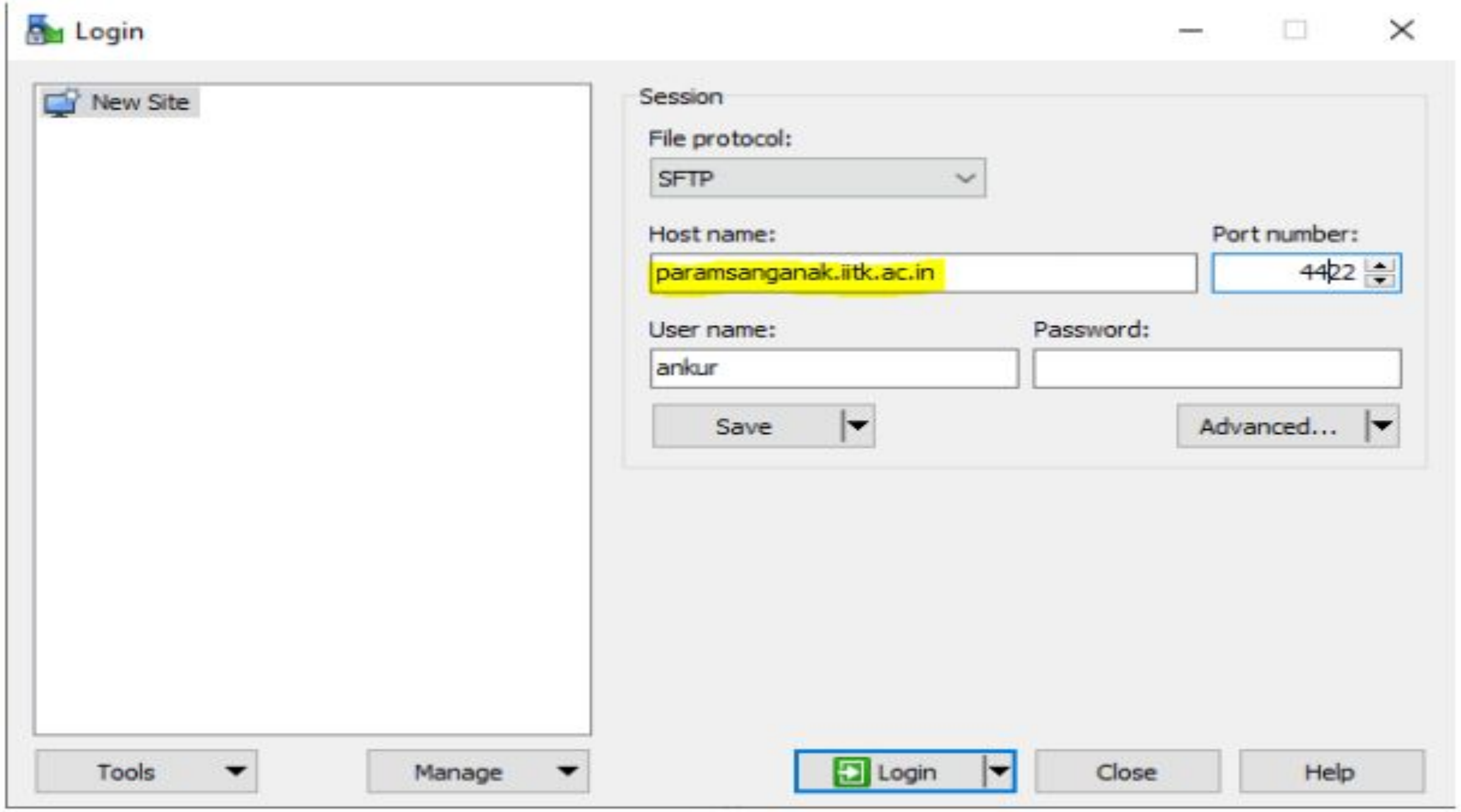


```
scp /drives/c/Users/All\ Users/Documents/My\ Pictures/desktop.ini 160010003@paramsanganak.iitk.ac.in:/home/160010003/
```

```
login as: 160010003
Using keyboard-interactive authentication.
If you truly desire access to this host, then you must indulge me in a simple ch
allenge.
-------------------------------------------------------------

Observe the picture below and answer the question listed afterwards:

  _   _   _   _   _   _   _   _
 / \ / \ / \ / \ / \ / \ / \ / \
( R | R | M | B | w | r | t | q )
 \_/ \_/ \_/ \_/ \_/ \_/ \_/ \_/

Type the string above: RRMBwrtq
Using keyboard-interactive authentication.
Password:
```

Copy files

WinScp (Windows):



Login

New Site

Session

File protocol: SFTP

Host name: paramsanganak.iitk.ac.in

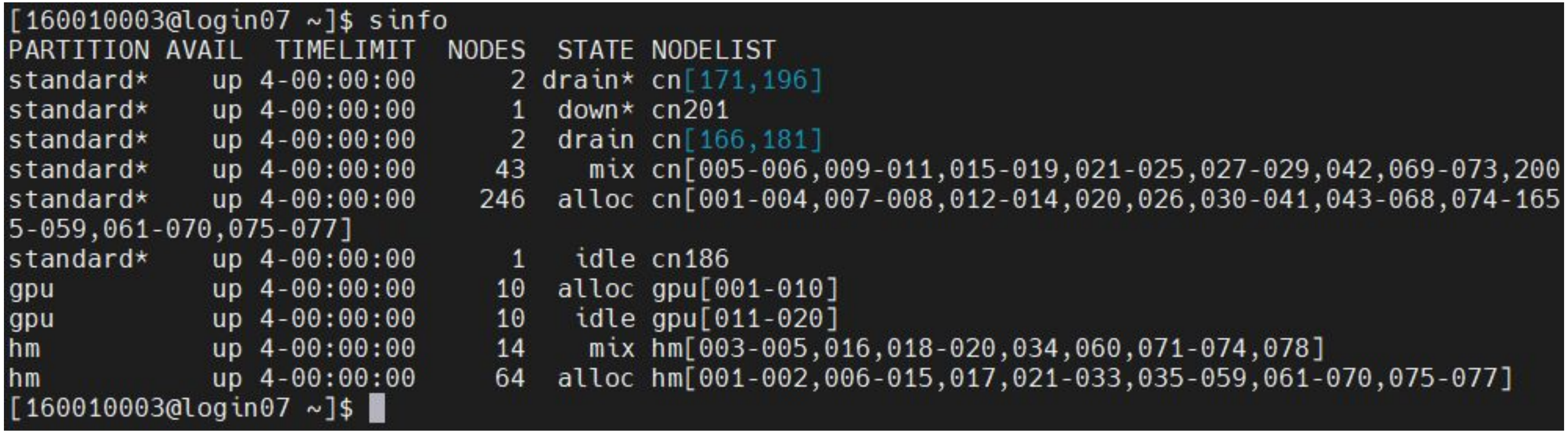
Port number: 4422

User name: ankur

Password:

Resource manager and scheduler (slurm)

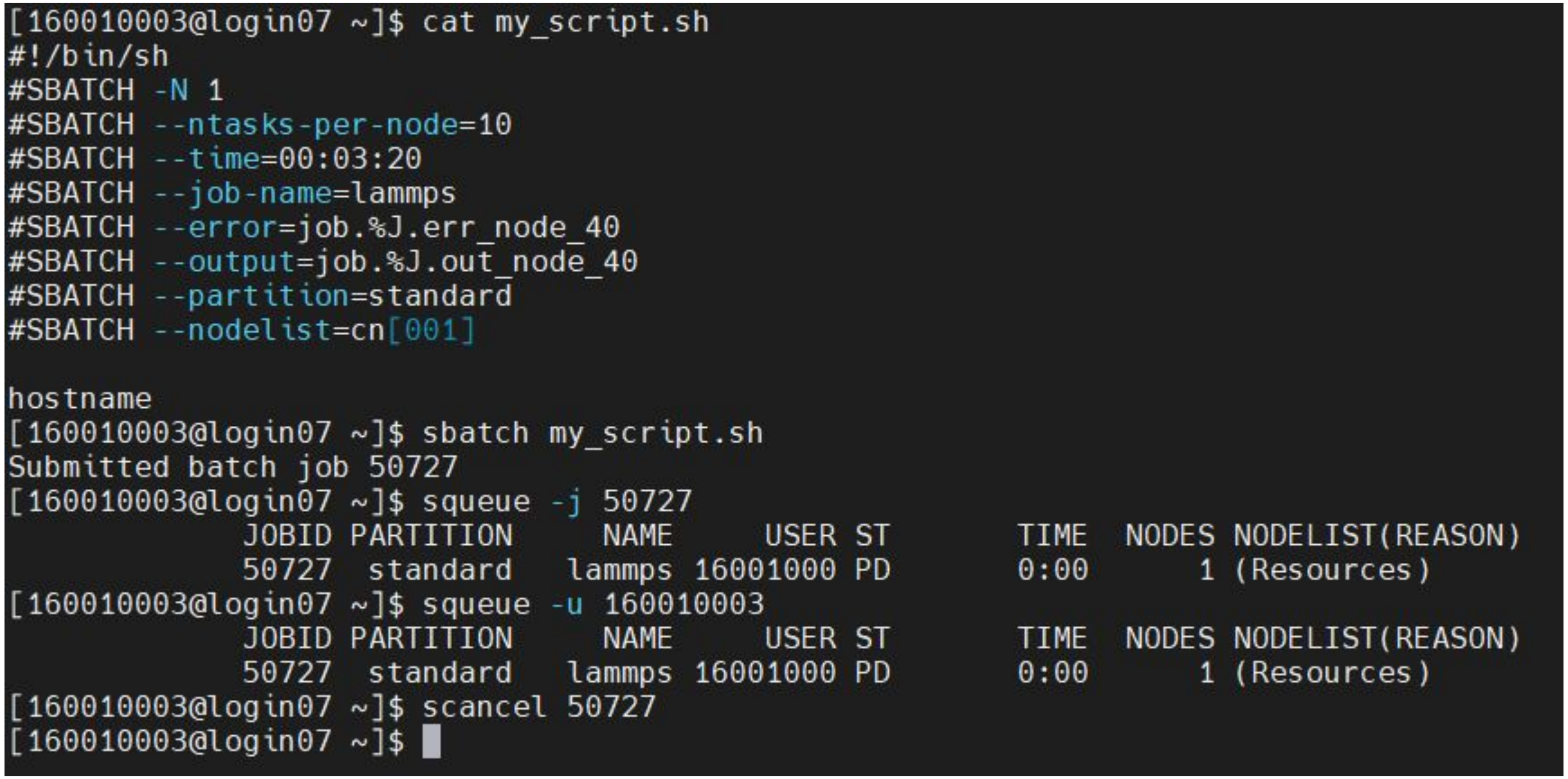
Command: Sinfo



```
[160010003@login07 ~]$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
standard*    up 4-00:00:00      2 drain* cn[171,196]
standard*    up 4-00:00:00      1  down* cn201
standard*    up 4-00:00:00      2  drain cn[166,181]
standard*    up 4-00:00:00     43    mix cn[005-006,009-011,015-019,021-025,027-029,042,069-073,200
standard*    up 4-00:00:00    246  alloc cn[001-004,007-008,012-014,020,026,030-041,043-068,074-165
5-059,061-070,075-077]
standard*    up 4-00:00:00      1   idle cn186
gpu          up 4-00:00:00     10  alloc gpu[001-010]
gpu          up 4-00:00:00     10   idle gpu[011-020]
hm           up 4-00:00:00     14    mix hm[003-005,016,018-020,034,060,071-074,078]
hm           up 4-00:00:00     64  alloc hm[001-002,006-015,017,021-033,035-059,061-070,075-077]
[160010003@login07 ~]$ 
```

Resource manager and scheduler (slurm)

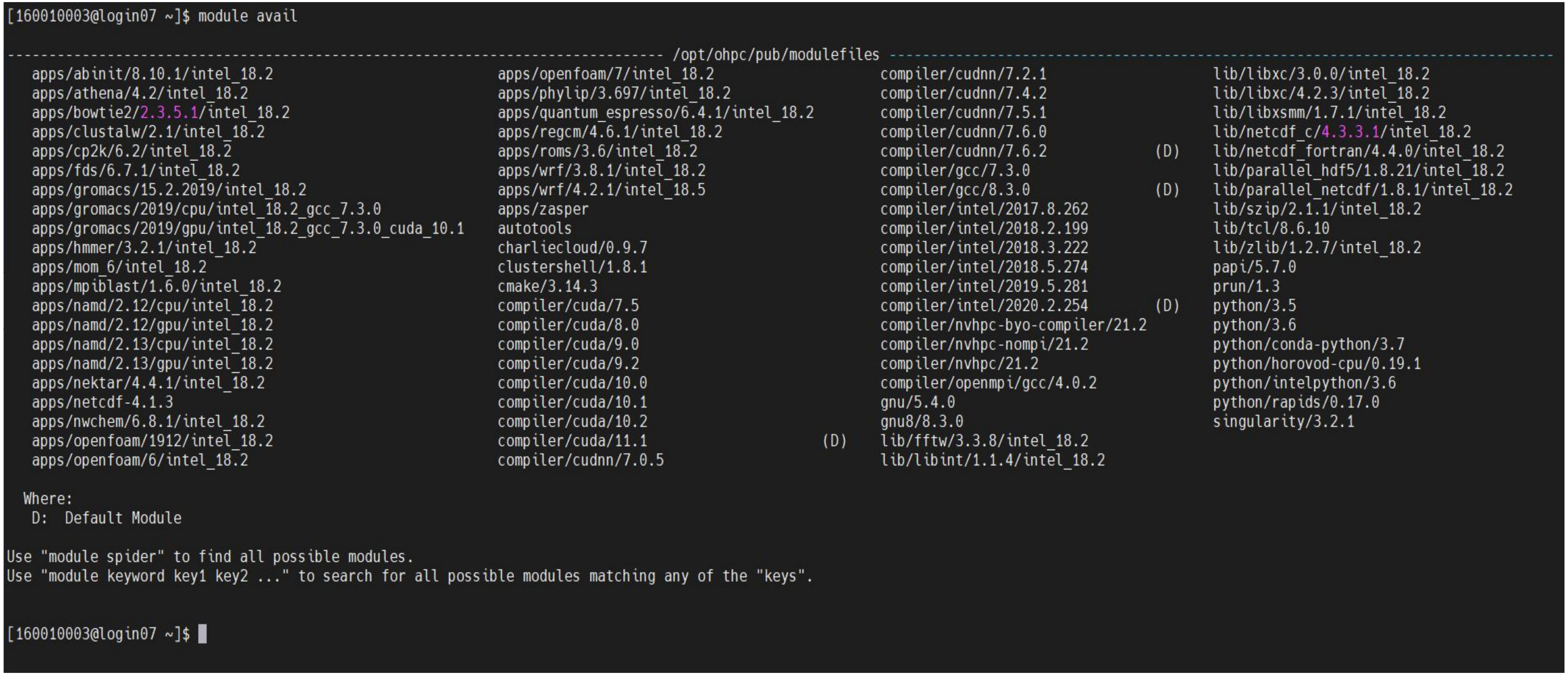
Command: sbatch, squeue, scancel, etc.



```
[160010003@login07 ~]$ cat my_script.sh
#!/bin/sh
#SBATCH -N 1
#SBATCH --ntasks-per-node=10
#SBATCH --time=00:03:20
#SBATCH --job-name=lammps
#SBATCH --error=job.%J.err_node_40
#SBATCH --output=job.%J.out_node_40
#SBATCH --partition=standard
#SBATCH --nodelist=cn[001]

hostname
[160010003@login07 ~]$ sbatch my_script.sh
Submitted batch job 50727
[160010003@login07 ~]$ squeue -j 50727
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             50727  standard   lammps 16001000 PD       0:00      1 (Resources)
[160010003@login07 ~]$ squeue -u 160010003
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             50727  standard   lammps 16001000 PD       0:00      1 (Resources)
[160010003@login07 ~]$ scancel 50727
[160010003@login07 ~]$ █
```

List the available modules

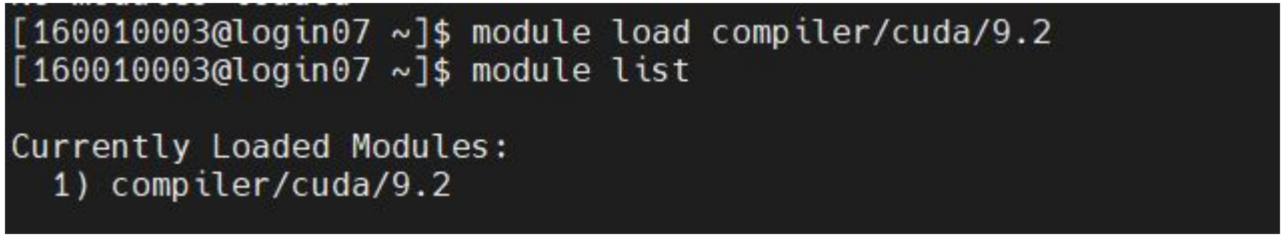
$ module avail



```
[160010003@login07 ~]$ module avail

------------------------------------------------------------------------------- /opt/ohpc/pub/modulefiles --------------------------------------------------------------------------------
   apps/abinit/8.10.1/intel_18.2                           apps/openfoam/7/intel_18.2                    compiler/cudnn/7.2.1                    lib/libxc/3.0.0/intel_18.2
   apps/athena/4.2/intel_18.2                              apps/phylip/3.697/intel_18.2                  compiler/cudnn/7.4.2                    lib/libxc/4.2.3/intel_18.2
   apps/bowtie2/2.3.5.1/intel_18.2                         apps/quantum_espresso/6.4.1/intel_18.2        compiler/cudnn/7.5.1                    lib/libxsmm/1.7.1/intel_18.2
   apps/clustalw/2.1/intel_18.2                            apps/regcm/4.6.1/intel_18.2                   compiler/cudnn/7.6.0                    lib/netcdf_c/4.3.3.1/intel_18.2
   apps/cp2k/6.2/intel_18.2                                apps/roms/3.6/intel_18.2                      compiler/cudnn/7.6.2             (D)    lib/netcdf_fortran/4.4.0/intel_18.2
   apps/fds/6.7.1/intel_18.2                               apps/wrf/3.8.1/intel_18.2                     compiler/gcc/7.3.0                      lib/parallel_hdf5/1.8.21/intel_18.2
   apps/gromacs/15.2.2019/intel_18.2                       apps/wrf/4.2.1/intel_18.5                     compiler/gcc/8.3.0               (D)    lib/parallel_netcdf/1.8.1/intel_18.2
   apps/gromacs/2019/cpu/intel_18.2_gcc_7.3.0              apps/zasper                                   compiler/intel/2017.8.262               lib/szip/2.1.1/intel_18.2
   apps/gromacs/2019/gpu/intel_18.2_gcc_7.3.0_cuda_10.1    autotools                                     compiler/intel/2018.2.199               lib/tcl/8.6.10
   apps/hmmer/3.2.1/intel_18.2                             charliecloud/0.9.7                            compiler/intel/2018.3.222               lib/zlib/1.2.7/intel_18.2
   apps/mom_6/intel_18.2                                   clustershell/1.8.1                            compiler/intel/2018.5.274               papi/5.7.0
   apps/mpiblast/1.6.0/intel_18.2                          cmake/3.14.3                                  compiler/intel/2019.5.281               prun/1.3
   apps/namd/2.12/cpu/intel_18.2                           compiler/cuda/7.5                             compiler/intel/2020.2.254        (D)    python/3.5
   apps/namd/2.12/gpu/intel_18.2                           compiler/cuda/8.0                             compiler/nvhpc-byo-compiler/21.2        python/3.6
   apps/namd/2.13/cpu/intel_18.2                           compiler/cuda/9.0                             compiler/nvhpc-nompi/21.2               python/conda-python/3.7
   apps/namd/2.13/gpu/intel_18.2                           compiler/cuda/9.2                             compiler/nvhpc/21.2                     python/horovod-cpu/0.19.1
   apps/nektar/4.4.1/intel_18.2                            compiler/cuda/10.0                            compiler/openmpi/gcc/4.0.2              python/intelpython/3.6
   apps/netcdf-4.1.3                                       compiler/cuda/10.1                            gnu/5.4.0                               python/rapids/0.17.0
   apps/nwchem/6.8.1/intel_18.2                            compiler/cuda/10.2                            gnu8/8.3.0                              singularity/3.2.1
   apps/openfoam/1912/intel_18.2                           compiler/cuda/11.1                     (D)    lib/fftw/3.3.8/intel_18.2
   apps/openfoam/6/intel_18.2                              compiler/cudnn/7.0.5                          lib/libint/1.1.4/intel_18.2

  Where:
   D:  Default Module

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".


[160010003@login07 ~]$ █
```

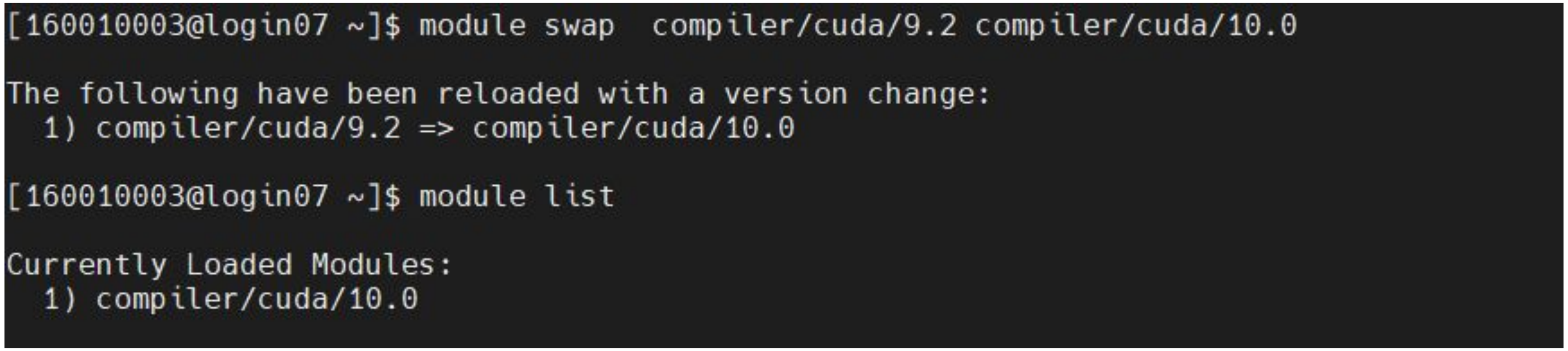
Load, list, swap modules

$ module load <module name>



```
[160010003@login07 ~]$ module load compiler/cuda/9.2
[160010003@login07 ~]$ module list

Currently Loaded Modules:
  1) compiler/cuda/9.2
```

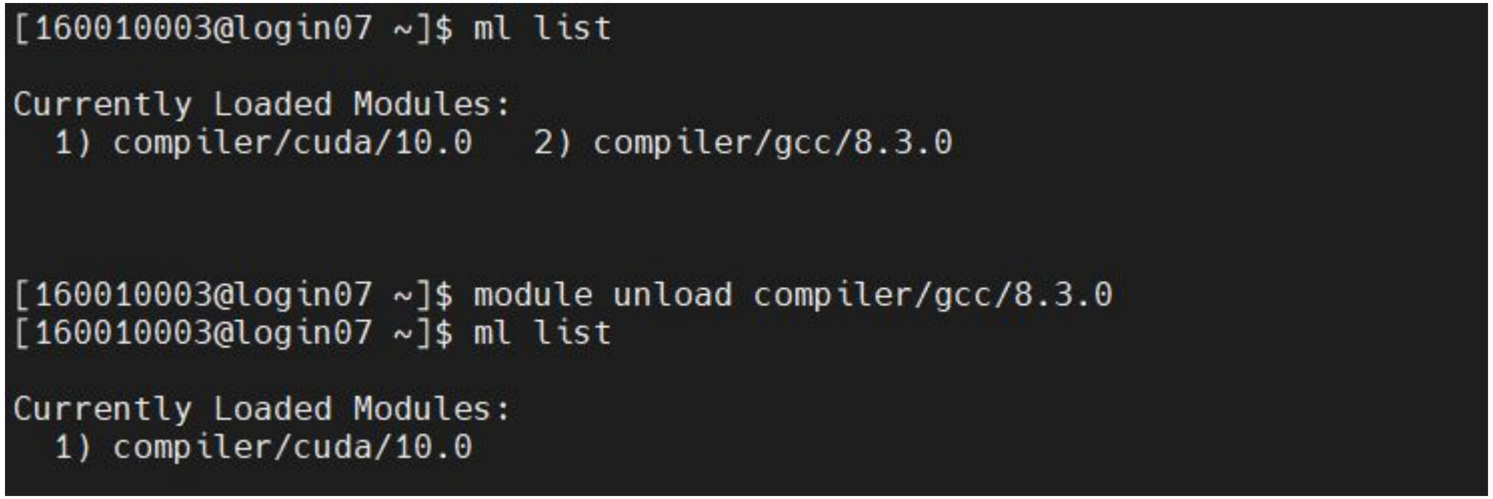
$ module swap <curr. module> <new module>



```
[160010003@login07 ~]$ module swap  compiler/cuda/9.2 compiler/cuda/10.0

The following have been reloaded with a version change:
  1) compiler/cuda/9.2 => compiler/cuda/10.0

[160010003@login07 ~]$ module list

Currently Loaded Modules:
  1) compiler/cuda/10.0
```

Unload a module

$ module unload <module name>



```
[160010003@login07 ~]$ ml list

Currently Loaded Modules:
  1) compiler/cuda/10.0   2) compiler/gcc/8.3.0



[160010003@login07 ~]$ module unload compiler/gcc/8.3.0
[160010003@login07 ~]$ ml list

Currently Loaded Modules:
  1) compiler/cuda/10.0
```