1. single.q

```
[mylee@fermi sge-examples]$ sudo cat /home/tilen/AGP/GUE_RP/CNN_project/L2000/training_data/high.sh
# For pure serial jobs, @YNT=1
#!/bin/sh

#$ -q single.q
#### Instead of 'single', you can use the follow queues ####
#### single.q : For NOT high memory jobs (below 14GB memory per node). It uses just a single
node.        ####
####          But your computation node may share with other user's
jobs.                              ####
#### highmem.q : For High memory jobs (beyond 14GB memory per node). You can use the node
exclusively,    ####
#### short_24.q

#$ -cwd
#$ -pe openmp 1         #### Instead of ' 12 ', input core number which you want to use, but there is a
limitation  ####
                         #### in both matlab and mathematica : Matlab : 12, Mathematica :
8                          ####

# Run job through bash shell

#$ -S /bin/bash

set -e

source /etc/profile.d/modules.sh

module load python/gcc-4.8.5/2.7.15

export OMP_NUM_THREADS=1   #### Instead of ' 12 ', input core number which you $
                            #### in both matlab and mathematica : Matlab : 12, $

#------------------------------------------------------------------
# My parameters

L=2000

R_init=511500
R=1

#iran=`od -vAn -N4 -tu4 < /dev/urandom`
iran=R_init

#------------------------------------------------------------------

PARAMS="$L $R_init $R"

# My commands
NEW_DIR2=runs_L"$L"_R_init_"$R_init"_"$R"
# by default there is a space at the beginning of iran, this bellow removes it
NEW_DIR="$(echo -e "${NEW_DIR2}" | tr -d '[:space:]')"

mkdir $NEW_DIR
cp high.sh ./$NEW_DIR
cp cluster-GUE-RP-model.py ./$NEW_DIR

cd $NEW_DIR
```

```
name2=info_GUE_RP_"$iran".out
# again by default there is a space at the beginning of iran, this bellow removes it
name="$(echo -e "${name2}" | tr -d '[:space:]')"


python ./cluster-GUE-RP-model.py $PARAMS > ./$name



####  Instead of 'command', input your corresponding command, such as matlab, math, and python  ####
####  : Input matlab (math) {python2.7, python3.5} for using Matlab (Mathematica) {Python2.7,
python3.5}, respectively ####

####  Instead of '/scratch/hscheon/source_file_name', input your source file name including the path
####

####  Instead of '/scratch/hscheon/output_file_name.out', input your output file name including the
path ####
```

2. gcc4.8/mvapich2

- The sample example files is in the /opt/sge-examples/jobs/Simple_mpi_test/

```
[dasan@fermi Simple_mpi_test]$ cat mvapich2-mpi-hello.sh
#!/bin/bash


#$ -S /bin/bash
#$  -cwd
#$  -V
#$  -N myjob

#$ -q  hm_long_40.q   ### max cores  slots=120

##$ -l   h=[dirac72][dirac-74]
##$ -l   h=dirac[72-73]

#$ -pe  mpi_40 80

cd $SGE_O_WORKDIR

export OMP_NUM_THREADS=1

export MV2_ENABLE_AFFINITY=0    ### mvapich2

module purge
module load  gcc-4.8.5/mvapich2/2.3

#mpirun  $PWD/mpi-hello
mpicc mpi-hello.c -o mpi-hello-mvapich2

mpirun  hostname

mpirun  ./mpi-hello-mvapich2

sleep 5

rm  mpi-hello-mvapich2
[dasan@fermi Simple_mpi_test]$
```

3. gcc8.2/openmpi4

- The sample example files is in the /opt/sge-examples/jobs/Simple_mpi_test/

```
[dasan@fermi Simple_mpi_test]$ cat openmpi4-mpi-hello.sh
#!/bin/bash


#$ -S /bin/bash
#$  -cwd
#$  -V
#$  -N myjob


#$ -q  hm_long_40.q
#$ -pe  mpi_40 80  ### max cores  slots=120


cd $SGE_O_WORKDIR


export OMP_NUM_THREADS=1


export OMPI_MCA_btl=openib,self,vader


module purge
module  load  gcc-8.2.0/openmpi/4.0.2  ###  WARNING: There was an error initializing an OpenFabrics
device.뜨지만 무시합니다.


#module load gcc-9.2.0/openmpi/4.0.2


mpicc mpi-hello.c -o mpi-hello-openmpi


mpirun  hostname


mpirun ./mpi-hello-openmpi


## 아래의 옵션 사용도 가능 합니다.
#mpirun  -x LD_LIBRARY_PATH  ./mpi-hello-openmpi
#mpirun --mca btl_openib_want_fork_support 1  -x LD_LIBRARY_PATH  ./mpi-hello-openmpi
#mpirun -np 2 --display-map --map-by node -H host1,host2
#mpirun --display-map ./mpi-hello-openmpi
##  --mca pml ob1 \
##  --mca btl_openib_if_include mlx5_0:1 \
##  --mca btl_openib_cpc_include rdmacm \
##  --mca btl_openib_allow_different_subnets 1 \
##  --mca btl self,sm,openib \
##  --mca btl_openib_gid_index 1 \


sleep 5
rm  mpi-hello-openmpi
[dasan@fermi Simple_mpi_test]$
```

4. intel mpi

- The sample example files is in the /opt/sge-examples/jobs/Simple_mpi_test/

```
[mylee@fermi Simple_mpi_test]$
[mylee@fermi Simple_mpi_test]$ cat  intel-impi-mpi-hello.sh
#!/bin/bash
```

```
#$ -S /bin/bash
#$  -cwd
#$  -V
#$  -N myjob


##$ -q  hm_long_40.q
#$ -q  hm_short_40.q  ### max cores  slots=120


#$ -pe  mpi_40 120    ### max cores  slots=120


cd $SGE_O_WORKDIR


export I_MPI_FABRICS=shm:dapl


module purge
module load intel-oneapi/compiler/2022.0.2  intel-oneapi/mpi/2021.5.1


mpicc mpi-hello.c -o mpi-hello-intelmpi


mpirun  hostname


mpirun ./mpi-hello-intelmpi


sleep 5
rm  mpi-hello-intelmpi
[mylee@fermi Simple_mpi_test]$
```

4. Other examples

a.

```
[root@fermi:~]# cat /home/scratch/dillip/SYK_proj/AubryAGP/sub1Para_AGP.sh
#!/bin/bash
#$ -S /bin/bash
#$ -l h_rt=160:00:00
#$ -q hm_long_40.q
#$ -pe mpi_40 40
#$ -v OMP_NUM_THREADS=1
#$ -cwd
echo "Preparing:"
echo "Checking:"
pwd
hostname
date
echo "Environment:"
export OMP_NUM_THREADS=1
echo "Starting:"


cd /home/scratch/dillip/SYK_proj/AubryAGP
source /home/dillip/.bashrc


module purge
module load sge
module load gcc/8.2.0
module load gcc-8.2.0/openmpi/4.0.2


module load julia/gcc-4.8.5/1.6.2
```

```
# MPI run
#mpirun -n 4 /home/scratch/dillip/CCSDpT_PmLike2.x



# run
#alias julia2="/home/scratch/dillip/Julia_Jobs/julia-
1.6.2/bin/julia"  /home/scratch/dillip/Julia_Jobs/0.jl

/home/scratch/dillip/julia-1.6.2/bin/julia  -p 16
/home/scratch/dillip/SYK_proj/AubryAGP/driv1_Aubry_AGP_gen_para.jl > out1_Aubry_para_AGP.txt

#matlab -nodesktop -nosplash -nodisplay -r "run driv_SYK_M4.m"

date
echo "Done."

exit 0
[root@fermi:~]#
```

b.

```
[mylee@fermi Simple_mpi_test]$
[mylee@fermi Simple_mpi_test]$ qstat -j  139142
==============================================================
job_number:                 139142
exec_file:                  job_scripts/139142
submission_time:            Sun Sep 18 22:00:49 2022
owner:                      dario
uid:                        1032
group:                      dario
gid:                        1032
sge_o_home:                 /home/dario
sge_o_log_name:             dario
sge_o_path:                 /opt/sge/bin:/opt/sge/bin/lx-amd64:/opt/openssl-3.0.5/bin:/opt/openssl-
3.0.5/ssl:/opt/anaconda3/condabin:/usr/lib64/qt-
3.3/bin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/opt/ibutils/bin:/home/dario/.local/bin:/home
/dario/bin
sge_o_shell:                /bin/bash
sge_o_workdir:              /home/scratch/dario/AA_cross_check
sge_o_host:                 fermi
account:                    sge
cwd:                        /home/scratch/dario/AA_cross_check
hard resource_list:         h_rt=172740
mail_list:                  dario@fermi
notify:                     FALSE
job_name:                   script_file.sh
jobshare:                   0
hard_queue_list:            hm_long_40.q
shell_list:                 NONE:/bin/bash
env_list:                   TERM=NONE,OMP_NUM_THREADS=40
script_file:                script_file.sh
parallel environment:  mpi_40 range: 40
binding:                    NONE
job_type:                   NONE
usage        1:             cpu=735:08:22, mem=85697973.77870 GB s, io=0.03839 GB, vmem=38.398G,
maxvmem=40.572G
binding      1:             NONE
scheduling info:            (Collecting of scheduler job information is turned off)
[mylee@fermi Simple_mpi_test]$


[mylee@fermi Simple_mpi_test]$
[mylee@fermi Simple_mpi_test]$
[mylee@fermi Simple_mpi_test]$ sudo  cat  /home/scratch/dario/AA_cross_check/script_file.sh
# For pure serial jobs, @YNT=1

#$ -S /bin/bash
#$ -l h_rt=47:59:00
#$ -q hm_long_40.q
#$ -pe mpi_40 40
#$ -v OMP_NUM_THREADS=40
#$ -cwd




# Run job through bash shell



set -e
export OMP_NUM_THREADS=40   #### Instead of ' 12 ', input core number which you want to use, but there
is a limitation  ####
                            #### in both matlab and mathematica : Matlab : 12, Mathematica :
8                          ####
####  load module which required to execute job  ####
####  for example: module load sge/8.1.8  ####
```

```
source /etc/profile.d/modules.sh
module load julia/gcc-4.8.5/1.8.0



julia -t
40  </home/scratch/dario/AA_cross_check/main_eigenvalues_filtered.jl>  /home/scratch/dario/AA_cross_che
ck/logs/output_file_name20_floor.out



####  Instead of 'command', input your corresponding command, such as matlab, math, and python  ####
####  : Input matlab (math) {python2.7, python3.5} for using Matlab (Mathematica) {Python2.7,
python3.5}, respectively ####

####  Instead of '/scratch/hscheon/source_file_name', input your source file name including the path
####

####  Instead of '/scratch/hscheon/output_file_name.out', input your output file name including the
path ####



[mylee@fermi Simple_mpi_test]$
```