

l) Submitting job in HPC cluster.

(a) Submitting Serial Job This example executes a.out command via job submit script method.

Create a script as follow:

```
[locuz@master1 ~]$ vi sleep.sh
#!/bin/bash
#PBS -S /bin/bash
#PBS -N Testjob
#PBS -l nodes=1:ppn=20
#PBS -j oe
cd $PBS_O_WORKDIR

./a.out > out.log
```

To submit this serial job script, you should use the qsub command.

```
[locuz@master1 ~]$ qsub sleep.sh
```

your job 29 ("sleep.sh") has been submitted

(b) Submitting Parallel Job Using job submit script:

```
[locuz@master1 ~]$ vi submit.sh
#!/bin/bash
#PBS -S /bin/bash
#PBS -N Gr_testjob
#PBS -q workq
#PBS -l nodes=1:ppn=20
#PBS -j oe
cd $PBS_O_WORKDIR
module load gromacs514-openmpiintel
echo "The nodefile for this job is stored at ${PBS_NODEFILE}"
cat ${PBS_NODEFILE}
np=$(wc -l < ${PBS_NODEFILE})
echo "Cores assigned: ${np}"
mpirun -np $np gmx_mpi mdrun -v -s /home/locuz/testgromacs/md.tpr
```

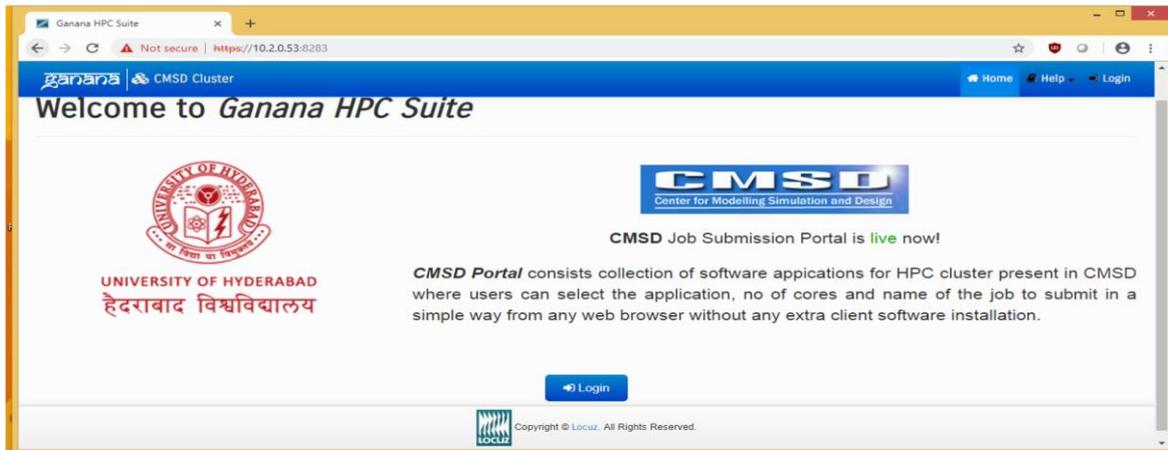
To submit the job:

```
[locuz@master1 ~]$ qsub submit.sh
```

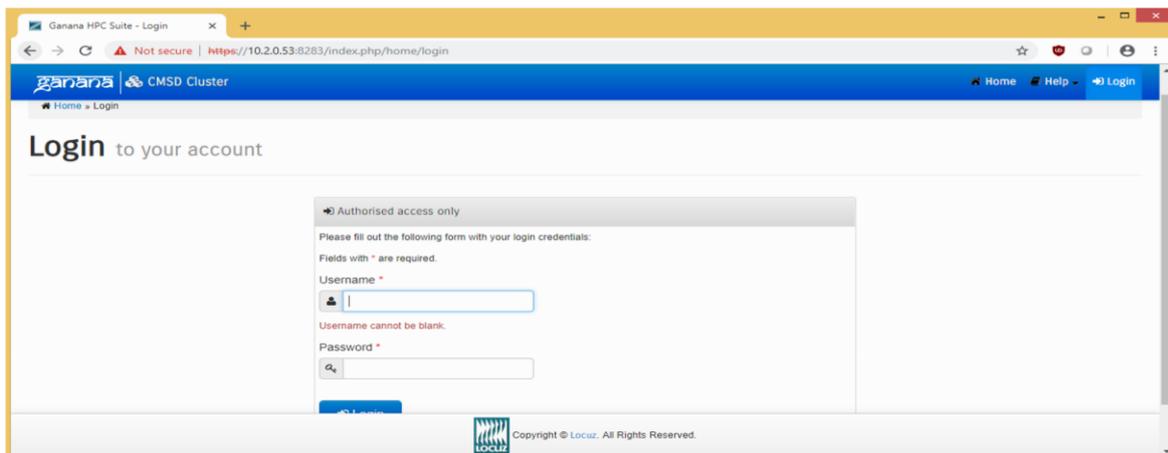
## Submitting jobs from Portal:-

Open the browser and type below address in URL.

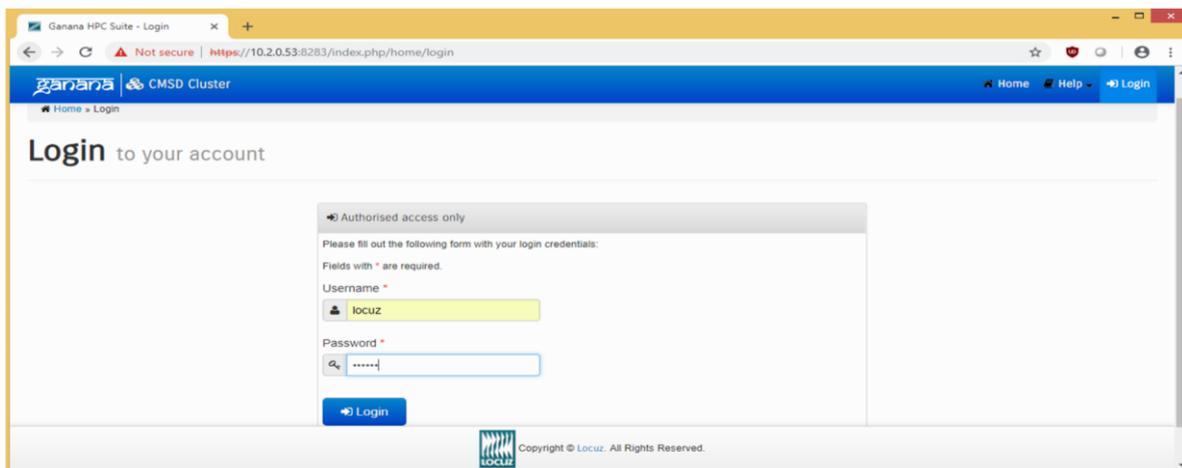
<https://10.2.0.53:8283/>



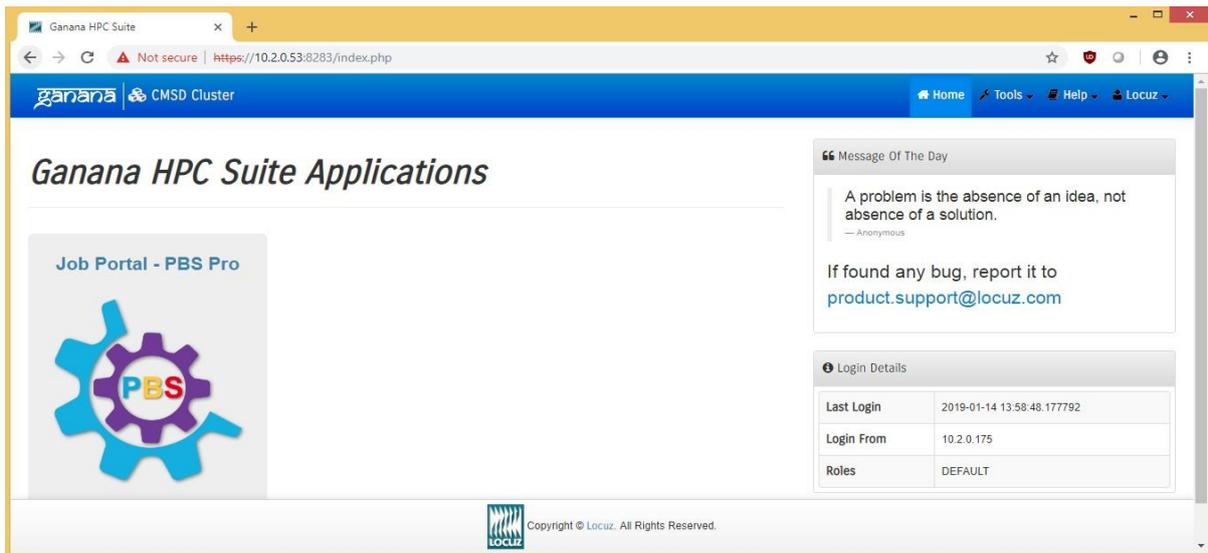
Click on the login tab enter the user credentials



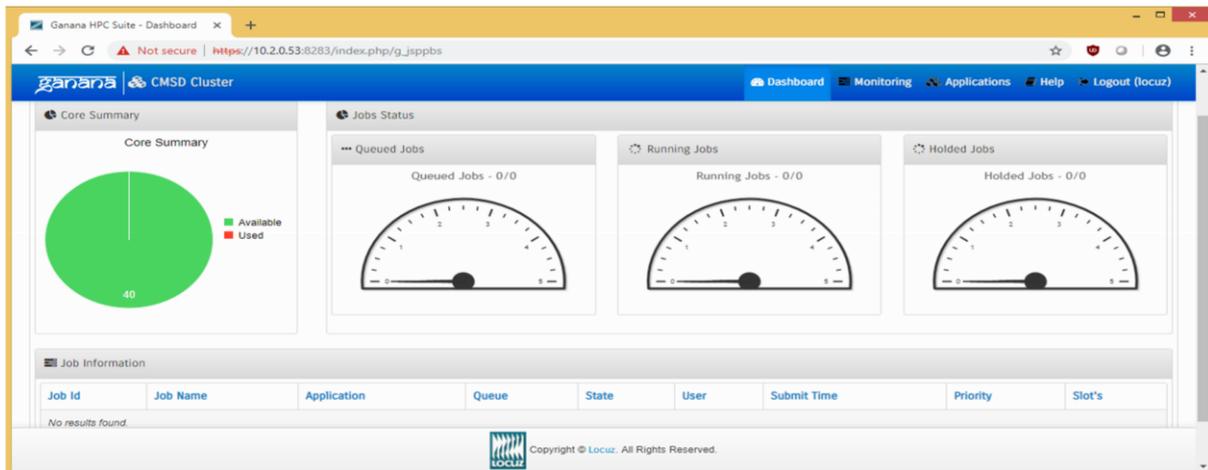
Enter the user name and password



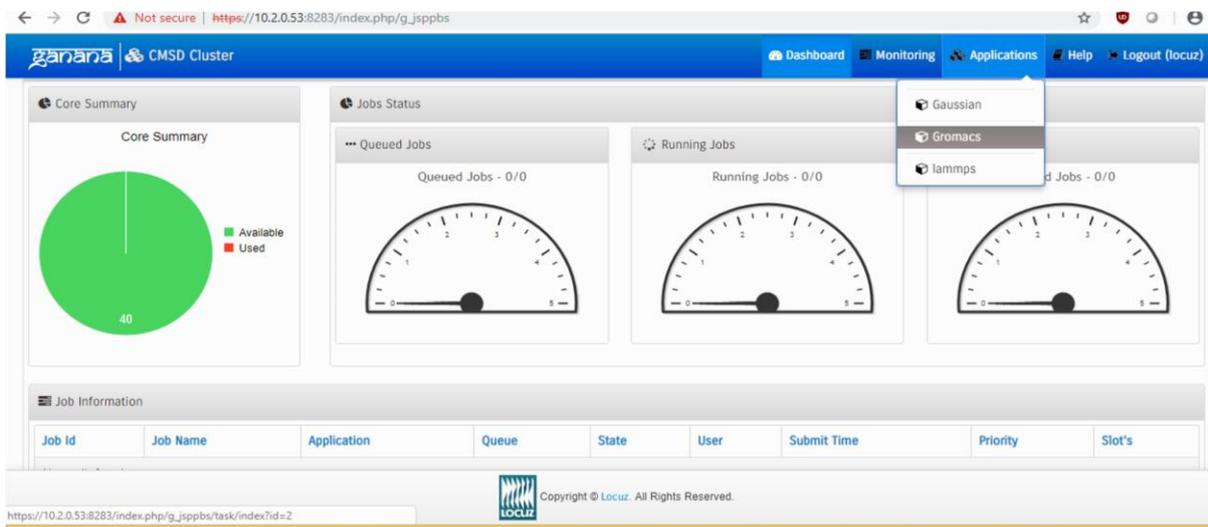
To submit and see the job information click on the job Portal-PBS Pro icon.



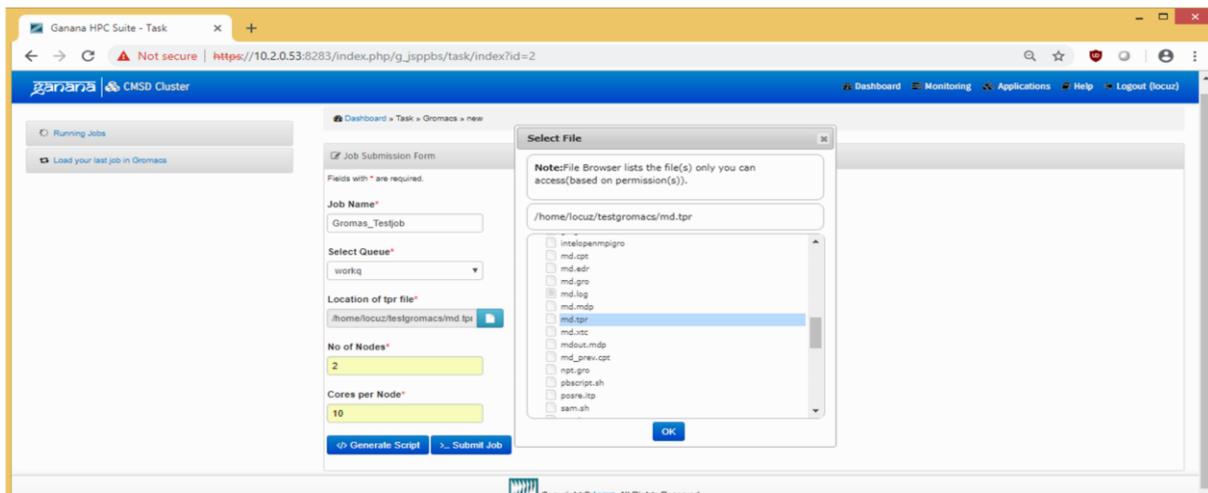
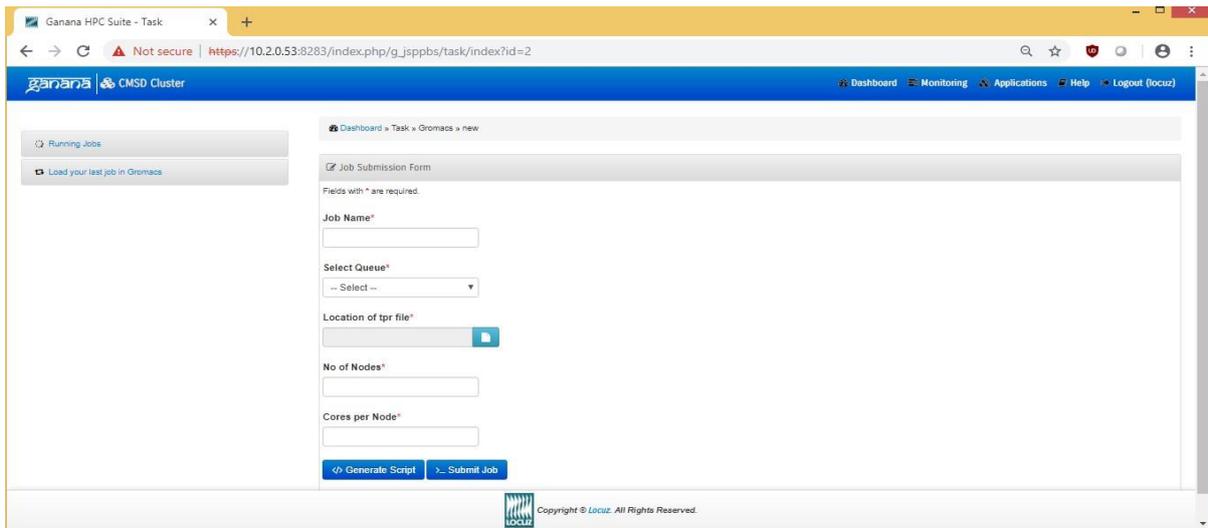
Click on Applications tab on top of the portal to submit jobs.



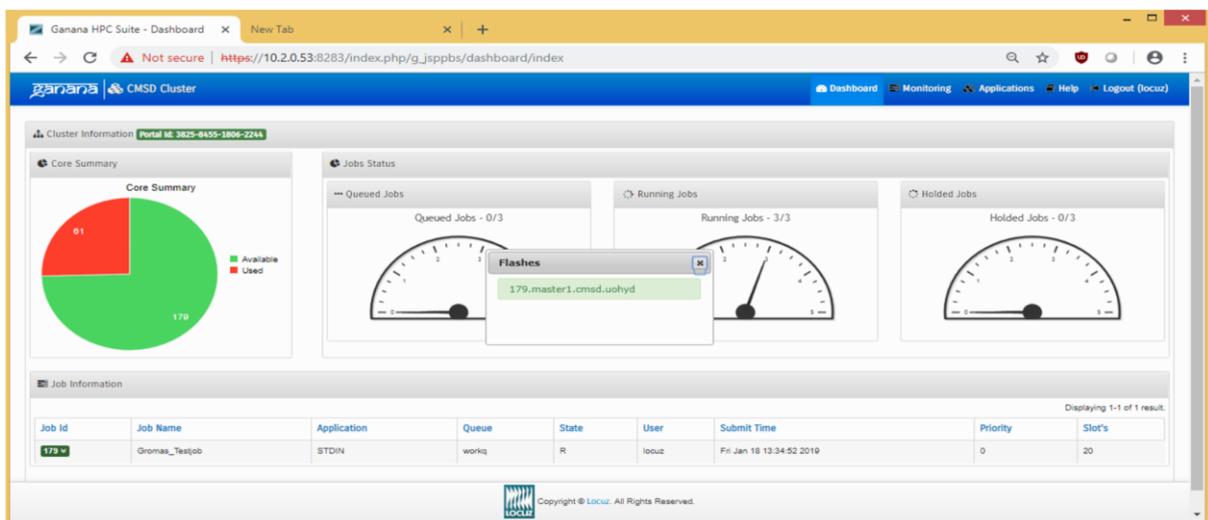
Select the application name.



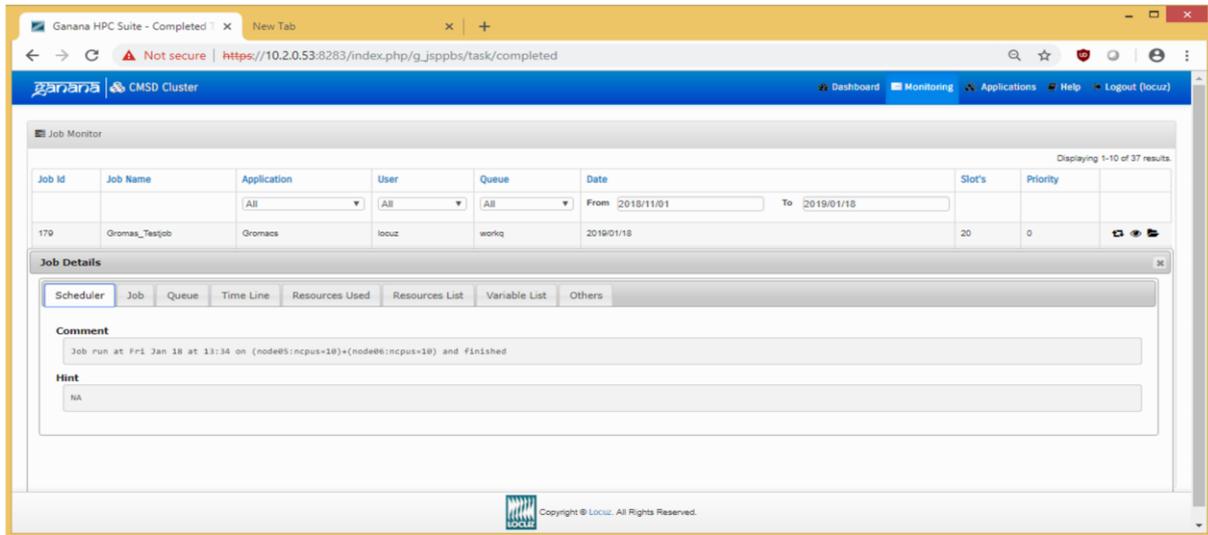
Give the job information and click on submit job



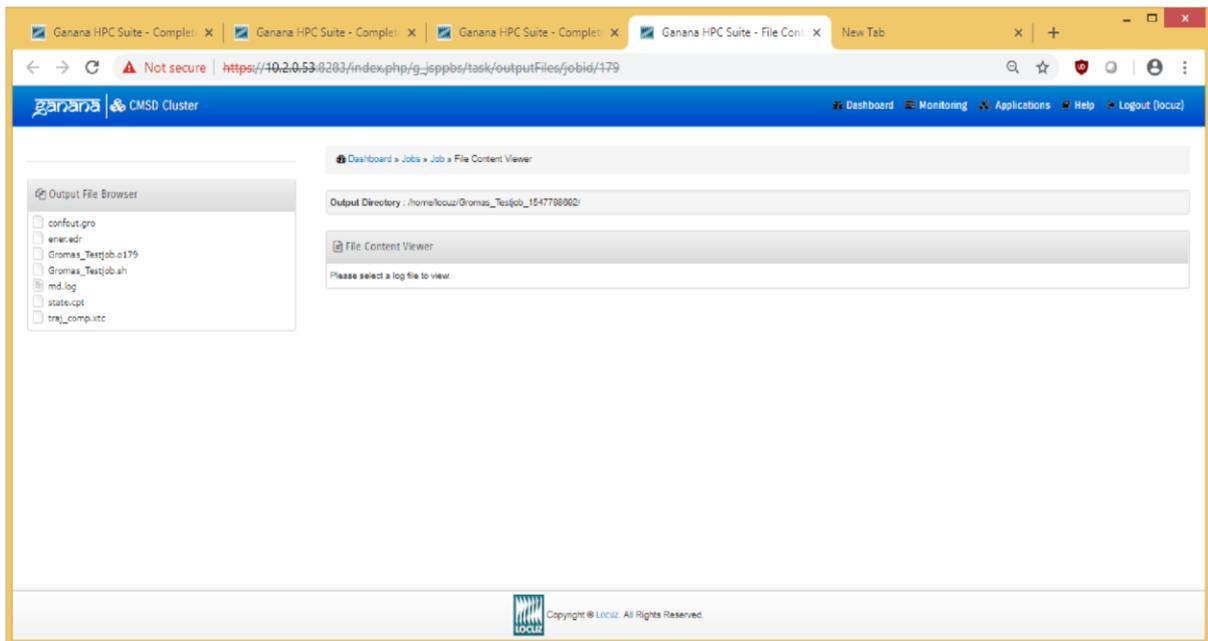
After Submitting the job we get job id information



We can monitor jobs information from monitoring Tab



Click on file browser Folder icon to job output details.



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