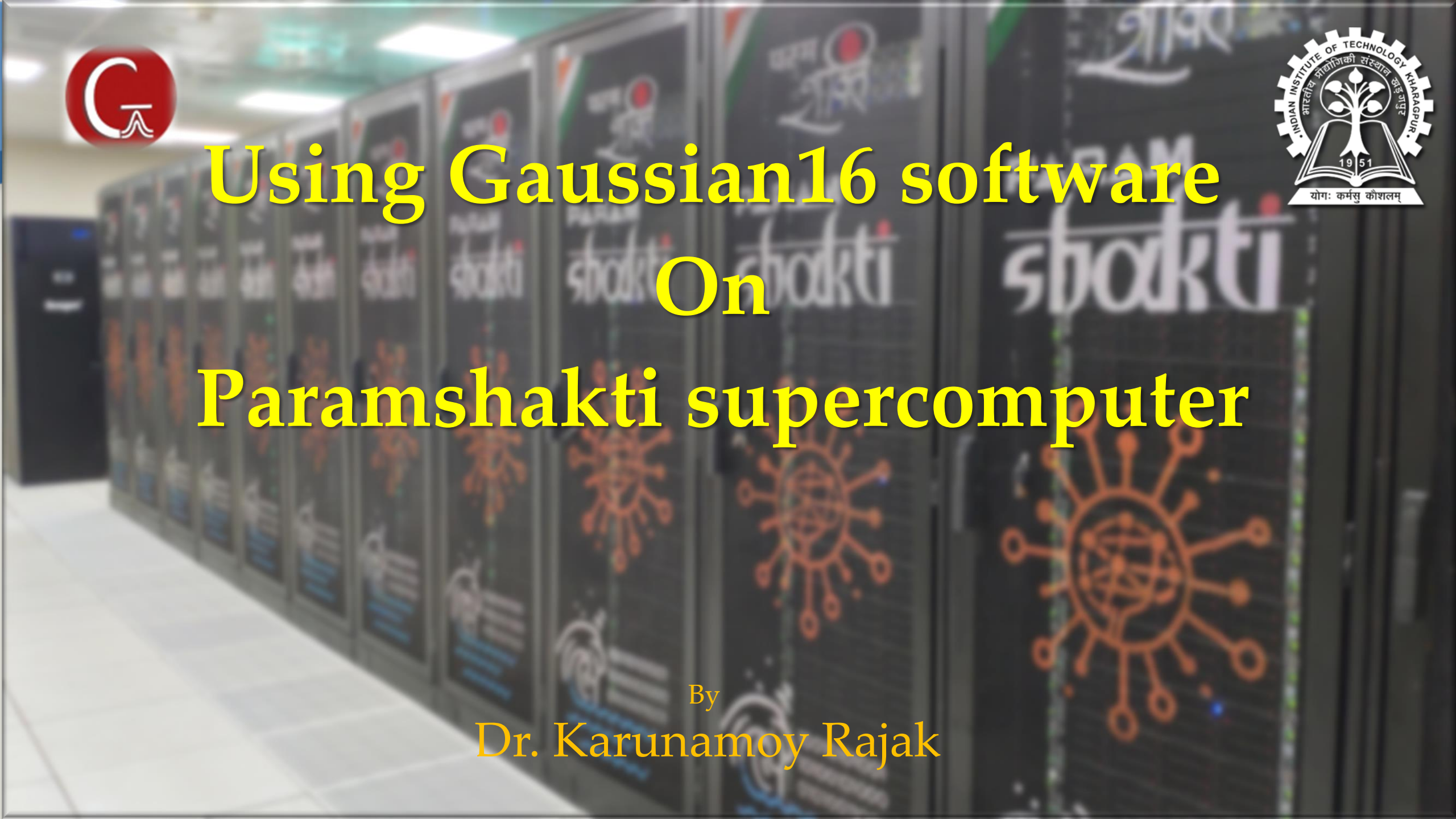


Using Gaussian16 software On Paramshakti supercomputer

By

Dr. Karunamoy Rajak

Outline

- About Gaussian Software
- Gaussian Input File Preparation
- Access of PARAMSHAKTI (PS)
    1. Create login at PS
    2. Connect with PS
- Submitting Gaussian jobs
    1. Generate batch script for SLURM workload manager
    2. Submitting job
- Monitor jobs in PS
- Gaussian16 performance on CPUs

About Gaussian 16

- Gaussian is a general purpose electronic structure package for use in computational chemistry.
- Most widely used computational chemistry package. The latest release is Gaussian16 Rev C.01
- Vendor's website: http://www.gaussian.com

About Gaussian 16

Pricing for Gaussian Products

USA	Outside the USA (excluding India, China & Hong Kong)	China & Hong Kong	India
Academic special bundle pricing	Academic special bundle pricing	Academic special bundle pricing	Academic special bundle pricing
Academic customers	Academic customers	Academic customers	Academic customers
Commercial customers	Commercial customers	Commercial customers	Commercial customers
US Government customers			

Due to recommendations by several international groups that monitor intellectual property protection laws and the enforcement of these laws, there are a number of countries to which Gaussian, Inc. does not license source code.

Maintenance pricing for Gaussian 16, GaussView 6, and Linda can be found by clicking this link.

Last updated on: 27 January 2017.

About Gaussian 16

LICENSING: A signed license is required prior to shipping Shrink wrap license

Gaussian 16 (New orders include *Exploring Chemistry*)

UNIX, Linux, Mac OS X			New License	Upgrade From G09
Site license	All machine types	Binary code	$6,950	$6,250
	Single Machine Type		$3,475	$2,775
			Add $1,400 for each addl. machine type	
Single computer	Mac OS 32-bit single core		$1,275	$975
Additional Charge for TCP Linda License			**New License**	**Upgrade From Linda 8**
Linda license	Each machine type		$2,775	$2,250

Gaussian 16 Functionality

Types of calculation:

- Gradients/Geometry optimizations
- Frequencies (IR/Raman, NMR, etc.)
- Transition state search
- IRC for reaction path
- Excited state calculation
- Spin-orbit coupling
- Several solvation models (PCM, SMD,etc), NonEquilibrium solvent model
- Two and three layer ONIOM model
- B-O molecular dynamics

Methods:

- Semiempirical: MNDO, AM1, PM3 etc.
- HF: restricted/unrestricted
- DFT: many pure/hybrid functionals
- MP: 2^{nd}-5^{th} order
- CI: single and double
- CC: single, double, triples contribution
- High accuracy methods: Gn, CBS, etc.
- MCSCF: including CASSCF
- MM: AMBER, Dreiding, UFF force field
- EOM-CCSD with analytic gradient
- DFTB and DFTBA methods

Gaussian Input File Structure

- .com, .inp, or .gjf (Windows version)
- Free format, case insensitive
- Spaces, commas, tabs, forward slash as delimiters between keywords
- ! as comment line/section
- Divided into sections (in order)
  - Link 0 commands (%)
  - Route section – Type of calculation
  - Title
  - Molecular specification
  - Optional additional sections

Input File - Example

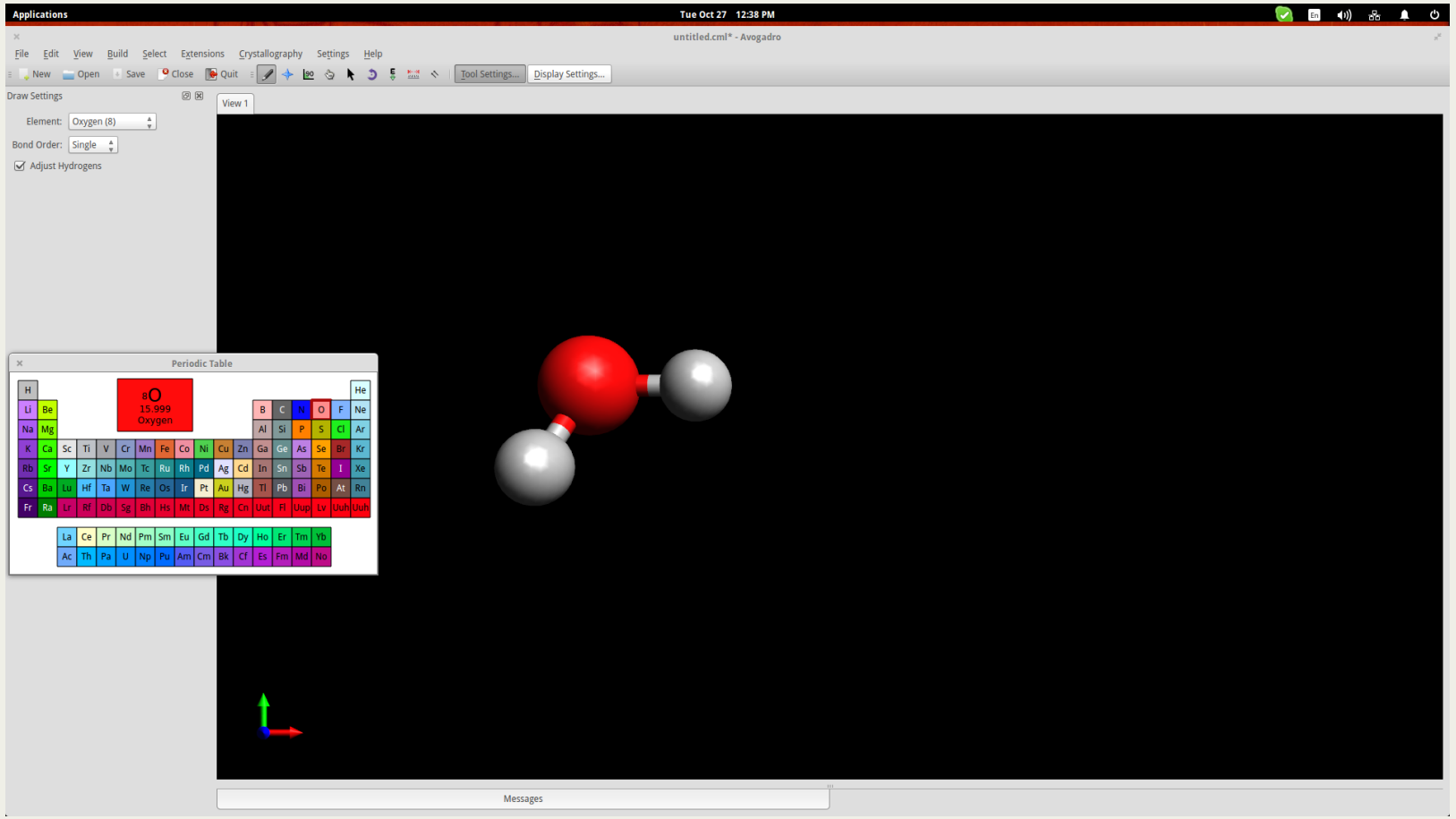
```
%nproc=8                        !Link 0 section
%mem=2GB
%chk=water.chk
# HF/6-31G(d) opt freq          !Route section
                                !Blank line
water energy                    !Title section
                                !Blank line
0 1                             !Charge & multiplicity
O -0.464 0.177 0.0              !Geometry in Cartesian Coordinate
H -0.464 1.137 0.0
H 0.441 -0.143 0.0
  Variable:                     !Blank line at the end
oh = 1.0
hoh = 120.0

                                !Blank line at the end
```

Molecular modeling and visualizer

Generate Cartesian Coordinate

- For Small molecules:
  - Avogadro
  - Gaussview
  - Jmol
  - Molekel
  - Molden
- For Biomolecules:
  - VMD
  - PyMOL
  - Chimera



Input File - Keyword Specification in the Route Section

- Keyword line(s) – specify calculation type and other job options
- Start with # symbol in the route section
- Can be multiple lines
- Terminate with a blank line
- Format
  - keyword=option
  - keyword(option)
  - keyword(option1,option2,…)
  - keyword=(option1,option2,…)
- User's guide provides list of keywords, options, and basis set notion

  https://gaussian.com/keywords/

Quick Links

Basis Sets
Density Functional (DFT) Methods
Solvents List SCRF
References

Users Ref Index

Keyword

[Keyword=]Option

List of Gaussian Keywords

- #
- ADMP
- BD
- BOMD
- CacheSize
- CASSCF
- CBS Methods
- CBSExtrapolate
- CCD and CCSD
- Charge
- ChkBasis
- CID and CISD
- CIS
- CNDO
- Complex
- Constants
- Counterpoise
- CPHF
- Density
- DensityFit and NoDensityFit
- DFT Methods
- DFTB and DFTBA
- EET
- EOMCCSD
- EPT
- External
- ExtraBasis & ExtraDensityBasis
- Field
- FMM
- Force
- Freq
- Gen and GenECP
- GenChk
- Geom
- GFInput
- GFPrint
- Gn Methods
- Guess
- GVB
- HF
- Huckel
- INDO
- Integral
- IOp
- IRC
- IRCmax
- Link0 Commands
- LSDA
- MaxDisk
- MINDO3
- MNDO
- MM Methods
- MP Methods
- Name
- NMR
- ONIOM
- Optimization
- Output
- PBC
- Polar
- Population
- Pressure
- Prop
- Pseudo
- Punch
- QCI
- Restart
- SAC-CI
- Scale
- Scan
- SCF
- SCRF
- Semi-Empirical Methods
- SP
- Sparse
- Stable
- Symmetry
- TD
- Temperature
- Test
- TestMO
- TrackIO
- Transformation
- Units
- Volume
- W1 Methods
- Window Keyword and Frozen Core Options
- ZIndo

Create login in PARAMSHAKTI

Not secure | hpc.iitkgp.ac.in/HPCF/quickGuide

Apps | Unit Converters - C... | parachem_server | buy | Reading list

IIT Kharagpur

High Performance Computing Facility

Indian Institute of Technology Kharagpur

HPCNC | User Support

- Home
- System Overview
- Quick Start Guide
- Using the System
- Tutorials
- User Guidelines
- Best Practices for HPC
- Publications
- HPC Advisory Committee
- Virtual Workshop
- User Support
- User Forms
- FAQs

Quick Start Guide

Quick Start Guide

1. All users are requested to go through the User policy and Best Practices to know the detailed guidelines approved by the Advisory Committee before requesting access to Paramshakti HPC systems

2. All the First Time Users will get access to the HPC systems through their respective Faculty/Project Investigator/Guide, who will be the account coordinator. The Faculty/Project Investigator/Guide must have submitted the User Forms as a pre-requisite.

3. Any User other than Faculty Adviser needs to follow the 2-step procedure for user account creation. For a particular user if the Faculty Adviser account is already registered then he can skip the Step-1.

Step -1

Faculty Adviser can submit a request using Faculty Form .The signed hard copy needs to be submitted at Room-F7, Lab1, First Floor JC Bose Annex building. Account creation of the Faculty Adviser may take upto 48 hours after the submission of the duly signed hard copy of the form. The Faculty Adviser will be notified via email after account creation is completed.

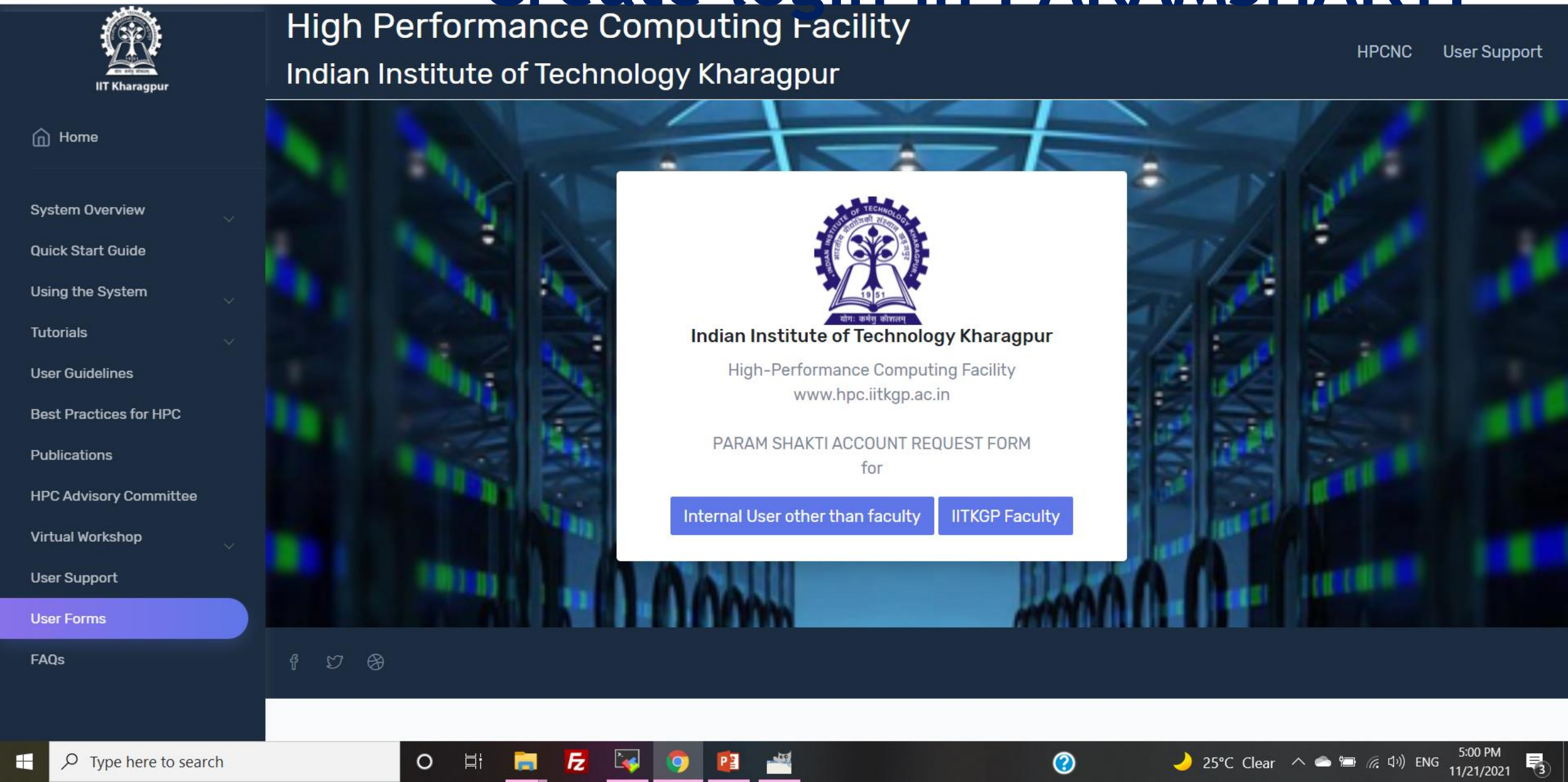
Step -2

After Faculty Adviser account creation is complete, the students/users other than Faculty in the respective group of the Faculty Adviser can start filling the User Forms and submit the duly signed hard copy at Room-F7, Lab1, First Floor JC Bose Annex building. The user will be notified via email after account creation is completed.

** Due to current pandemic situation users may send the scanned copy of the signed form duly endorsed by the respective Head of the Department/Centre/School by e-mail to:shaktisupport@iitkgp.ac.in .

Type here to search | 25°C Clear | ENG | 4:59 PM 11/21/2021

Create login in PARAMSHAKTI



Create login in PARAMSHAKTI

Not secure | hpc.iitkgp.ac.in/HPCF/user_form

Apps | Unit Converters - C... | parachem_server | buy | Reading list

Indian Institute of Technology Kharagpur
High-Performance Computing Facility
www.hpc.iitkgp.ac.in

PARAM SHAKTI ACCOUNT REQUEST FORM

(internal users other than IIT Kharagpur faculty)

1. User Details

Name(Full)

Name of the Project Guide/Advisor

Please type few characters of the first name of Faculty Advisor and select from available list. Manual Entry is invalid *

Department/School/Center

Select Department/School/Center

Degree Registered/Designation

Roll No. / Institute ID

Date of joining the

mm/dd/yyyy

Type here to search

25°C Clear

ENG

5:00 PM
11/21/2021

Connect with PARAMSHAKTI

Remote System Access

✓ Connect PS through ssh via port 22 (Inside Campus) or 4422 (Outside Campus)

Linux OS:

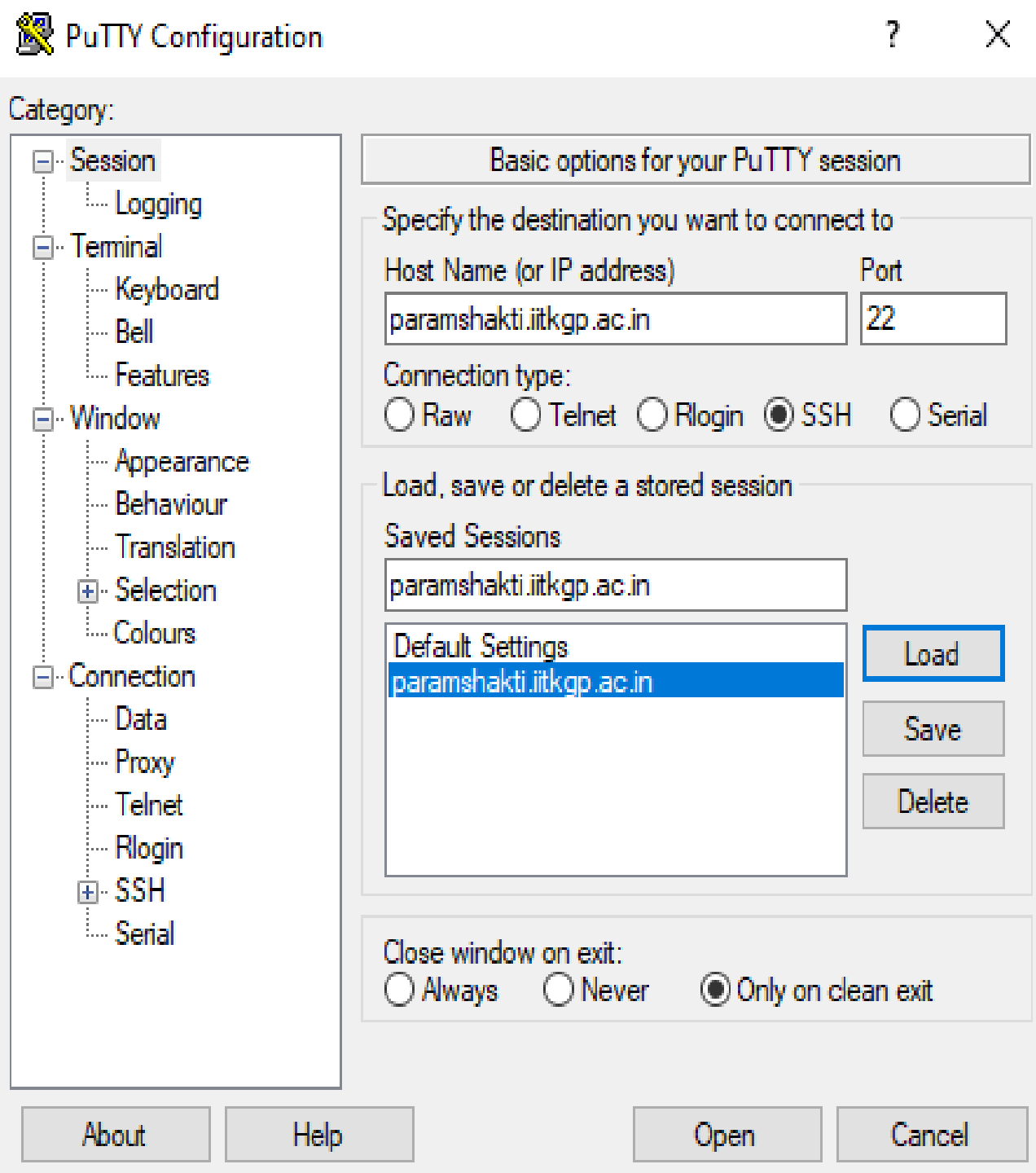
- ❑ ssh command to login/access from terminal
- ❑ sftp/scp command to copy file and directory
- ❑ vi command for editing file

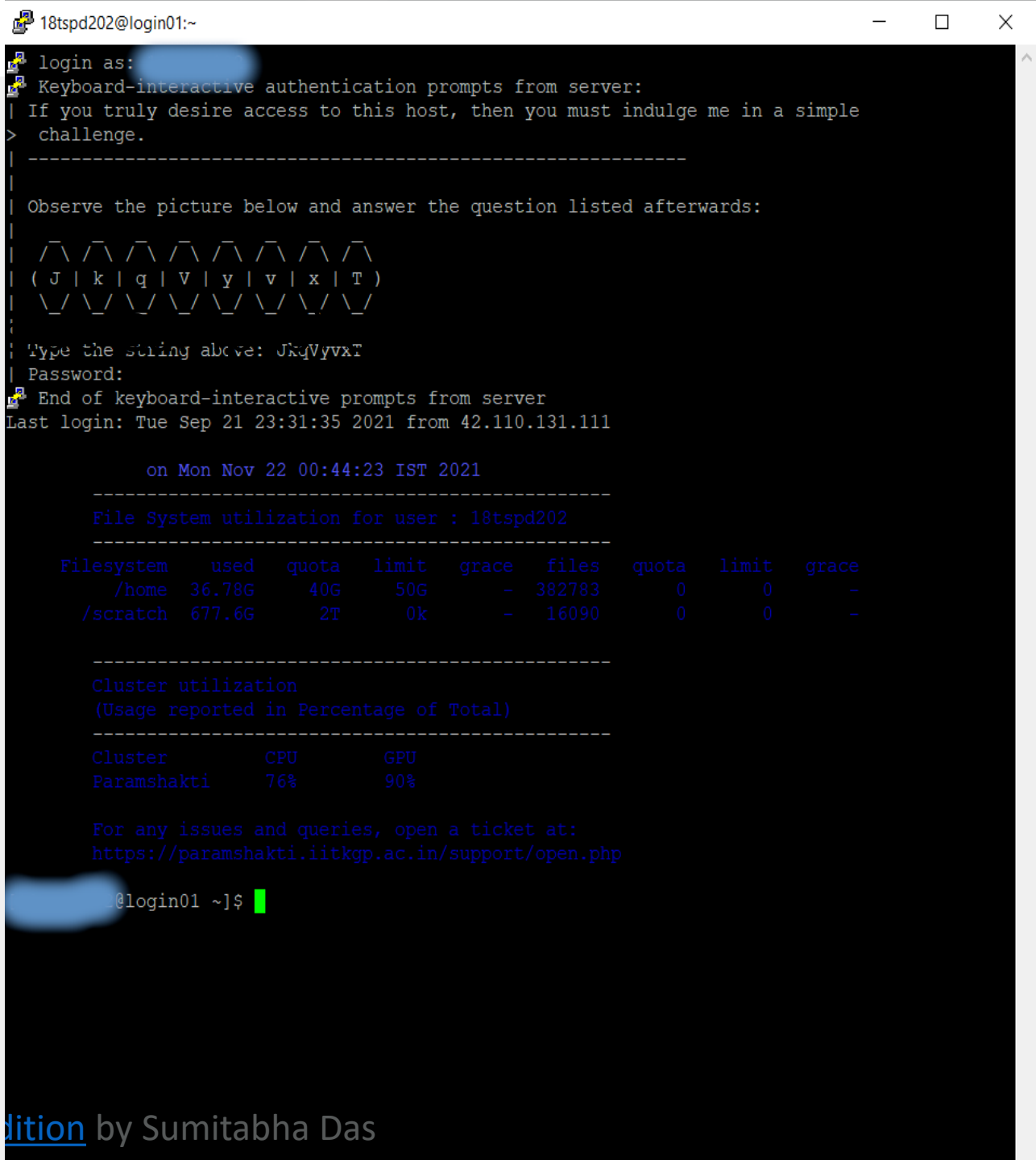
```
ssh –p 4422 user1@paramshakti.iitkgp.ac.in
scp  -P 4422 user2@hostname:[address2] user1@paramshakti.iitkgp.ac.in:[address1]
```

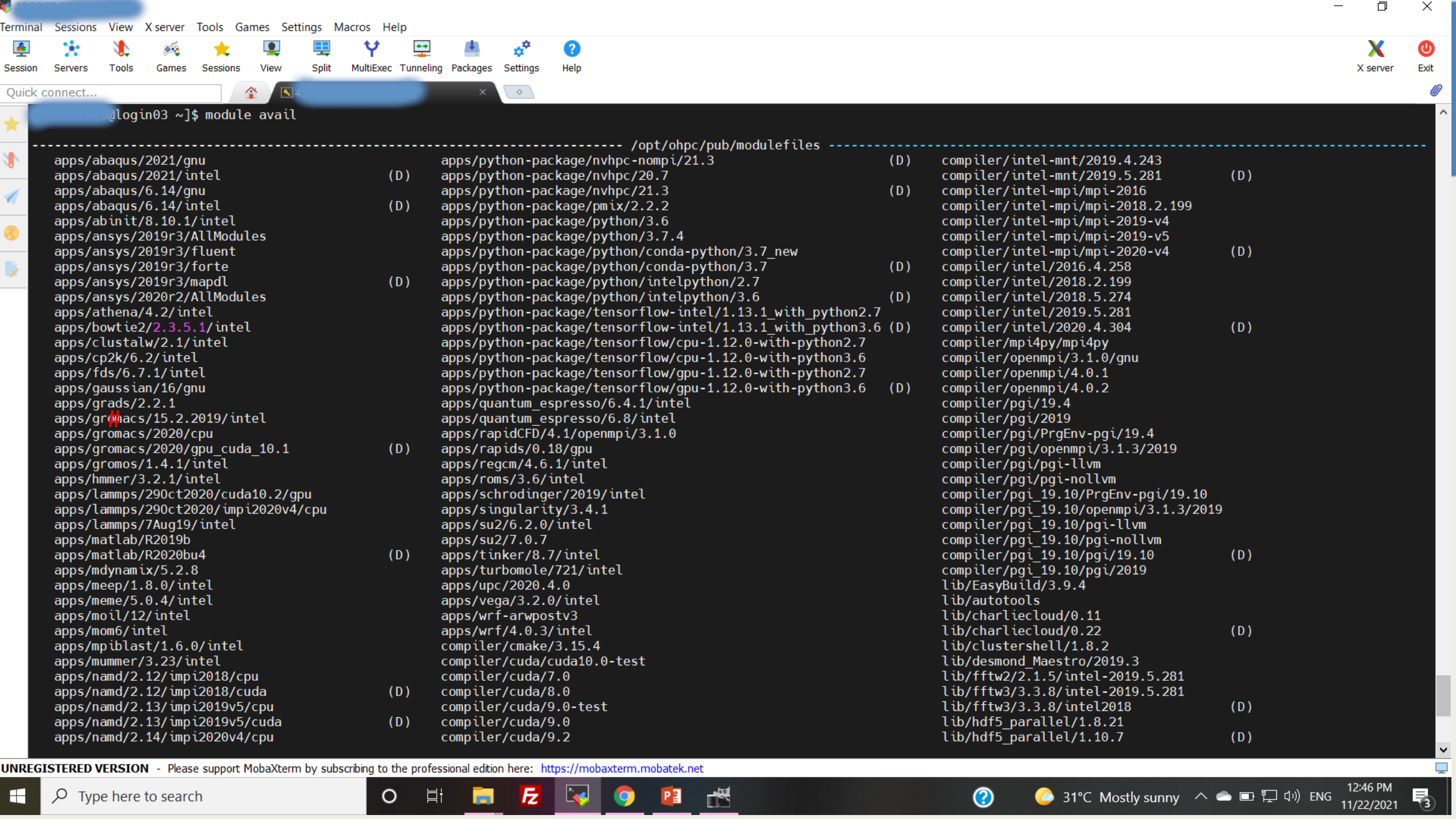
Windows OS:

- ❑ login via ssh from Putty, MobaXterm, Tera Term etc.
- ❑ copy file between servers using FileZilla, WinSCP etc.

UNIX : Concepts and Applications | 4th Edition by Sumitabha Das






Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help
X server Exit
Quick connect...
login03 ~]$ module avail
/opt/ohpc/pub/modulefiles
apps/abaqus/2021/gnu
apps/abaqus/2021/intel (D)
apps/abaqus/6.14/gnu
apps/abaqus/6.14/intel (D)
apps/abinit/8.10.1/intel
apps/ansys/2019r3/AllModules
apps/ansys/2019r3/fluent
apps/ansys/2019r3/forte
apps/ansys/2019r3/mapdl (D)
apps/ansys/2020r2/AllModules
apps/athena/4.2/intel
apps/bowtie2/2.3.5.1/intel
apps/clustalw/2.1/intel
apps/cp2k/6.2/intel
apps/fds/6.7.1/intel
apps/gaussian/16/gnu
apps/grads/2.2.1
apps/gromacs/15.2.2019/intel
apps/gromacs/2020/cpu
apps/gromacs/2020/gpu_cuda_10.1 (D)
apps/gromos/1.4.1/intel
apps/hmmer/3.2.1/intel
apps/lammps/29Oct2020/cuda10.2/gpu
apps/lammps/29Oct2020/impi2020v4/cpu
apps/lammps/7Aug19/intel
apps/matlab/R2019b
apps/matlab/R2020bu4 (D)
apps/mdynamix/5.2.8
apps/meep/1.8.0/intel
apps/meme/5.0.4/intel
apps/moil/12/intel
apps/mom6/intel
apps/mpiblast/1.6.0/intel
apps/mummer/3.23/intel
apps/namd/2.12/impi2018/cpu
apps/namd/2.12/impi2018/cuda (D)
apps/namd/2.13/impi2019v5/cpu
apps/namd/2.13/impi2019v5/cuda (D)
apps/namd/2.14/impi2020v4/cpu
apps/python-package/nvhpc-nompi/21.3 (D)
apps/python-package/nvhpc/20.7
apps/python-package/nvhpc/21.3 (D)
apps/python-package/pmix/2.2.2
apps/python-package/python/3.6
apps/python-package/python/3.7.4
apps/python-package/python/conda-python/3.7_new
apps/python-package/python/conda-python/3.7 (D)
apps/python-package/python/intelpython/2.7
apps/python-package/python/intelpython/3.6 (D)
apps/python-package/tensorflow-intel/1.13.1_with_python2.7
apps/python-package/tensorflow-intel/1.13.1_with_python3.6 (D)
apps/python-package/tensorflow/cpu-1.12.0-with-python2.7
apps/python-package/tensorflow/cpu-1.12.0-with-python3.6
apps/python-package/tensorflow/gpu-1.12.0-with-python2.7
apps/python-package/tensorflow/gpu-1.12.0-with-python3.6 (D)
apps/quantum_espresso/6.4.1/intel
apps/quantum_espresso/6.8/intel
apps/rapidCFD/4.1/openmpi/3.1.0
apps/rapids/0.18/gpu
apps/regcm/4.6.1/intel
apps/roms/3.6/intel
apps/schrodinger/2019/intel
apps/singularity/3.4.1
apps/su2/6.2.0/intel
apps/su2/7.0.7
apps/tinker/8.7/intel
apps/turbomole/721/intel
apps/upc/2020.4.0
apps/vega/3.2.0/intel
apps/wrf-arwpostv3
apps/wrf/4.0.3/intel
compiler/cmake/3.15.4
compiler/cuda/cuda10.0-test
compiler/cuda/7.0
compiler/cuda/8.0
compiler/cuda/9.0-test
compiler/cuda/9.0
compiler/cuda/9.2
compiler/intel-mnt/2019.4.243
compiler/intel-mnt/2019.5.281 (D)
compiler/intel-mpi/mpi-2016
compiler/intel-mpi/mpi-2018.2.199
compiler/intel-mpi/mpi-2019-v4
compiler/intel-mpi/mpi-2019-v5
compiler/intel-mpi/mpi-2020-v4 (D)
compiler/intel/2016.4.258
compiler/intel/2018.2.199
compiler/intel/2018.5.274
compiler/intel/2019.5.281
compiler/intel/2020.4.304 (D)
compiler/mpi4py/mpi4py
compiler/openmpi/3.1.0/gnu
compiler/openmpi/4.0.1
compiler/openmpi/4.0.2
compiler/pgi/19.4
compiler/pgi/2019
compiler/pgi/PrgEnv-pgi/19.4
compiler/pgi/openmpi/3.1.3/2019
compiler/pgi/pgi-llvm
compiler/pgi/pgi-nollvm
compiler/pgi_19.10/PrgEnv-pgi/19.10
compiler/pgi_19.10/openmpi/3.1.3/2019
compiler/pgi_19.10/pgi-llvm
compiler/pgi_19.10/pgi-nollvm
compiler/pgi_19.10/pgi/19.10 (D)
compiler/pgi_19.10/pgi/2019
lib/EasyBuild/3.9.4
lib/autotools
lib/charliecloud/0.11
lib/charliecloud/0.22 (D)
lib/clustershell/1.8.2
lib/desmond_Maestro/2019.3
lib/fftw2/2.1.5/intel-2019.5.281
lib/fftw3/3.3.8/intel-2019.5.281
lib/fftw3/3.3.8/intel2018 (D)
lib/hdf5_parallel/1.8.21
lib/hdf5_parallel/1.10.7 (D)
UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: https://mobaxterm.mobatek.net
Type here to search
31°C Mostly sunny
ENG
12:46 PM
11/22/2021

Job-file/batch-script

```
[user@hostname ~]$ module avail                          # lists all the available modules
[user@hostname ~]$ module load apps/gaussian/16/gnu      # load modules the gaussian with gnu compilers into
                                                           your environment
[user@hostname ~]$ module unload apps/gaussian/16/gnu    # remove all environment related to
                                                           apps/gaussian/16/gnu
```

Serial/Minimal batch script for Slurm Workload manager:

```
#!/bin/bash
#SBATCH -J job_name            # name of the job
#SBATCH -p standard-low        # name of the partition: available options "standard,standard-low,gpu,gpu-low,hm"
#SBATCH -t 01:00:00            # walltime in HH:MM:SS, Max value 72:00:00
#SBATCH --nodes=1              # number of nodes (-N) should be 1 for serial)
#SBATCH -n 1                   # no of processes

#list of modules you want to use, for example
module load apps/gaussian/16/gnu

#name of the executable
exe=g16                                # name of the executable

#run the application
$exe input.com
```

Batch script for parallel gaussian job:

[user@hostname ~]$ vi job_name.sh

```
#!/bin/bash
#SBATCH -J job_name                    #Job name(--job-name)
#SBATCH -o %j-out-myjob                #Name of stdout output file(--output)
#SBATCH -e %j-err-myjob                #Name of stderr error file(--error)
#SBATCH -p standard-low                #Queue (--partition) name
#SBATCH –N 1                           #number of nodes should be 1 for g16 without linda)
#SBATCH -n 10                          # Number of procs
#SBATCH -t 72:00:00                    # specifies walltime(--time maximum duration)of run
#SBATCH --mem=10000                    # Memory per node specification is in MB. It is optional.
#SBATCH --mail-user=user@email.com     # user email ID where job status info will be sent
#SBATCH --mail-type=ALL                # Send Mail for all type of event regarding the job

# list of modules you want to use, for example
#             module load apps/gaussian/16/gnu
# name of the executable
             g16root="/home/apps"
             GAUSS_SCRDIR="/scratch/$USER/gaussian"
             export g16root GAUSS_SCRDIR
             . $g16root/g16/bsd/g16.profile
             exe=g16
# Executables along with right Parameters and right input files
#mpirun -bootstrap slurm -n $SLURM_NTASKS $exe < input.com > output.log
             $exe input.com
```

[user@hostname ~]$ sbatch job_name.sh
[user@hostname ~]$ Submitted batch job 546965

Monitor Jobs Status

by

SLURM WORKLOAD MANAGER

[user@hostname ~]$ squeue # lists all the submitted jobs

```
[ y@login08 ~]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            545616 standard- pdi-thio 1      j0  R 1-04:28:58      1 cn308
            545472 standard- pdi_q4.c 1      j0  R 1-13:30:03      1 hm027
            545584 standard- pdi_q4.c 1      j0  R 1-13:21:42      1 hm025
            545587 standard- pdi_q4.c 1      j0  R 1-13:18:35      1 hm033
            545583 standard- pdi-tri- 1      j0  R 2-10:59:23      1 cn076
            545588 standard- pdi-tri- 1      j0  R 2-10:59:23      1 cn276
            545615 standard- pdi-thio 1      j0  R 2-10:59:23      1 hm008
            545572 standard- trimer_1 1      j0  R 2-13:49:09      1 cn031
            545271 standard- Fe-2b-W4 1      j1  R 2-23:44:06     12 cn[010,032-033,037,039-040,084,093,138,273-275]
[ y@login08 ~]$
```

[user@hostname ~]$ scontrol show jobid <job id> # Show the details of the job

[user@hostname ~]$ scancel <job id> # Kill a job

http://www.hpc.iitkgp.ac.in/HPCF/jobControl

https://slurm.schedmd.com/tutorials.html

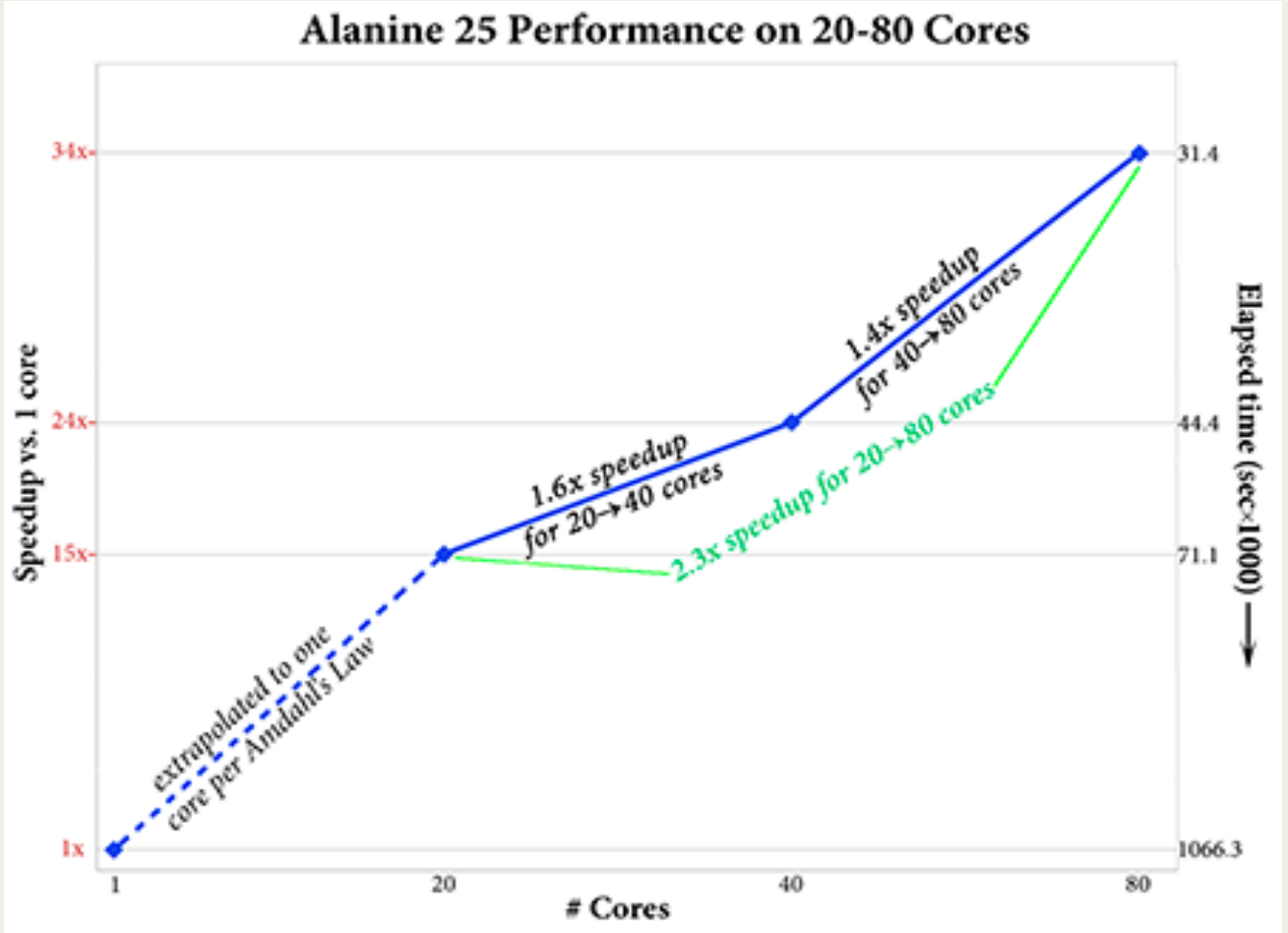
https://slurm.schedmd.com/documentation.html

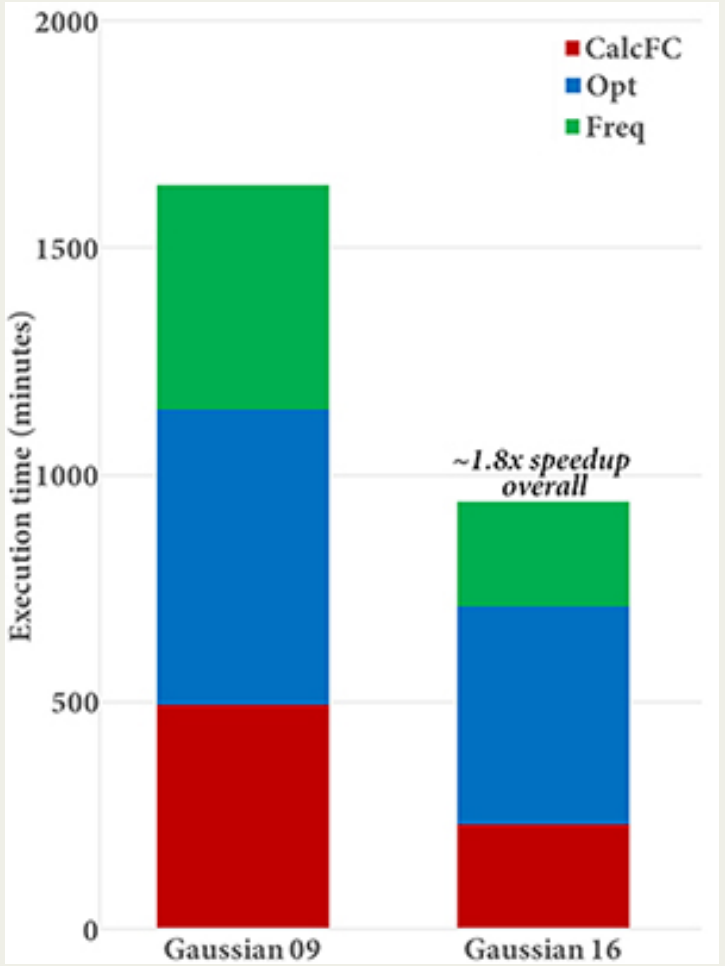
Monitor Jobs Status

[user@hostname ~]$ less job-name.log

```
Any fool can criticize, condemn, and complain -- and most do.
-- Dale Carnegie
Job cpu time:       0 days  0 hours  0 minutes 25.3 seconds.
Elapsed time:       0 days  0 hours  0 minutes  7.5 seconds.
File lengths (MBytes):  RWF=      6 Int=      0 D2E=      0 Chk=     93 Scr=      1
Normal termination of Gaussian 16 at Thu Nov 25 10:19:45 2021.
```

Gaussian 16 on CPUs





https://gaussian.com/g16new/

THANK YOU