

# USER GUIDE

## HPC user help guide

### Abstract

This guide provides concise instructions for users on Introduction of Linux, how to access and utilize the IITGN HPC facility, how to copy & paste data on Linux, how to create job submission scripts, supercomputer job submission related useful commands and FAQs.

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## HIGH PERFORMANCE COMPUTING CLUSTER (HPCC) – SPECIFICATION'S

Fully Qualified Domain Name	hpc.iitgn.ac.in
IP Address of HPC cluster	10.0.138.33
<b>Each node in the cluster is as follows:</b>	
Master/Head Node (01)	CPU - 2 x Intel(R) Xeon(R) Gold 5215 CPU 10-Core Processor with 96 GB RAM/Memory
I/O Nodes (01-02)	CPU - 2 x Intel(R) Xeon(R) Gold 6230 CPU 20-Core Processor with 64 GB RAM/Memory
Compute Nodes (01-05) (small partition)	CPU - 2 x Intel(R) Xeon(R) Gold 6230 CPU 20-Core Processor with 96 GB RAM/Memory
Compute Nodes (06-16) (medium partition)	CPU - 2 x Intel(R) Xeon(R) Gold 6230 CPU 16-Core Processor with 192 GB RAM/Memory
Compute Nodes (17) (test partition)	CPU - 2 x Intel(R) Xeon(R) Gold 6130 CPU 16-Core Processor with 160 GB RAM/Memory
Compute Nodes (18-28) (large partition)	CPU - 2 x Intel(R) Xeon(R) Gold 6130 CPU 20-Core Processor with 192 GB RAM/Memory
GPU Nodes (01-02) (p100gpu partition)	CPU - 2 x Intel(R) Xeon(R) Gold 6130 CPU 16-Core Processor with 192 GB RAM/Memory 1 x Tesla P100-PCIE-16GB
GPU Nodes (03-06) (v100gpu partition)	CPU - 2 x Intel(R) Xeon(R) Gold 6130 CPU 20-Core Processor with 192 GB RAM/Memory 1 x Tesla V100-PCIE-32GB
Usable Storage	~60 TB Usable SAN storage
Total CPU	1248 cores
Total Compute Nodes	34
High-Speed Interconnect	Mellanox EDR Infiniband 100Gbps
User Level Quota	200 GB per user in home directory
Operating System	Rocky 8.8

## INTRODUCTION TO LINUX

LINUX is an Open Source Operating System (OS). Its file system is ext3/ext4 format, likewise in Windows you would see FAT/NTFS format. A shell or popularly called a "terminal" is an interface between the kernel (the heart of the OS) where, user types in command, to execute certain tasks. Normal users generally get a "\$" (dollar) prompt to work in a shell. Root or Super-users get "#" (hash) prompt to manage, modifying, monitor almost everything about a system. For any doubts or clarifications of commands, please see the

```
[user1@HPC ~]$ <command> --help
```

```
E.g. [user1@HPC ~]$ ls --help
```

### Basic commands to enhance your skills:

- How to check operating system(OS) version in Linux?

Answer:

```
[user1@ HPC ~]$ lsb_release -a
```

- How to check kernel version in Linux?

Answer:

```
[user1@ HPC ~]$ uname -rso
```

- How to see the current path or working directory?

Answer:

```
[user1@ HPC~]$ pwd
```

- How to list all files and directories?

Answer:

```
[user1@ HPC~]$ ls -la
```

- How to go back to previous folder?

Answer:

```
[user1@ HPC~]$ cd ..
```

- How to go back to parent directory?

Answer:

```
[user1@ HPC~]$ cd
```

- How to view content of any file?

Answer:

```
[user1@ HPC~]$ cat <file_name>
```

- How to copy & paste data on Linux?

Answer:

Case-A:

```
[user1@ HPC~]$ cp /home/admin/Desktop/myfolder/myfile /new-location
```

Case-B:

```
[user1@ HPC~]$ cp -rpvf /home/admin/Desktop/myfolder/myfile /new-location
```

Note: In Case-B, an option "-rpvf" is used. "r" stands for recursively, "p" stands for parent, "v" stand for verbose, "f" stands for forcefully. Using this option, a user can see the process and progress of 'copying' from one location to other showing the complete path from where-and-to it is copying.

- How to check available storage in system?

Answer:

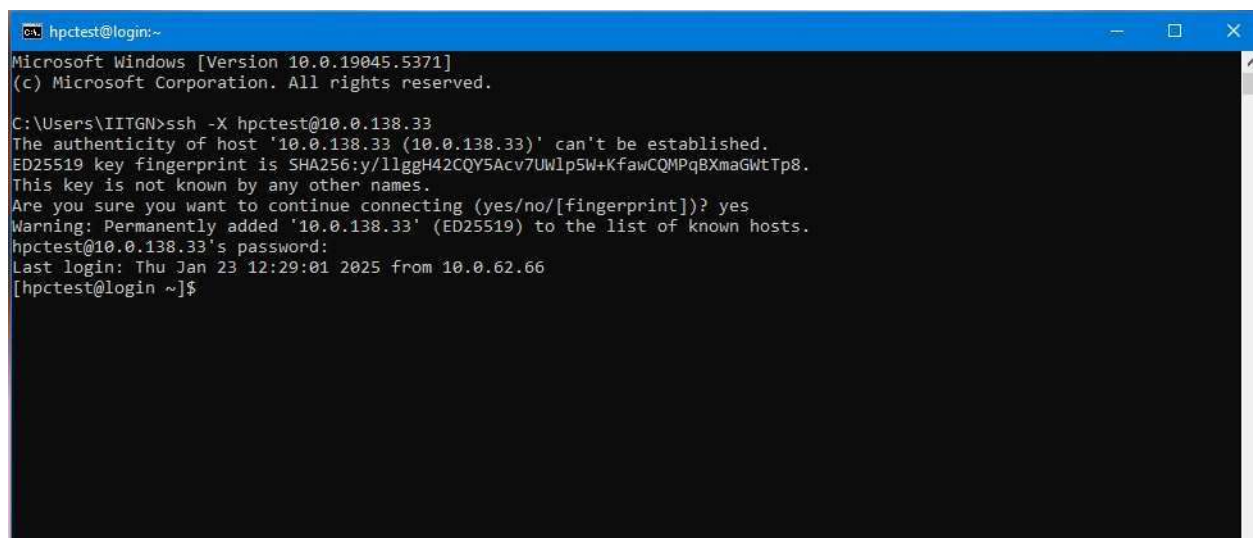
```
[user1@ HPC~]$ free -h
```

## How to access the HPC facility?

❖ Please use your **SSO/Network ID** credentials for the username and password.

- Using SSH in Windows

To access the IITGN HPC cluster on a Windows system, open the "Command Prompt," and log in with your provided "Username" and "IP\_address" (e.g., Username: hpctest, IP\_address: 10.0.138.33 for the IITGN HPC Cluster) as provided in the email.



```
hpctest@login:~
Microsoft Windows [Version 10.0.19045.5371]
(c) Microsoft Corporation. All rights reserved.

C:\Users\IITGN>ssh -X hpctest@10.0.138.33
The authenticity of host '10.0.138.33 (10.0.138.33)' can't be established.
ED25519 key fingerprint is SHA256:y/llggH42CQY5Acv7UWlp5W+KfawCQMPqBXmaGwtTp8.
This key is not known by any other names.
Are you sure you want to continue connecting (yes/no/[fingerprint])? yes
Warning: Permanently added '10.0.138.33' (ED25519) to the list of known hosts.
hpctest@10.0.138.33's password:
Last login: Thu Jan 23 12:29:01 2025 from 10.0.62.66
[hpctest@login ~]$
```

Figure 1 - A snapshot of instruction using Windows command prompt

- Using SSH in Mac or Linux

Both Mac and Linux systems provide a built-in SSH client, so there is no need to install any additional package. Open the terminal, connect to SSH server by typing the following command:

```
[user1@ HPC~]$ ssh <username>@<IP_address>
```

For example, to connect to the IITGN HPC cluster, with the username

```
[user1@ HPC~]$ ssh user1@10.0.138.33
```

You will be prompted for a password, and then will be connected to the server.

- Using tools like MobaXterm, WinSCP, PuTTY etc.

These are the third-party tools that haven't been configured by default in your system. You'll need to download them from the browser.

## MobaXterm

It is a third party freely available tool which can be used to access the IITGN HPC system and transfer file to IITGN HPC cluster through your local systems (laptop/desktop).

Link to download this tool:

[https://download.mobatek.net/2502024121622306/MobaXterm\\_Portable\\_v25.0.zip](https://download.mobatek.net/2502024121622306/MobaXterm_Portable_v25.0.zip)

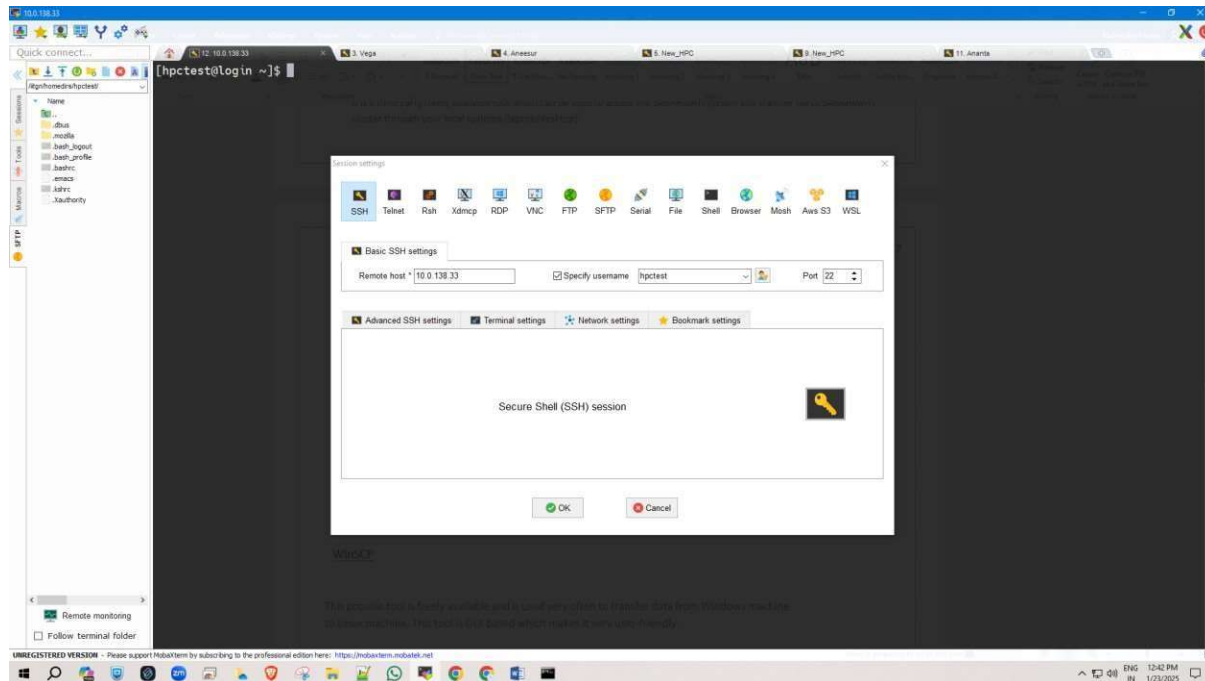


Figure 2 - A snapshot of instruction using MobaXterm

## WinSCP

This popular tool is freely available and is used very often to transfer data from Windows machine to Linux machine. This tool is GUI based which makes it very user-friendly.

Link for this tool is:

<https://winscp.net/download/WinSCP-6.3.6-Setup.exe/download>

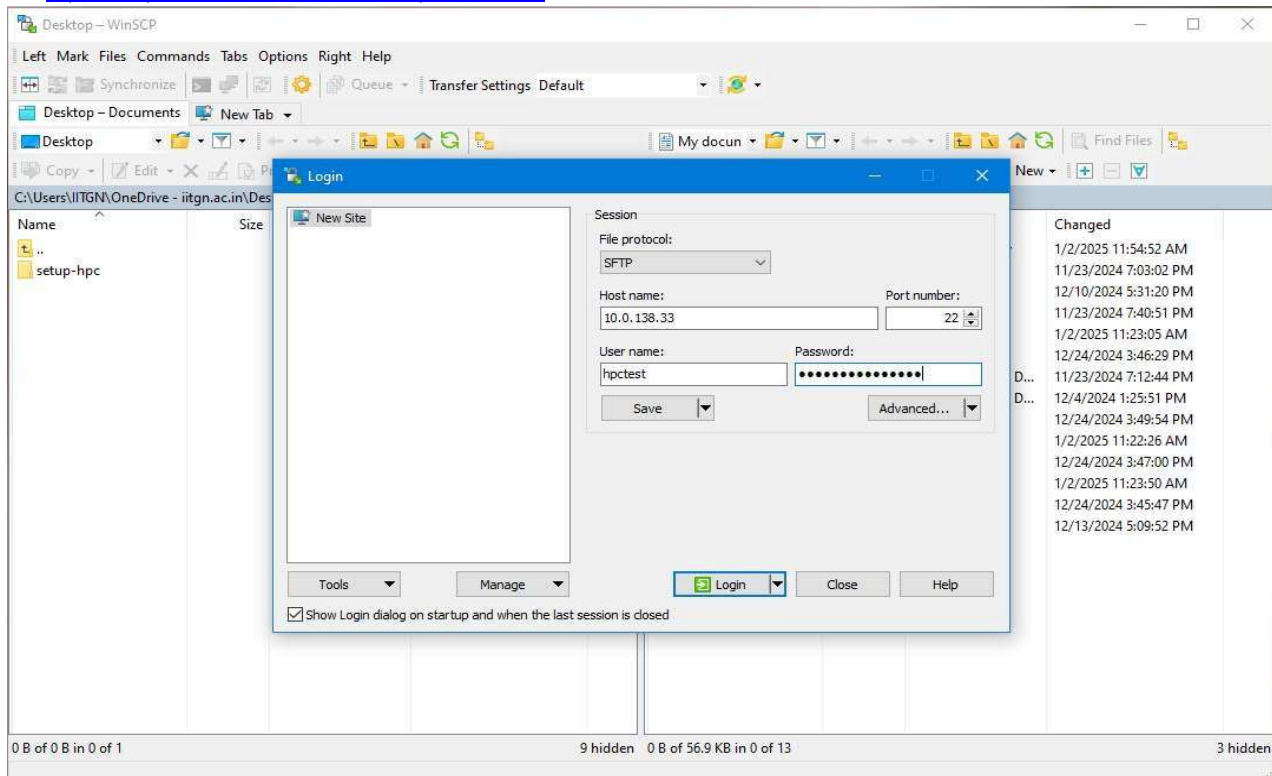


Figure 3 - A snapshot of instruction using WinSCP



## PuTTY

PuTTY is the most popular open source “ssh” client application for Windows. Once PuTTY is installed, access the system by entering the “IP\_address”, after which an interface will prompt you for the “username and password” of the user.

Link for this tool is:

[https://www.puttygen.com/download-putty#google\\_vignette](https://www.puttygen.com/download-putty#google_vignette)

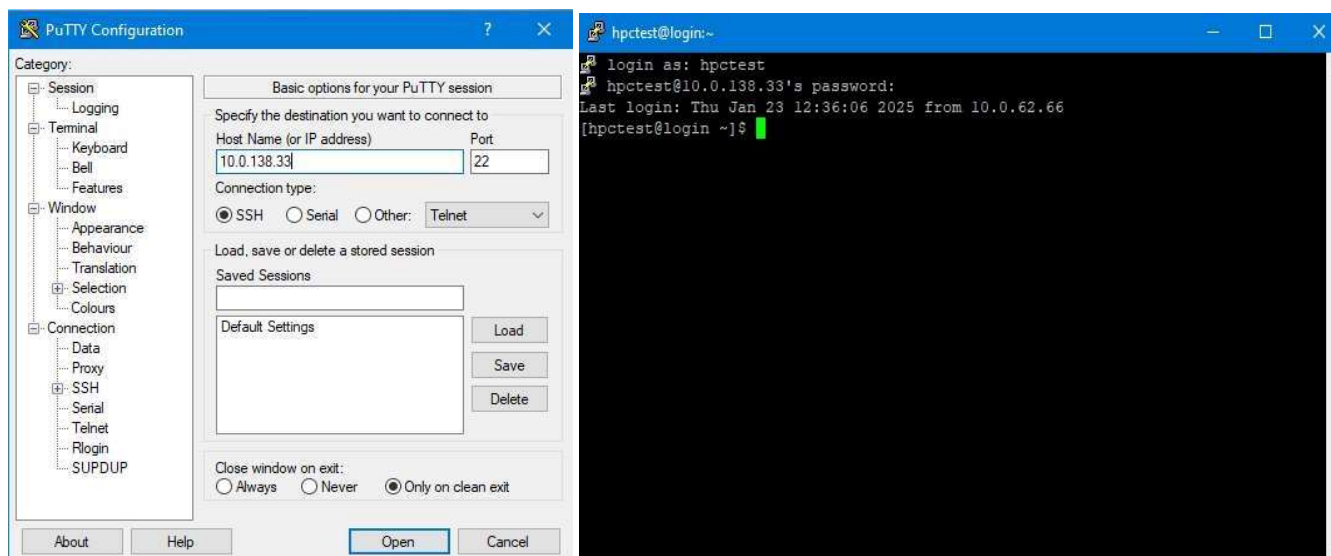


Figure 4 - A snapshot of instruction using PuTTY

## Transferring files between local machine and IITGN HPC cluster

To store the data special directories have been made available to the users with the name “home” the path to this directory is “/home/username”. Whereas these directories are common to all the users, a user will get his own directory with their username in /home/ Username directories where they can store their data.

/home/<username>/: This directory is generally used by the user to install applications.

However, there is a limit to the storage provided to the users, the limits have been defined according to quota over these directories, all users will be allotted the same quota by default. When a user wishes to transfer data from their local system (laptop/desktop) to the IITGN HPC system, they can use various methods and tools.

A user using ‘Windows’ operating system will get methods and tools that are native to Microsoft Windows and tools that could be installed on your Microsoft windows machine. Linux operating system users do not require any tool.

They can just use the “scp” command on their terminal, as mentioned below.

```
$ scp -r <path to the local data directory> <Username>@IP_address:<path to directory on HPC where to save the data>
```

Users are advised to keep a copy of their data with themselves, once the project/research work is completed by transferring the

data in from IITGN HPC cluster to their local system (laptop/desktop). The command shown below can be used for effecting file transfers (in all the tools):

#### Example:

Same Command could be used to transfer data from the IITGN HPC system to your local system (laptop/desktop).

```
$ scp -r /dir/dir/file username@<IP_address>:/home/username
```

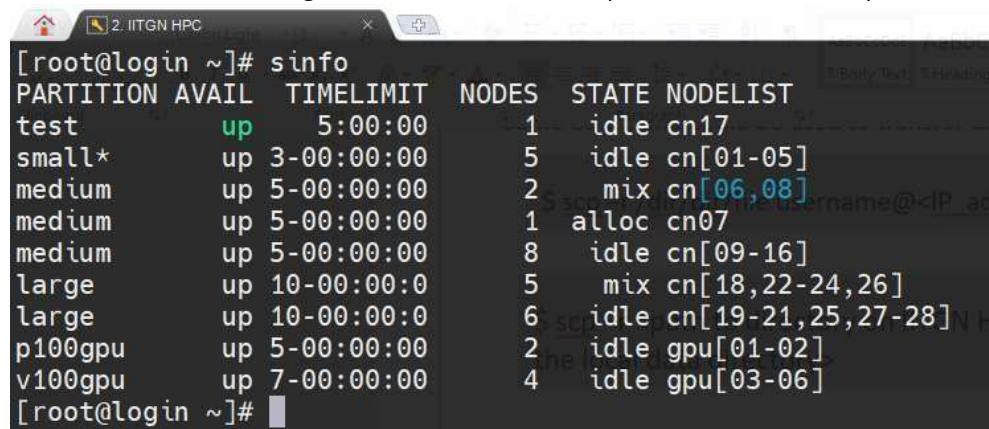
```
$ scp -r <path to directory on HPC> <username>@<IP of localsystem>:<path to the local data directory>
```

**Note:** The Local system (laptop/desktop) should be connected to the network with which it can access the IITGN HPC system.

#### Walltime of the cluster:

Walltime parameter defines as to how long your job will run. The maximum runtime of a job allowed as per QoS policy. If more than 7 days are required, a special request needs to be sent to HPC coordinator and it will be dealt with on a case-to-case basis.

The command to check standard walltime assigned, state of the nodes and partion available in the system:



```
[root@login ~]# sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
test      up      5:00:00    1     idle cn17
small*    up    3-00:00:00    5     idle cn[01-05]
medium    up    5-00:00:00    2     mix  cn[06,08]
medium    up    5-00:00:00    1     alloc cn07
medium    up    5-00:00:00    8     idle cn[09-16]
large     up   10-00:00:00    5     mix  cn[18,22-24,26]
large     up   10-00:00:00    6     idle cn[19-21,25,27-28]
p100gpu   up    5-00:00:00    2     idle gpu[01-02]
v100gpu   up    7-00:00:00    4     idle gpu[03-06]
[root@login ~]#
```

Figure 4 - A snapshot of time-limit

The command line to specify walltime is given below.

```
$ srun -t walltime <days-hours:mins:seconds>
```

and also, as part of the submit scripts described in the manual. If a job does not get completed within the walltime specified in the script, it will get terminated.

The biggest advantage of specifying appropriate walltime is that the efficiency of scheduling improves resulting in improved throughput in all jobs including yours. You are encouraging to arrive at the appropriate walltime for your job by executing your jobs few times.

NOTE: You are requested to explicitly specify the walltime in your command lines and scripts.

#### How to create job submission scripts?

Script files contain the information that SLURM needs to run your job. It has directives about names of files, how many cpus/gpus to use, which queue to run the job on.

You can create your script files directly in your respective directory on the cluster using: vi, vim, nano etc. Or you can create them on your computer using Macintosh: Text-Edit and Windows: Notepad and then move the file to the cluster via above shown methods.

The following is an example of a script file's content:

<code>#!/bin/bash</code>	Tells the OS which shell to run this script in
<code>#SBATCH --job-name &lt;my_job_name&gt;</code>	Assigns the name "my_job_name" to the job
<code>#SBATCH -p &lt;partition_name&gt;</code>	Run "sinfo" command to see the list of available partition
<code>#SBATCH --mail-user=&lt;your_email&gt;</code>	Email address to send job-related status (optional: may not work)
<code>#SBATCH --nodes=1</code>	Run all processes on a single node
<code>#SBATCH --ntasks=1</code>	Run a single task
<code>#SBATCH --cpus-per-task=4</code>	Number of CPU cores per task
<code>#SBATCH --gres=gpu</code>	Include gpu for the task (optional only for GPU jobs)
<code>#SBATCH --mem=6gb</code>	Total memory limit (optional)
<code>#SBATCH --time=00:00:05:00</code>	Time limit days:hrs:min:sec (optional)
<code>#SBATCH --output=first_%j.log</code>	Standard output and error log
<code>myprogram</code>	Your program information goes on the following line

### Sample job script:

```
#!/bin/bash
#SBATCH --job-name=test_job           # Job name
#SBATCH --partition=small             # Run "sinfo" command to see the list of available partition
#SBATCH --nodes=1                     # Run all processes on a single node
#SBATCH --ntasks=1                    # Run a single task
#SBATCH --cpus-per-task=20            # Number of CPU cores per task
#SBATCH --gres=gpu                    # Include gpu for the task (optional only for GPU jobs)
#SBATCH --mem=6gb                     # Total memory limit (optional)
#SBATCH --time=00:05:00               # Time limit hrs:min:sec (optional)
#SBATCH --output=first_%j.log         # Standard output and error log

date;hostname;pwd

module load openmpi4
<Executable PATH> INPUT OUTPUT
```

### IITGN HPC Jobs related Useful Commands

- For submitting a job: `$ sbatch <your_script_file.sh>`
- For checking jobs in queue status: `$ squeue -l`
- For checking the available module files: `$ module avail`
- To load the module file: `$ module load <module_name>`
- For checking node status: `$ sinfo --all`
- For checking status of the running job: `$ scontrol show jobid <job_id_number>`
- For checking any job status in queue: `$ sacct -j <job-id>`
- For cancelling the job: `$ scancel <job-id>`
- For checking whether the job is running in GPU: `$ nvidia-smi`
- For checking the generation of output at runtime: `$ tail -f output.log`

## FAQs

1. How to request for an HPC account?  
Answer: Please send an email to [support.hpc@iitgn.ac.in](mailto:support.hpc@iitgn.ac.in)
2. How many Jobs can I run and with how many cores?
3. Answer: There is no limit on the number of jobs per user. The maximum number of cores per job is currently set as 80.
4. What is the default storage allocation for my account?  
Answer: The quota for each user is 200 GB in the home directory.
5. What should I do if my job fails?  
Answer: Check the job output and error files for clues. Review your job script for errors. If you still need help, contact support with the error logs.
6. How do I check my job status?  
Answer: by using command (squeue -u <username>)
7. What is a job script?  
Answer: A job script is a text file containing instructions for the scheduler, including resource requests (e.g., CPUs, memory), runtime, and the program or script to execute.
8. What software is available on the HPC cluster?  
Answer: Use the module avail command to view the available modules.
9. What happens if I exceed resource limits?  
Answer: Your job may be queued, throttled, or terminated depending on the system's policies. You can resubmit your job with suitable changes.
10. Can I access the HPC system from outside the campus?  
Answer: Yes, but you must use a VPN connection or follow the institution's remote access policies.
11. Can I run Jobs on the master node or in any other node in an interactive manner without using script and bypassing the scheduler?  
Answer: No, Users are strictly NOT ALLOWED to run any jobs on the Master Nodes/login or any other node in an interactive manner. Users MUST ONLY run jobs only using the scripts through the job scheduler.
12. Whom should I contact for any issue?  
Answer: For any issue or requests pertaining to HPC cluster, please send your email with your working-path, error logs and error screenshots and submit-script only at [support.hpc@iitgn.ac.in](mailto:support.hpc@iitgn.ac.in)

More Details can be found on the website: <https://istf.iitgn.ac.in/hpc/>