SOPs – IIT HPC access and JOB Submission

1. IIT HPC

OS Version: Rocky linux 8.7 with slurm as workload manager

Login Instructions:

- **"ssh username@172.30.3.10 "**
- Type your password and you will be able to login.

To check the install applications run following commands.

- **“module use /opt/modulefiles”** list of directories where the module system looks for modulefiles.
- **"module avail"** run this command to see available modules.
- **"module load <modulename>"** run this command to load module/application.

once you load module you can simply type the application name and run it example

- "<**modulename**> **--version**" command to check version.

Keep this terminal open until you are accessing HPC

```
[amit@cn01 ~]$ module use /opt/modulefiles/
[amit@cn01 ~]$ module avail
------------------------------------------------------------ /opt/modulefiles -------------------------------------------------------------
advisor/2025.4                compiler/2025.2.1       dnnl/3.8.1      gromacs/2025.3              lammps/2025           python/3.12.4
advisor/latest                compiler/2025.3.0       dnnl/3.9.1      hdf5/1.12.2                 lapack/3.12.0         tbb/2022.2
ccl/2021.16.1                 compiler/latest         dnnl/latest     intel_ipp_intel64/2022.2    mkl/2025.2            tbb/2022.3
ccl/2021.17.0                 dal/2025.8              dpct/2025.2.0   intel_ipp_intel64/2022.3    mkl/2025.3            tbb/latest
ccl/latest                    dal/2025.9              dpct/2025.3.0   intel_ipp_intel64/latest    mkl/latest            umf/0.11.0
cmake/3.28.2                  dal/latest              dpct/latest     intel_ippcp_intel64/2025.2  mpi/2021.7            umf/1.0.2
compiler-intel-llvm/2025.2.1  debugger/2025.2.0       dpl/2022.9      intel_ippcp_intel64/2025.3  mpi/2021.16           umf/latest
compiler-intel-llvm/2025.3.0  debugger/2025.3.0       dpl/2022.10     intel_ippcp_intel64/latest  mpi/2021.17           vasp/5.4.4
compiler-intel-llvm/latest    debugger/latest         dpl/latest      ishmem/1.3.0                namd/2.14             vaspkit/1.5.0
compiler-rt/2025.2.1          dev-utilities/2025.2.0  fftw/3.3.10     ishmem/1.5.0                netcdf-fortran/4.6.1  vtune/2025.7
compiler-rt/2025.3.0          dev-utilities/2025.3.0  gcc/8.5         ishmem/latest               netcdf/4.9.2          vtune/latest
compiler-rt/latest            dev-utilities/latest    gcc/12.2.0      laamps/22jul2025            openmpi/5.0.8

------------------------------------------------- /usr/share/Modules/modulefiles --------------------------------------------------
dot  module-git  module-info  modules  null  use.own
```

Windows

To login into cluster firstly you have to connect with campus Wi-Fi

Once you connect with the Wi-Fi open terminal and type the following command to login.

- Download Open MobaXtream Portable application(https://download.mobatek.net/2432024101610907/MobaXterm_Portable_v24.3.zip)
- Double click on icon and allow permission then click on session icon on top left corner choose ssh option and enter your server ip address (192.168.1.33) and then click ok
- It will ask for you password submit your password you will be able to login into the server.

Else you can you window terminal or PowerShell terminal to login into the server.

- Open your windows terminal/PowerShell terminal and type following command.
- "ssh username@172.30.3.10"
  enter your user password you will be able to login to the server.

MacOS

- User terminal to login to the HPC through server user id and password
- "ssh username@172.30.3.10"

2. Use slurm scripts to submit JOB in HPC

```
#############################################################################
# Template slurm script to submit a job on HPC
#############################################################################
#!/bin/bash
#SBATCH --job-name=gmx_md          # Job name, appears in queue
#SBATCH --output=gmx_md.out        # Standard output file
#SBATCH --error=gmx_md.err         # Standard error file
#SBATCH --partition=small       # Partition: small (default) or highmemory
#SBATCH --qos=small               # QOS: small, medium, highmemory
#SBATCH –account=small_acct     # small: max 1 node, 10 days
                                   # medium: max 2 nodes, 4 days
#SBATCH --nodes=2                # Number of nodes to allocate
#SBATCH --ntasks-per-node=32        # MPI tasks per node
#SBATCH --time=48:00:00            # Job runtime (HH:MM:SS)
```

```
# Load modules
module use /opt/modulefiles/
module purge                    # Clear all loaded modules
module load gcc/12.2.0
module load openmpi/5.0.8
module load gromacs/2025.3-openmpi

# Add FFTW path (if not picked up automatically)
export LD_LIBRARY_PATH=/opt/fftw-3.3.10/lib:$LD_LIBRARY_PATH
export PATH=/opt/fftw-3.3.10/bin:$PATH
export OMPI_MCA_coll_hcoll_enable=0
# GROMACS env
export OMP_NUM_THREADS=1
export GMX_MAXCONSTRWARN=-1
# Check GROMACS executable
which gmx_mpi
gmx_mpi --version
# Run multi-node simulation
srun --mpi=pmix gmx_mpi mdrun -deffnm md_0_10
```

Utility commands

- **sbatch <scriptname>** # To submit job using slurm script
- **squeue** # To check job status
- **sinfo -l** # detailed list of Slurm partitions and nodes

sinfo

User

```
(base) [root@master01 ~]# sinfo
PARTITION  AVAIL  TIMELIMIT  NODES  STATE NODELIST
small*        up 10-00:00:0      4    mix cn[04-05,07,19]
small*        up 10-00:00:0     13  alloc cn[01-03,06,08-16]
small*        up 10-00:00:0      2   idle cn[17-18]
medium        up 4-00:00:00      4    mix cn[04-05,07,19]
medium        up 4-00:00:00     13  alloc cn[01-03,06,08-16]
medium        up 4-00:00:00      2   idle cn[17-18]
highmemory    up 1-00:00:00      2   idle hm[01-02]
```

Home Directory PATH/User Data Directory Path: -

- /scratch/home/username
- /scratch/user_data/(department_name/username)

(Note: User only have their specific deticated path allowed by the admin, user only access to that directory. **(cd /*scratch*/user_data/(department_name/username))**

All the operational scripts are stored at: /scratch/software/scripts

Master Node Access (Failure Scenario)

In case the primary master node is not accessible or users are unable to log in to the master node, users must connect to the fallback master node using SSH.

Use the following command to log in:

ssh <username>@172.30.3.11

Slurm QoS & Partition Submission Guidelines

Small Partition

Use the following Slurm directives:

#SBATCH --partition=small

#SBATCH --qos=small

#SBATCH –account=small_acct

Limits:

- Maximum **1 node**
- Maximum **64 CPU cores**
- Maximum **2 running jobs at a time**

Medium Partition

Use the following Slurm directives:

#SBATCH --partition=medium

#SBATCH --qos=medium

#SBATCH –account=medium_acct

Limits:

- Maximum **2 nodes**
- Maximum **128 CPU cores**
- Maximum **1 running job at a time**

High-Memory Partition

Use the following Slurm directives:

#SBATCH --partition=highmemory

#SBATCH --qos=highmemory

#SBATCH –account=highmemory_acct

Limits:

- Maximum **2 nodes**
- Maximum **128 CPU cores**
- Maximum **1 running job at a time**

Example to Access Compute Nodes

- First, log in to the cluster master/login node:

  ssh username@IP_address

- After logging in, connect to any compute node (cn01 to cn19):

  ssh cn01

Cluster Usage Policy and Execution Guidelines

Do NOT run jobs interactively on the head node or login node.
All computational workloads must be submitted through the Slurm scheduler using sbatch, srun, or appropriate Slurm commands.

Running heavy processes directly on the Master node:

• Degrades system performance for all users
• May result in process termination without notice
• If an interactive session is required:
(Request resources using Slurm (e.g., srun --pty bash in computes nodes)
• Ensure the session runs only on allocated compute nodes, not on the master node.
• Login in compute node and run directly the interactive job in compute node.

Policy Enforcement

Users activitity and the jobs are monitor by the Admin.

- Unauthorized interactive computations may lead to Immediate job termination

(Note: Do not run Python or other computational jobs on the login node. Always run them on a compute node (e.g., ssh cn06), or the job will be terminated without warning.)