Logging into Server

```
# Connecting to server using SSH

$ ssh node1@ubuntu-server

$ password: password
```

Sending Files to Server

```
# copy a file from your local system to a remote system

$ scp /path/to/local/file   node1@ubuntu-server:/path/to/remote/directory

# copy a directory recursively from your local system to a remote system

$ scp  -r  /path/to/local/directory   node1@ubuntu-serverr:/path/to/remote/directory
```

Submitting a Job to the SLURM

Simple Linux Utility for Resource Management (SLURM)

When using a cluster, jobs can be submitted in two main ways: as batch jobs or interactive jobs. In the following sections, we are going to discuss about both modes, their differences, and how to submit jobs effectively

Batch Job

A batch job allows you to submit a job script that will run without direct user interaction. You specify the required resources (like CPU, memory, and time), and the job is queued until those resources become available. Steps to perform a batch job are as follows:

1. Write a SLURM Job Script

A job script is a shell script that includes both SLURM directives and the commands you want to execute.

Example:

```
$ vi md.sh

#!/bin/bash

#SBATCH --job-name=mdrun_job              # Job name

#SBATCH --output=mdrun_output.log         # Standard output and error log

#SBATCH --error=error_%j.log              # log specifically to display error in running jobs

#SBATCH --nodes=1                         # Use 1 node

#SBATCH --ntasks=1                        # Run a single task

#SBATCH --cpus-per-task=24                # Request 24 CPU cores
```

```
#SBATCH --gres=gpu:1                          # Request 1 GPU
#SBATCH --mem-per-cpu=400                     # Memory per CPU
#SBATCH --time=02:00:00                       # Time limit
#module load gromacs                          # Load if any required modules
cd /home/node1/5P9I-8.20-Pongachromene        # Change to the directory containing your .tpfile
gmx  mdrun  -s  MD-100ns.tpr    -deffnm md_run  # Run mdrun with the specified tpr file
```

2. Submiting a job to a cluster

Once you've written your job script, use the sbatch command to submit it to the cluster.

```
$ sbatch   md.sh
```

SLURM will queue the job and execute it when resources become available.

3. Monitor the Job

You can monitor the job's progress using the squeue command:

```
$  squeue  -u  node1.
```

Interactive Job

An interactive job allows you to work directly on the compute nodes of a cluster in real time. This is useful for testing code, debugging, or running jobs that require user input or observation. While you can use both salloc and srun to run interactive jobs, salloc is generally the preferred method, as it provides more flexibility and control over resource allocation.

Using salloc for interactive Jobs The salloc command is used to request resources from SLURM and grants you an interactive shell on the allocated compute node. From this shell, you can run your tasks manually, providing a real-time environment for experimentation or debugging.

```
$ salloc  --ntasks=1 --cpus-per-task=4 --mem=8G --time=02:00:00
```

The above block of code requests for 4 CPU cores and 8 GB of memory and 2 hours of time from any node in normal partition to run a single task.

Using srun for Interactive Jobs

The srun command is commonly used for running individual tasks within a job (allocated using sbatch and salloc). But using a Psuedo-Terminal, srun command can also be used run jobs interactively. Example of using srun in interactive jobs:

```
 $ srun --ntasks=1 --cpus-per-task=4 --mem=8G --time=02:00:00 -- partition=general
```

Slurm User & Admin Commands

$ sinfo : display characteristics of partitions

$ squeue : display jobs and their state

$ scancel : cancel a job or set of jobs.

eg ; $ scancel < jobid >

# sacct : command can be used to retrieve information about jobs that have completed, including their status, resource usage, and more

$ scontrol : display and changes characteristics of jobs, nodes, partitions

eg; scontrol show job < job id >

Slurm Job logs

Job logs can be found in /var/log.

```
$  cat /var/log/slurm_jobcomp.log
```