HPC GUIDE FOR OPENFOAM V-2012

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1. Every time: qsub -I -q fpt-small -l nodes=1:ppn=16 to enter the node
2. Every time that a new terminal to the hpc is open to type *source .bashrc* and then *of2012.* Need to type source.bashrc and of2012 also when connected to a node
3. To give permission for a file to run *chmod +x nameofthefile* and the file should become green
4. How to copy files from your laptop to the hpc?

* First way is to open power shell on the laptop and type the following

Text

Description automatically generated

* Second way is to open WinSCP and then just copy paste the files.

1. How to run a simulation on the cluster?

**Non-interactive Jobs:** this is the most common PBS job. A job script is created that contains PBS resource requests and the commands necessary to execute the job. The job script is then submitted to PBS to be run non-interactively. Use this to execute all calculations if possible.

qsub ‘myJob.pbs’

**Interactive Jobs:** this is a way to get an interactive terminal on one or more of the compute nodes of the cluster. Commands can then be run interactively through that terminal directly on the compute nodes for the duration of the job. Use this for work that needs user input such as grid operations or post-processing.

qsub –I –X –l –q ‘queue\_name’ nodes=1:ppn=1:typeg

A sample script for OpenFoam is given below. If you are running your own OpenFOAM executable, make sure that it is saved in the folder:

/home/<yourNetID>/OpenFOAM/<yourNetID>-<version>/platforms/<systemOptions>/bin

################# Cut and paste from line below #########################

#!/bin/bash

#PBS -j oe

###PBS -o qsub.${PBS\_JOBID}.log ##this is not necessary

#PBS -N jobname #specify name of the job

#PBS -l nodes=4:ppn=32:typej,walltime=02:30:00

### Replace the command above with the following to change memory and num. of proc. per node #######

###PBS -l nodes=n12-05:ppn=2:typeg,pmem=1000mb,walltime=2:00:00

#PBS -m abe

#PBS -M l.scarlatti@tudelft.nl

set –e

echo Job started on `uname -n` at `date`

nproc=128 #Choose the number so that nproc = (num. of nodes) x (cores per node)

Application=waveFoam #Change the name with that of your application ‘waveFoam’

Output=info.log

######## Uncomment the following if you want to use your own version of OpenFoam (installed manually) #######

######## Note: as OpenFoam is heavy, it is assumed it is installed in your scratch folder ######################

source /home/lascarlatti/OpenFOAM/OpenFOAM-v2012/etc/bashrc #need to change this

####### make sure any symbolic links are resolved to absolute path and move to working directory ############

export PBS\_O\_WORKDIR=$(readlink -f $PBS\_O\_WORKDIR)

cd $PBS\_O\_WORKDIR

#touch ./${PBS\_JOBID}.txt # Not needed – the PBS system automatically create it

######## Start the solver ###############

if [ $nproc -gt 1 ]; then

mpirun -np $nproc $Application –parallel > $Output 2>&1

else

$Application > $Output 2>&1

fi

###################### End of script ##################################