# HPC – Running Gaussian 09 through Job Scheduler -PBS

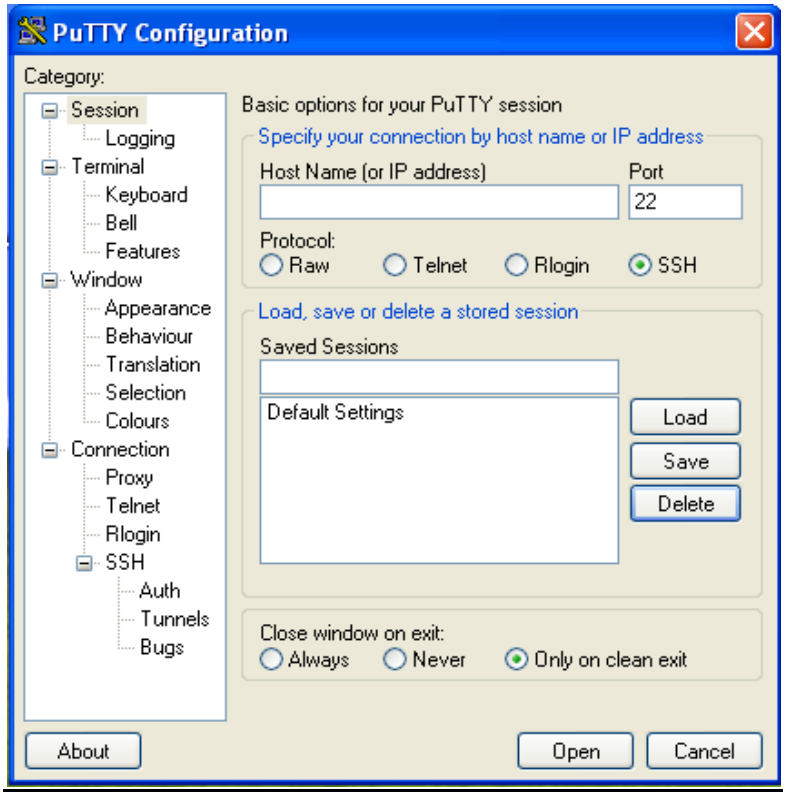
## Gaussian 09 (g09) job submission through Job scheduler

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


## 1) Running a Serial Gaussian Job

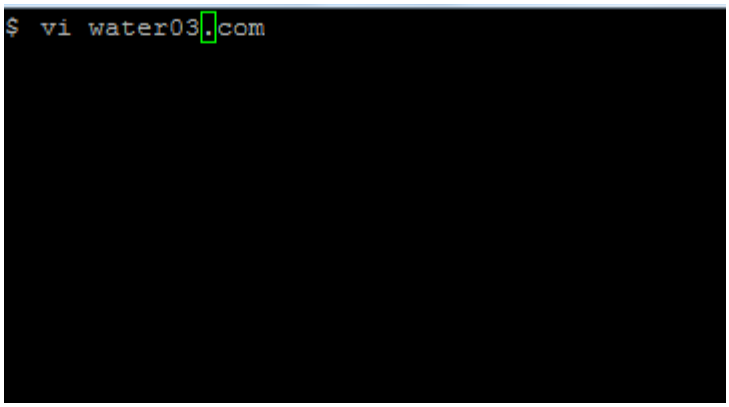
To run Gaussian Job user needs to follow the below steps

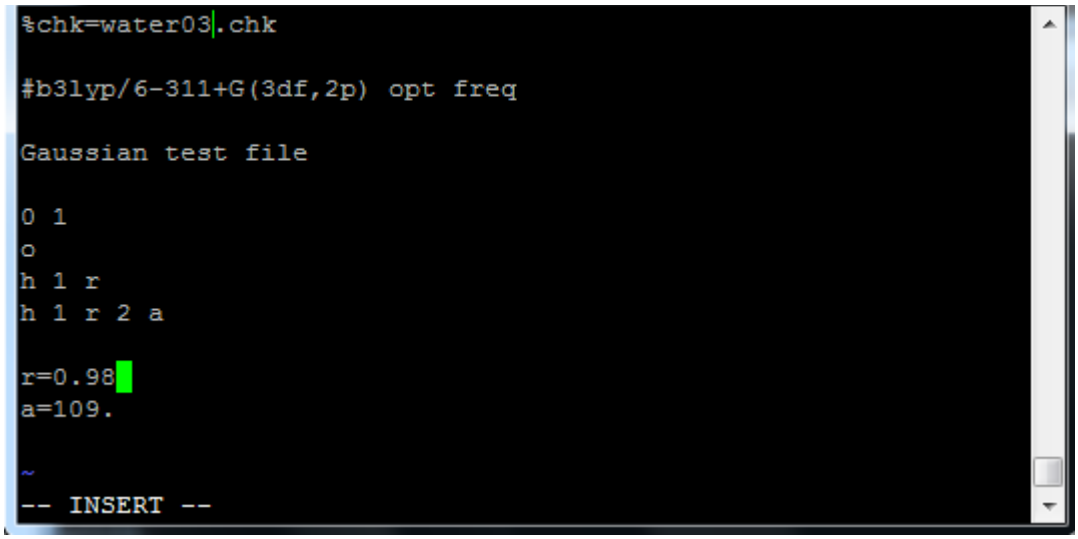
### a) Creating an input file:

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:**

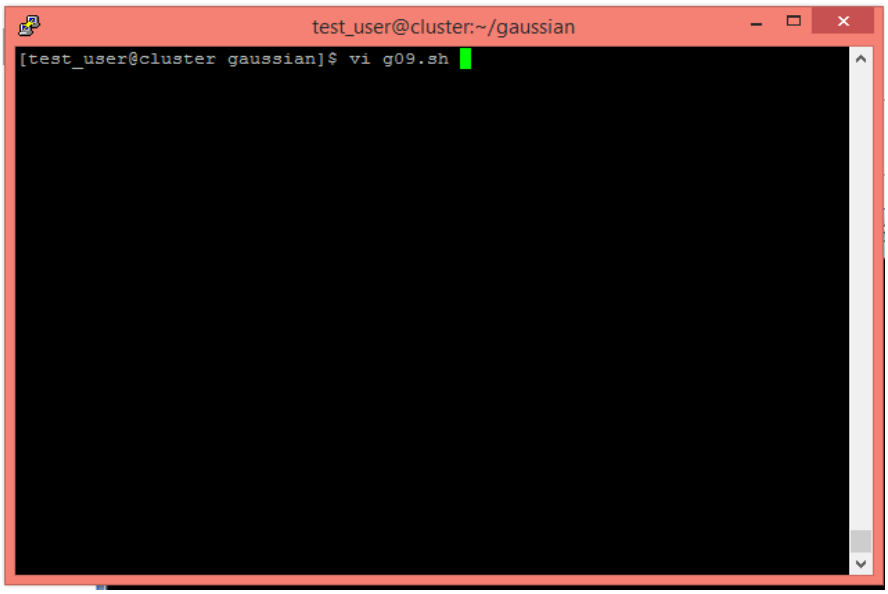


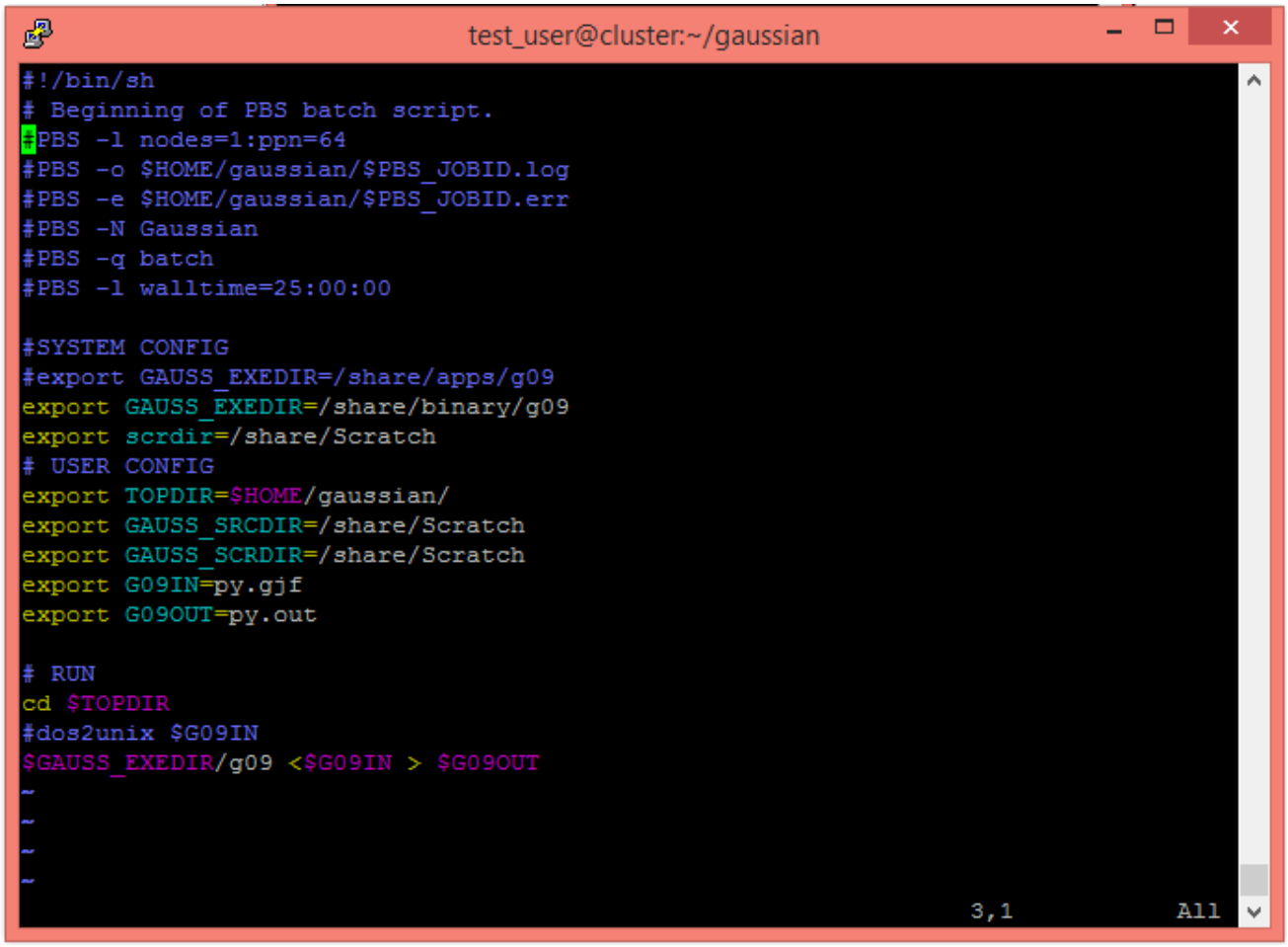




```
%chk=water03.chk

 #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.



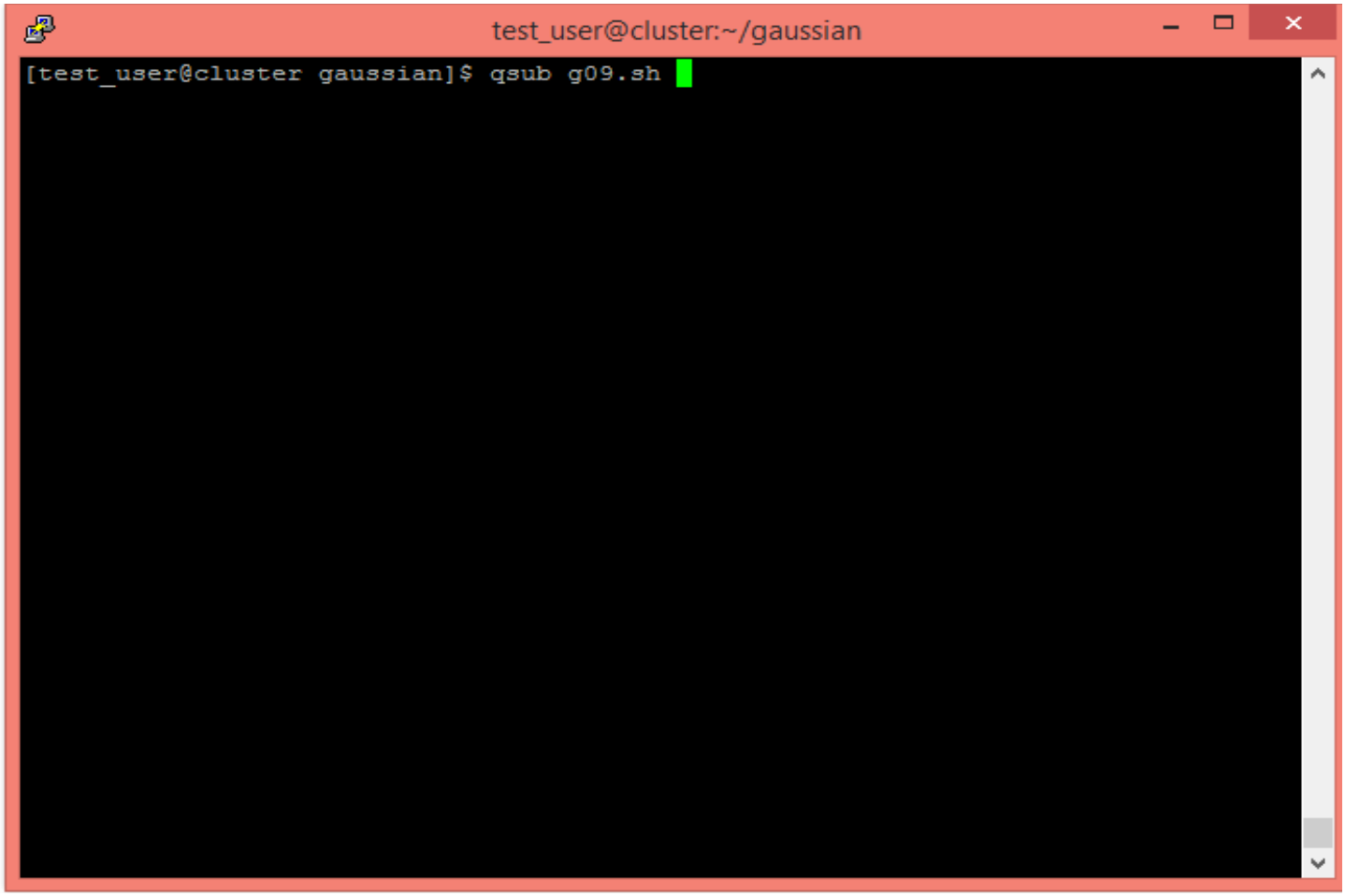
Save the file and exit (esc+shift :, then wq to save the file)

**c) Submitting the Job:**

Users can submit their jobs by using qsub command followed by pbsscript name, as shown below

User can use qstat command to check his job as shown below, basic commands related to PBS can be found here.

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.



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