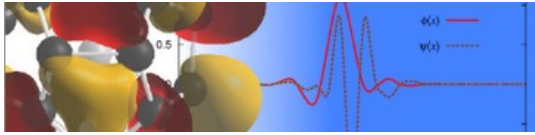


BigDFT hands on

Connect to CINECA : ssh login.plx.cineca.it

Go to http://bigdft.org

To the webpage Tutorials and First runs with BigDFT

job.sub file

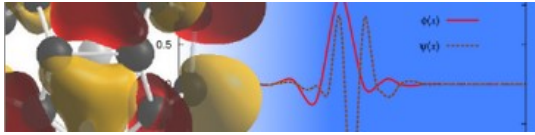
```
#!/bin/bash
#PBS -A train_wkms2013
#PBS -N bigdft
#PBS -l walltime=30:00
#PBS -l select=1:mpiprocs=6:ncpus=6
#PBS -o job.out
#PBS -q parallel

# start from launch dir
cd $PBS_O_WORKDIR

# load BigDFT module
module load autoload bigdft
mpirun -n 6 bigdft
```

1 node

6 MPI processes/node

6 cores/node

Indicate also the total number of MPI processes

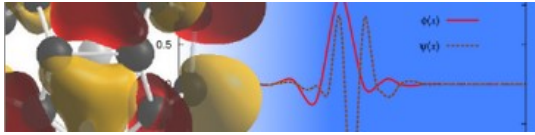


N2 molecule

- posinp.xyz

```
2 angstroem
free
N 0. 0. 0.
N 0. 0. 1.11499
```

- qsub job.sub
- qstat
- Look at job.out
- See also default.xxx files

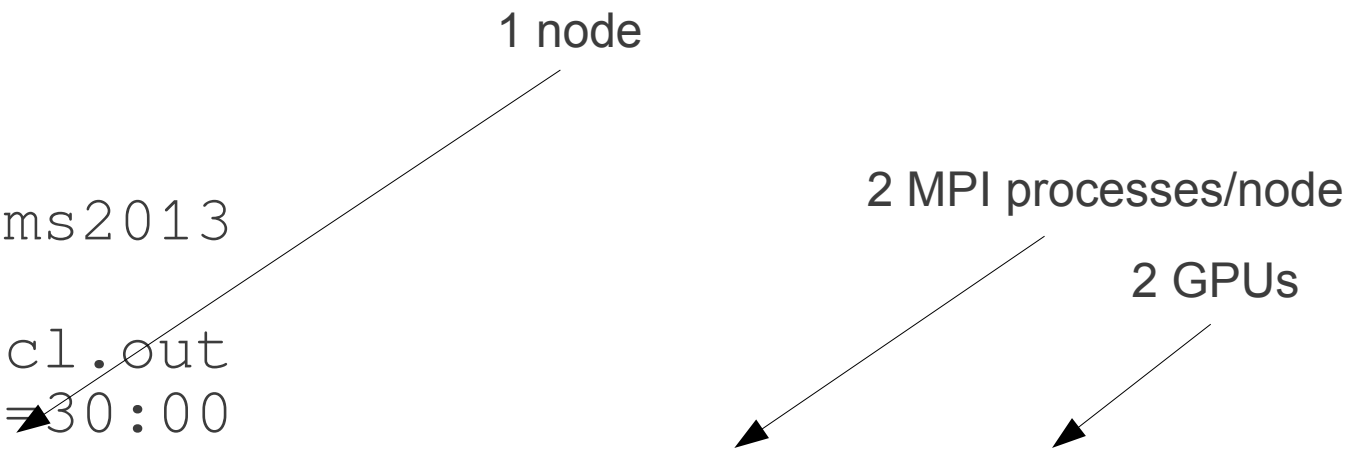


Job.out

```
Number of MPI processes 12

MPI process does not use OpenMP

No material acceleration (iproc=0)

....

FINAL iter,total energy,gnrm    11  -1.988348372590913O2E+01  3.36E-05

 ------------------------------------ Kohn-Sham Eigenvalues and Occupation Numbers

 e(   1)= -1.03189260251871E+00 2.0000

 e(   2)= -4.97010644365110E-01 2.0000

 e(   3)= -4.30727629604671E-01 2.0000

 e(   4)= -4.30727289584172E-01 2.0000

 e(   5)= -3.81210771917243E-01 2.0000

...

Final values of the Forces for each atom

     1      N -3.38813E-21 -1.69407E-21  5.67055E-02

     2      N -8.47033E-21 -8.47033E-21 -5.67055E-02
```

OpenCL (GPU)

job-opencl.sub




```
#!/bin/bash
#PBS -A train_wkms2013
#PBS -N bigdft
#PBS -o job-opencl.out
#PBS -l walltime=30:00
#PBS -l select=1:ncpus=2:mpiprocs=2:ngpus=2
# the following line ensures entire nodes are
reserved
#PBS -l place=free:excl

# start from launch dir
cd $PBS_O_WORKDIR

# load BigDFT module
module load autoload bigdft
mpirun -n 2 bigdft
```

OpenCL run

- In input.perf, add the following line :

  ACCEL OCLGPU

- job-opencl.out

```
Number of MPI processes 2
MPI process does not use OpenMP
OpenCL support activated, No. devices per node (used, available):     2     2
```