सत्यमेव जयते
Department of Biotechnology
Ministry of Science and Technology,
Government of India

United Nations
Educational, Scientific and
Cultural Organization

क्षेत्रीय जैव प्रौद्योगिकी केन्द्र
Regional Centre
for Biotechnology

Indian Biological Data Centre

BRAHM

High Performance Computing (HPC)

The Indian Biological Data Centre (IBDC)
Regional Centre for Biotechnology (RCB), NCR Biotech Science Cluster, 3rd Milestone, Faridabad-Gurugram Expressway, Faridabad – 121 001, INDIA
Phone: 0129-2848672
Email: support@ibdc.rcb.res.in
Website: https://ibdc.rcb.res.in/

General Guidelines for 'BRAHM' HPC users

Please ensure you read the HPC usage guidelines and SOP given below before using the BRAHM High-Performance Computing Facility of the Indian Biological Data Centre.

1. All the communication regarding the HPC access, analysis and account renewal will be sent to IBDC support (support@ibdc.rcb.res.in).
2. All new users should complete the HPC usage training before submitting any jobs to the cluster.
3. The User Server account login credential will be valid for one month, and you are requested to renew your account monthly.
4. After six months, the user has to submit the usage report and justify why he/she needs further HPC access.
5. After HPC Upgradation, Now user need to add one additional attribute in PBS Script (see the PBS template section) to submit the job such as (**Ex: #PBS –P bric , #PBS -P external**).
6. Users are requested to remove or kill the jobs with E status otherwise, they will be auto-killed after 24 Hrs.
7. Intensive tasks must not be run on the head/login nodes; these should be reserved for editing code and job scripts, code compilation, data movement, submitting jobs and managing the queuing system.
8. Any suspicious job that is having an adverse effect on the cluster may be deleted without any prior notification.
9. If the required software or tools are not available in the cluster, kindly email the details of the required software along with the link to its source and execution details to IBDC support at support@ibdc.rcb.res.in.
10. User accounts that remain inactive for 90 consecutive days will be automatically deactivated. All associated data and files will be permanently deleted after an additional 30 days retention period. Users are responsible for backing up any critical data before the retention period expires.
11. Users are strictly prohibited from executing computational jobs on the login node. Any job detected running on the login node will be automatically terminated without prior notice. All jobs must be submitted and executed through the PBS scheduler using a valid PBS script.
12. Provide details of your research articles published on research work conducted using the 'BRAHM-HPC' facility to IBDC (support@ibdc.rcb.res.in).

13. **Acknowledging BRAHM HPC in Publications**

When you write articles about your research for publication, conference proceedings or other reports, kindly acknowledge the use of the BRAHM HPC facility by including the following:

We acknowledge the BRAHM: High-Performance Computational facility of the Indian Biological Data Centre, Regional Centre for Biotechnology, Faridabad, INDIA

(https://ibdc.rcb.res.in/; DBT Grant no. BT/TCB/IBDC/2019) to carry out the ….. Name your computational analysis you performed at BRAHM ….

HPC access and JOB Submission

1. IBDC BRAHM HPC ACCESS THROUGH VPN

1.1 Ubuntu

Please install the openvpn package in your computer and follow the instructions to connect with IBDC BRAHM

- **`sudo apt install openvpn -y`** #Install openvpn
- Download Linux SSL VPN configuration file by using VPN user id and password mentioned in the login credential email at https://14.139.42.241
- **`sudo openvpn --config config.ovpn`** # replace config.ovpn file with the name of the downloaded .ovpn file
- Use VPN username and password in the terminal.
- Successful VPN connection would show a dialog Initialization Sequence Completed (Figure 1).
  Note: Keep this terminal open until you are accessing HPC

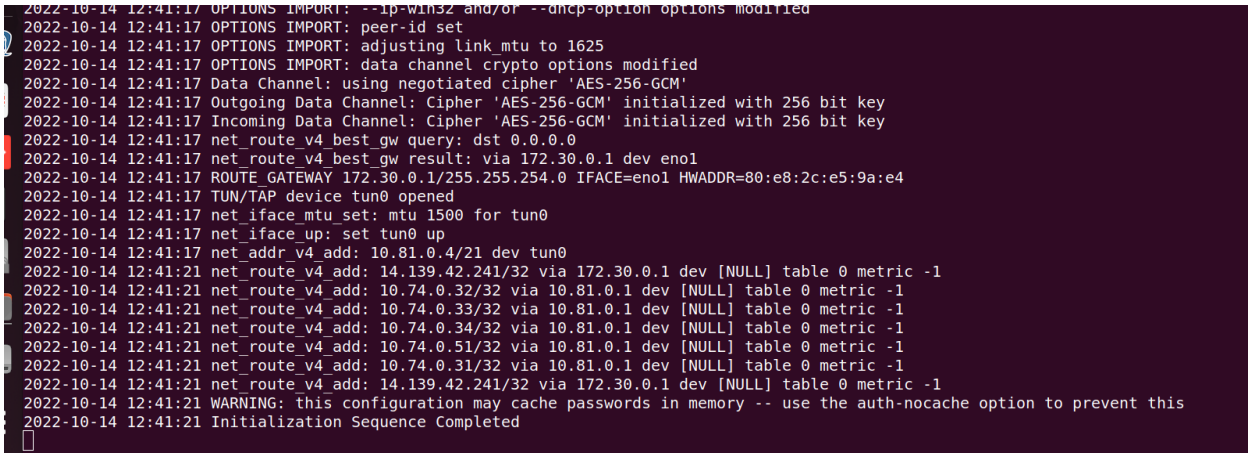

Figure 1: Snapshot of terminal showing VPN connected in Linux Machine

- Open a new Terminal to access the server with ssh through the login node (IP: 10.74.0.51) using server username and password.
  - **`ssh -X -Y userid@10.74.0.51`**

1.2 Windows

- Download Windows SSL VPN configuration file by using VPN user-id and password at https://14.139.42.241
- Import the OVPN Certificate on Open VPN client by clicking on the browse button (**Figure 2)**

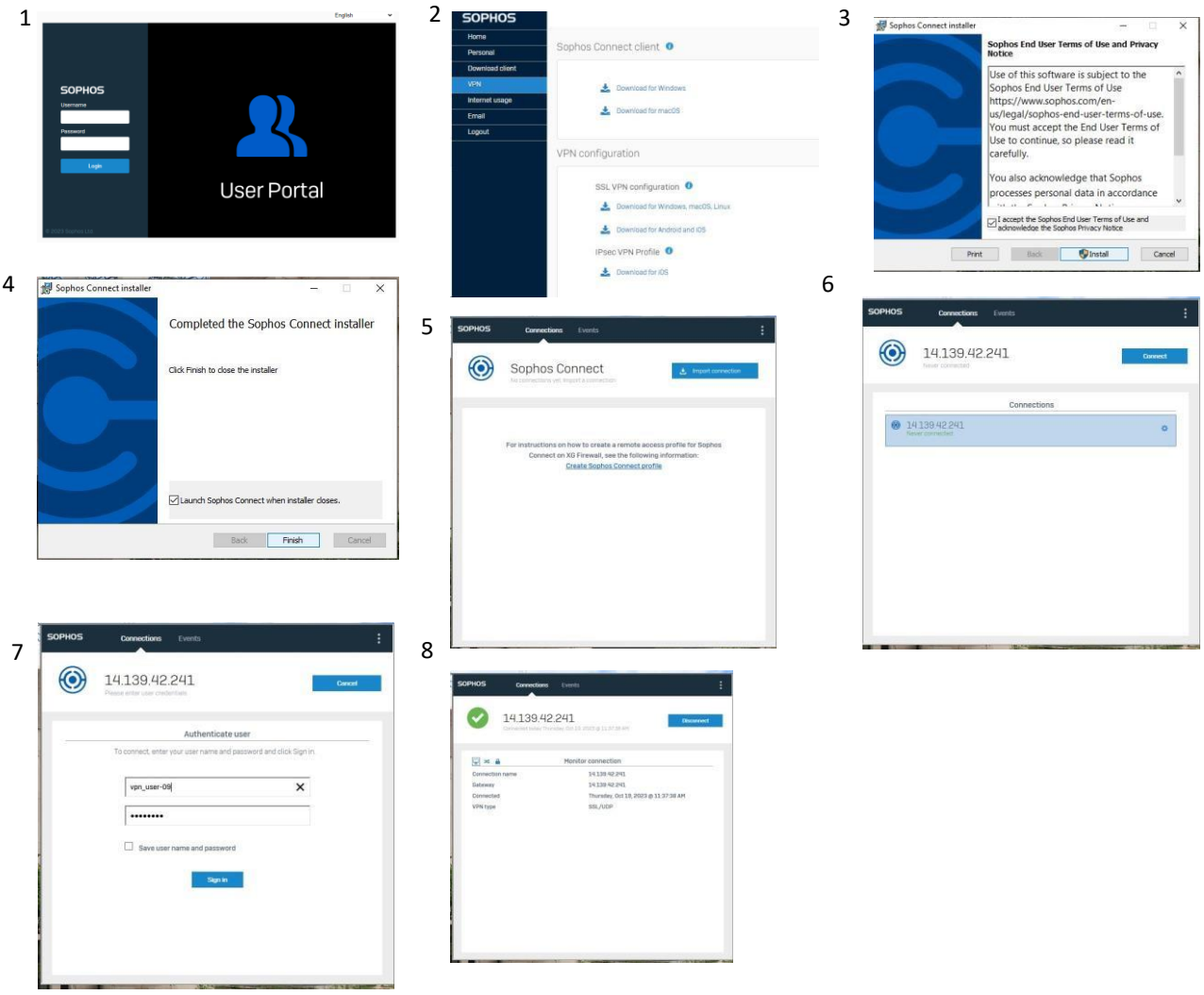

Figure 2: Snapshots of process of setting up of VPN connection

- Add your user VPN user-id and password to connect to IBDC HPC network.
  - *Note: Keep the VPN client connected throughout the duration of HPC access.*
- Open user Windows power shell/putty/WinSCP terminal to login to the HPC through server user id and password
  - **`ssh -X -Y userid@10.74.0.51`**

1.3 MacOS

- Download Open VPN Client (MacOS: https://openvpn.net/downloads/openvpn-connect-v3-macos.dmg) and install
- Download MacOS SSL VPN configuration file by using VPN user-id and password at https://14.139.42.241

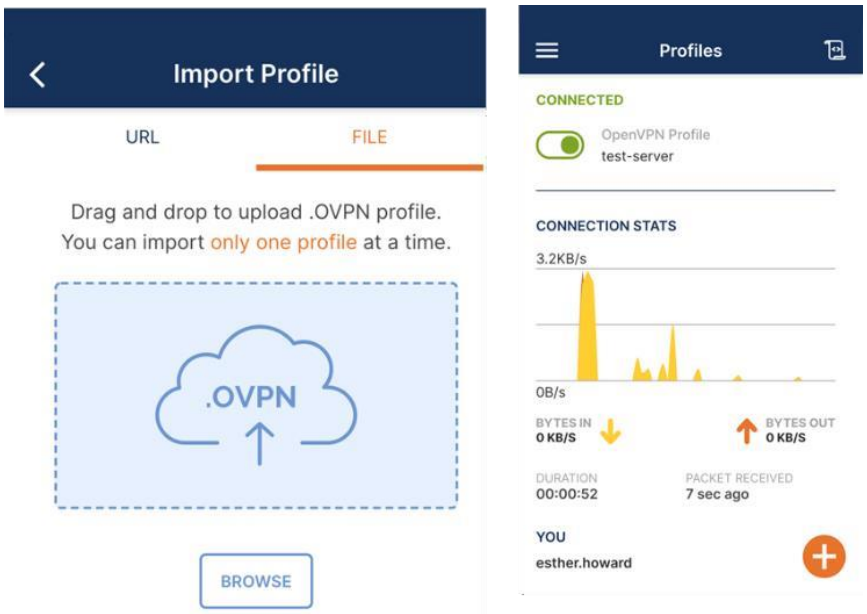

Figure 3: Snapshots showing the OpenVPN client to browse .OVPN configuration file and the successful OpenVPN connection.

- Import the OVPN Certificate on OpenVPN client similar to **Figure 2**
- Add user VPN user id and password to connect to HPC network.
    - *Note: Keep the VPN client connected throughout the duration of HPC access.*
- User terminal to login to the HPC through server user id and password
  `ssh -X -Y userid@10.74.0.51`

2. Use PBS scripts to submit Job in HPC

Number of queues available at the IBDC 'BRAHM' HPC

Queue Name	CPUs	GPUs	Walltime	Description
shortq	24	0	24 Hrs	Use this queue for testing the script or scripts requiring a short time duration to run.
mediumq	64	0	72 Hrs	MPI based job submission for maximum 3 days.
highq	48	2	96 Hrs	Jobs having CPU+GPU mix requirement.
simulationq	24	1	96 Hrs	This queue can be used specifically for MD Simulation

3. Utility commands

Description	Command
To submit the job using PBS script	`qsub singlenode.pbs`
To check the job status	`qstat`
To check all software installed in HPC from the source code	`module avail`
Load conda environment	`module load anaconda3/2022.05`
To check software installed through conda environment	`conda env list`

Template PBS script to submit a cpu only job

sample1.pbs

```
#PBS -S /bin/bash
#PBS -q shortq
#PBS -l select=1:ncpus=20      ## or select=2:ncpus=10 to run 20 cpus job on 2
nodes
#PBS -l walltime=24:00:00      ## this should not be more than defined walltime
for a queue
#PBS -P bric                   ## This is only for BRIC Community Users
#PBS -P external               ## This is only for External Users

#PBS -N myscript
#PBS -o myscript.out
#PBS -e myscript.err

cd $PBS_O_WORKDIR/

#Load the required package such as bowtie package
module load bowtie2/2.4.5

# To use a software from Conda environment
source activate /opt/apps/anaconda3/envs/Stringtie

#Execute the script
bash comand.sh #Execute
```

Template PBS script to submit a job with GPU

sample2.pbs
Submission of MD simulations production run
highq and simulationq queues both can be used for GPU related jobs.
##

```
#!/bin/bash
#PBS -N testjob
#PBS -q simulationq
#PBS -l ngpus=1
#PBS -l walltime=24:00:00
#PBS -joe
#PBS -P bric                    ## This is only for BRIC Community Users
#PBS -P external                ## This is only for External Users
cd $PBS_O_WORKDIR

module load gromacs/gpu/2022.3
export GMX_GPU_DD_COMMS=true
export GMX_FORCE_UPDATE_DEFAULT_GPU=true
gmx mdrun -deffnm md_0_1 -nb gpu


##########################################################################
```

IBDC Support

Contact IBDC support (support@ibdc.rcb.res.in) for any issue related to HPC access.