I) 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 -I 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

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

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

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Give the job information and click on submit job

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After Submitting the job we get job id information

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