Parallel Materials Modelling Packages
GPAW Exercises

1 Introduction

This handout contains specific instructions for running GPAW calculations on ARCHER. The actual exercises can be found on the web at:

```
https://wiki.fysik.dtu.dk/gpaw/exercises/exercises.html
```

2 Setup

At the start of the session you should load the ASE and GPAW modules:

```
guest01@eslogin002:~> module load ase
guest01@eslogin002:~> module load gpaw
```

3 Running ASE Scripts

Please note that the ASE GUI does not work on ARCHER - please save the scripts on the website as python scripts and run them using the python interpreter according to the instructions below. Alternative, the scripts can be edited and run within an interactive python session. E.g. for the first exercise:

```
guest01@eslogin002:~> cat example.py
from ase import Atoms
from ase.calculators.emt import EMT
from ase.optimize import QuasiNewton

system = Atoms('H2', positions=[[0.0, 0.0, 0.0],
                                [0.0, 0.0, 1.0]])
calc = EMT()

system.set_calculator(calc)

opt = QuasiNewton(system, trajectory='h2.emt.traj')

opt.run(fmax=0.05)

guest01@eslogin002:~> python example.py
BFGSLineSearch:    0[  0]  22:15:13        2.299029        8.0358
BFGSLineSearch:    1[  2]  22:15:13        1.129250        2.9257
BFGSLineSearch:    2[  4]  22:15:13        1.070800        0.2142
```

```
BFGSLineSearch:    3[  5]  22:15:13        1.070549        0.0367
guest01@eslogin002:~>
```

Please note that only very small (<10 second) jobs should be run interactively on the ARCHER front-end. Remember this is a shared resource between ALL ARCHER users!

To run your python script on the backend, please use the batch script in the next section.

4   Running GPAW in parallel

To run a GPAW job on ARCHER, you will need a batch script similar to the following. See the general instructions handout and/or the ARCHER website if you need to modify it:

```
guest02@eslogin003:/work/y14/y14/guest02> cat gpaw.pbs
#!/bin/bash --login

#PBS -N test_gpaw
#PBS -l select=1
#PBS -l walltime=0:5:0
#PBS -A y14

cd $PBS_O_WORKDIR

module load gpaw
module load ase

aprun -n 24 gpaw-python input.py
```