

# HPC – Running Gaussian 09 through Job Scheduler -PBS



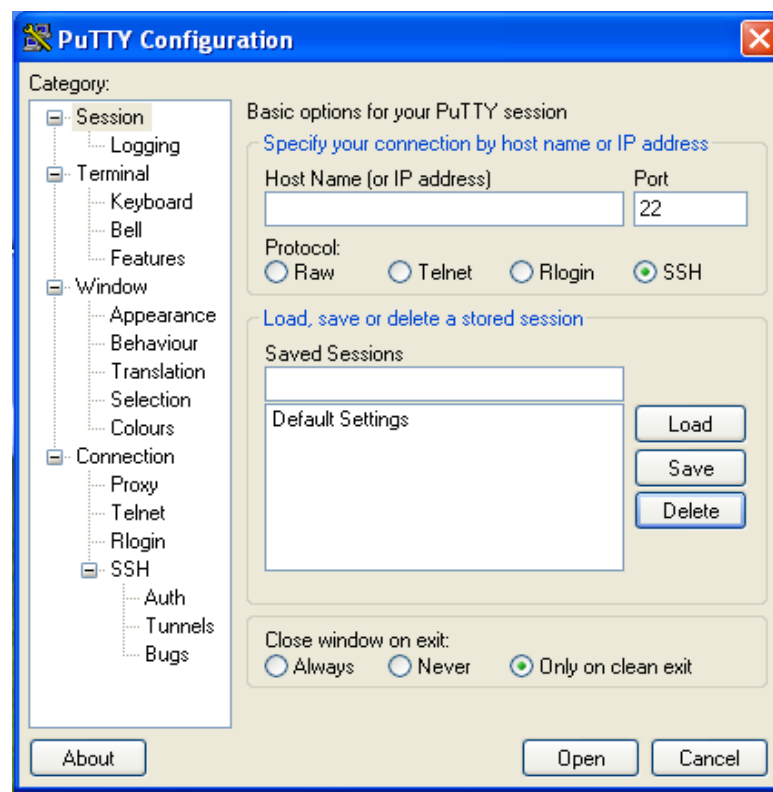
## Gaussian 09 (g09) job submission through Job scheduler

Gaussian g09 is a software package for molecular dynamics. Gaussian g09 is installed for serial (single-processor) use, for parallel (multi-processor, shared memory) use within a single compute node, and for distributed (multi-processor, distributed memory) use.

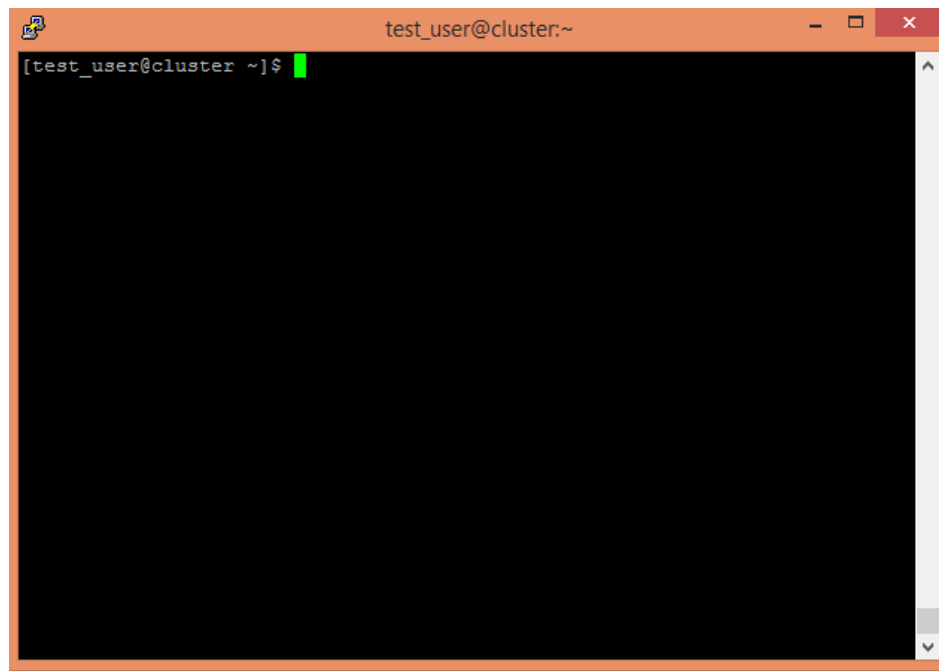
.In order to use Gaussian g09 on HPC Cluster at SBU user needs to login using Putty or SSH client first

### Login using Putty Client:

Login using PUTTY as shown below by typing the hostname as 192.168.220.100 with port 22



Then login using your **username** and **password** provided by the Administrator. After login user will see the screen as shown below

A terminal window titled 'test\_user@cluster:~' with a black background and a green cursor. The prompt is '[test\_user@cluster ~]\$'. A red box with the number '2' is in the top right corner of the page.

## 1) Running a Serial Gaussian Job

To run Gaussian Job user needs to follow the below steps

### a) **Creating an input file:**

User can use vi or vim editor to create input files or can create input files on their local PC and transfer them on to the HPC cluster using winscp ([Click Here](#) for the procedure to transfer files from local machine to the HPC). e

To run a Gaussian job you must specify in the input file **(1)** the name of the checkpoint file (.chk); **(2)** the Route section lines (# commands); **(3)** the title line; **(4)** the charge and spin multiplicity line; **(5)** the molecule specifications in a symbolic Z-matrix, a standard Z-matrix, or Cartesian coordinates; and **(6)** any additional input needed for your job.

Sample input file using VI editor:

```
$ vi water03.com
```

```
%chk=water03.chk  
#b3lyp/6-311+G(3df,2p) opt freq  
Gaussian test file  
0 1  
o  
h 1 r  
h 1 r 2 a  
  
r=0.98  
a=109.  
~  
-- INSERT --
```

```
%chk=water03.chk
```

```
#b3lyp/6-311+G(3df,2p) opt freq
```

```
Gaussian test file
```

```
0 1
```

```
o
```

```
h 1 r
```

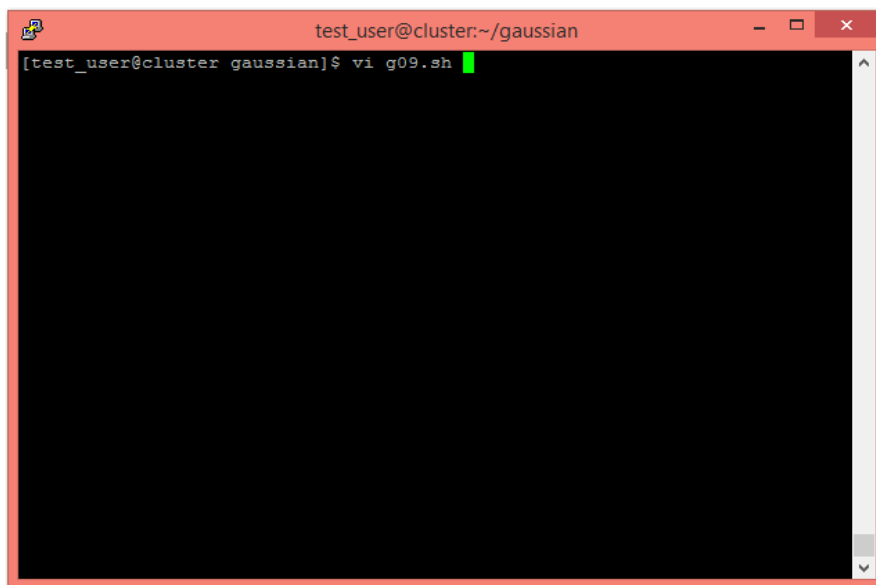
```
h 1 r 2 a
```

```
r=0.98
```

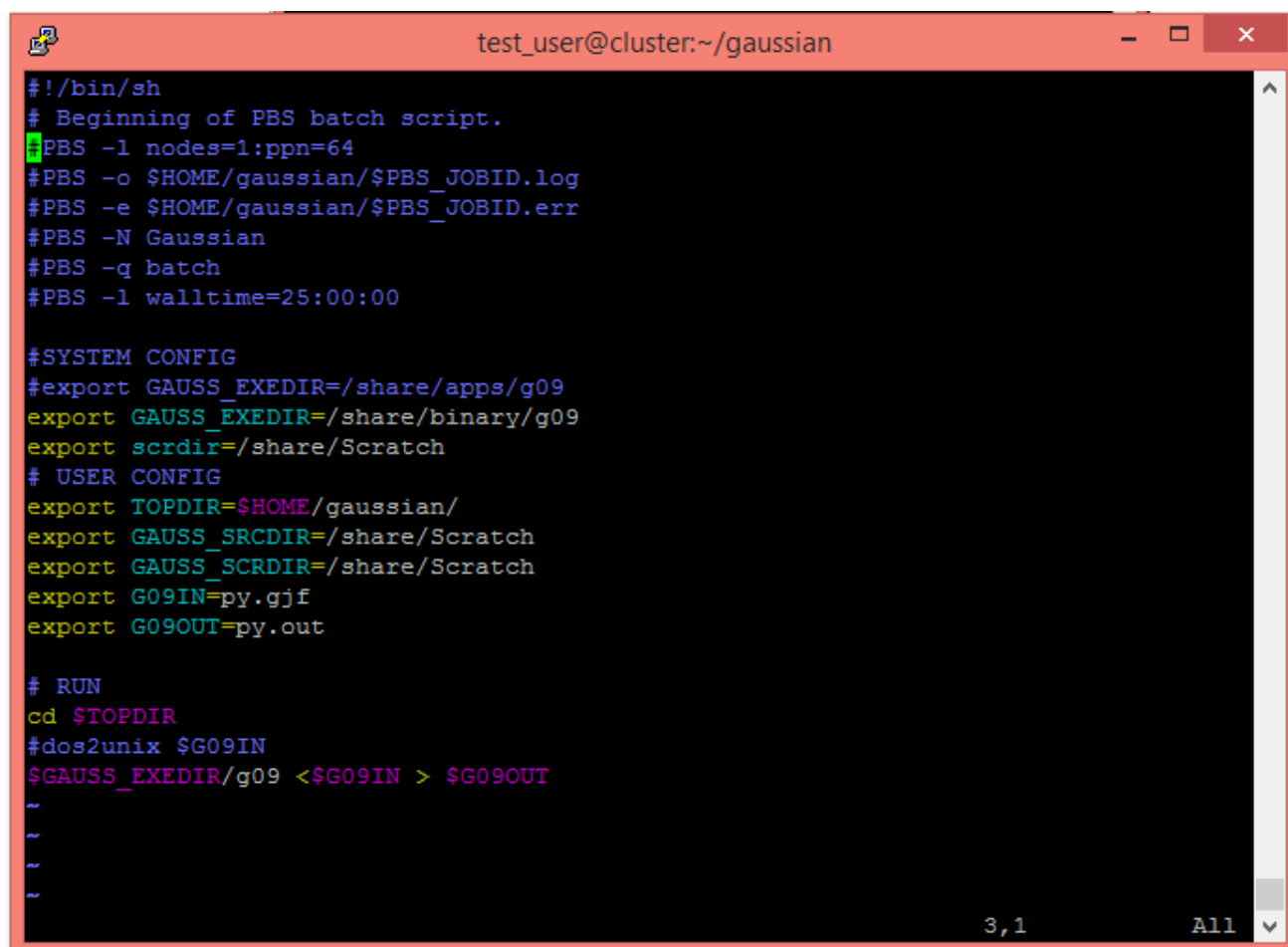
```
a=109.
```

**b) Creating Job scheduler (PBS) script:**

To run a Gaussian g09 batch job on the cluster, user needs to create a PBS script for it. The sample script below includes a request for one processor in a single compute node.



```
test_user@cluster:~/gaussian
[test_user@cluster gaussian]$ vi g09.sh
```



```
test_user@cluster:~/gaussian
#!/bin/sh
# Beginning of PBS batch script.
PBS -l nodes=1:ppn=64
#PBS -o $HOME/gaussian/$PBS_JOBID.log
#PBS -e $HOME/gaussian/$PBS_JOBID.err
#PBS -N Gaussian
#PBS -q batch
#PBS -l walltime=25:00:00

#SYSTEM CONFIG
#export GAUSS_EXEDIR=/share/apps/g09
export GAUSS_EXEDIR=/share/binary/g09
export scrdir=/share/Scratch
# USER CONFIG
export TOPDIR=$HOME/gaussian/
export GAUSS_SRCDIR=/share/Scratch
export GAUSS_SCRDIR=/share/Scratch
export G09IN=py.gjf
export G09OUT=py.out

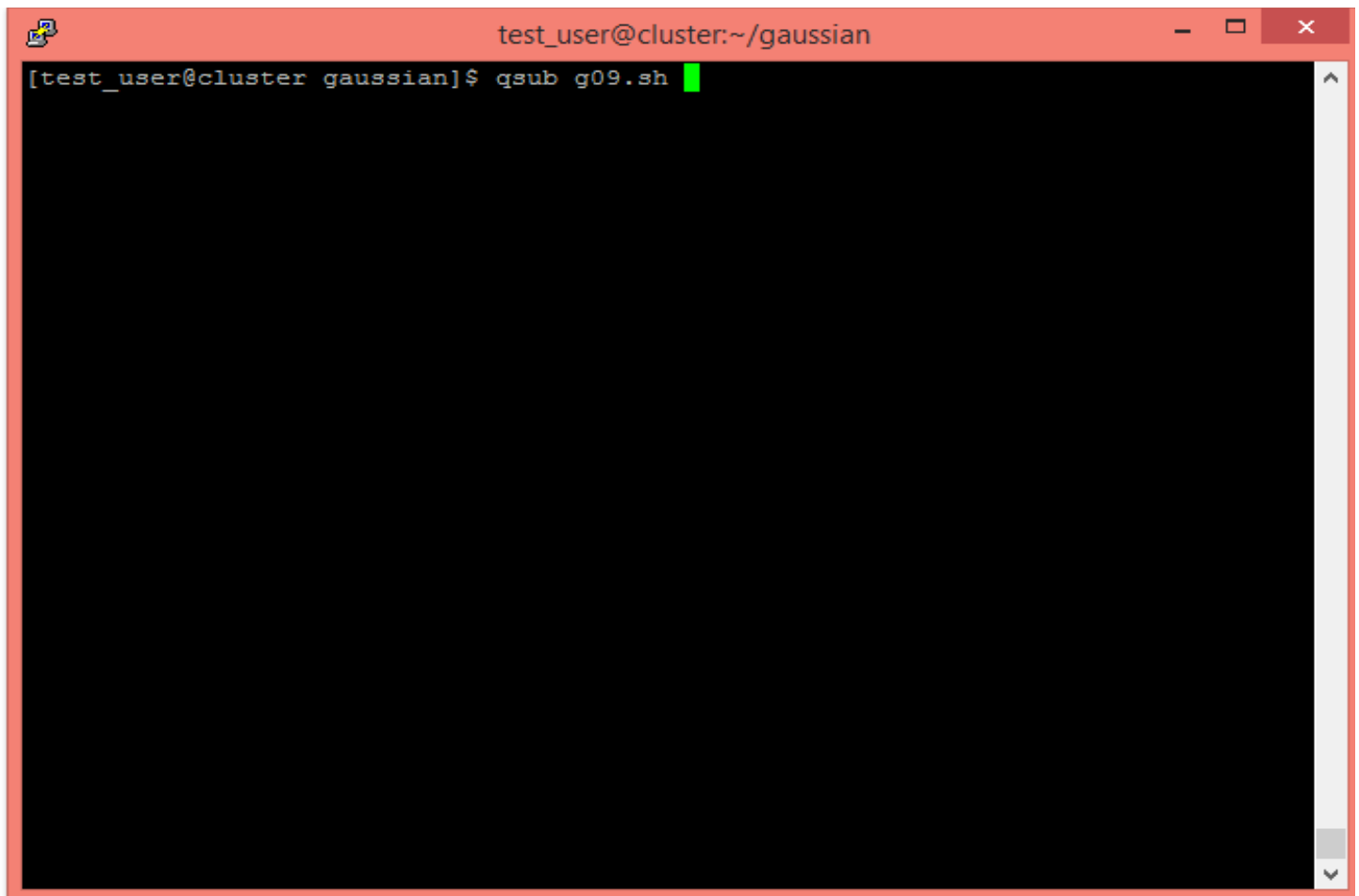
# RUN
cd $TOPDIR
#dos2unix $G09IN
$GAUSS_EXEDIR/g09 <$G09IN > $G09OUT
~
~
~
~
3,1 All
```

Save the file and exit (esc+shift :, then wq to save the file)

c) **Submitting the Job:**

User can use `qstat` command to check his job as shown below, basic commands related to PBS can be found [here](#).  
Users can submit their jobs by using `qsub` command followed by pbscript name, as shown below

User can check if their job is running or not by typing `qstat` command, if he doesn't find his job in the list it means his job has completed, now he can check his result file with the name `water03.out` in his home folder, user can open this file in vi editor or can copy this file from his home folder to his local machine using `winscp`.

A terminal window titled "test\_user@cluster:~/gaussian" with standard window controls. The terminal shows the command "[test\_user@cluster gaussian]\$ qsub g09.sh" followed by a green cursor. The rest of the terminal is black.

```
test_user@cluster:~/gaussian
[test_user@cluster gaussian]$ qsub g09.sh
```

User can use `qstat` command to check his job as shown below, basic commands related to PBS  
User can check if their job is running or not by typing `qstat` command, if he doesn't find his job in the list it means his job has completed, now he can check his result file with the name `*.out` in his home folder, user can open this file in vi editor or can copy this file from his home folder to his local machine using `.winscp`