

# Parallel Materials Modelling Packages

## CP2K Exercises

### 1 Introduction

This handout contains specific instructions for running CP2K calculations on ARCHER. Details of the exercises themselves are available on the CP2K web site:

<http://www.cp2k.org/exercise>

The exercises grouped under ‘Lecture 1’ are a good introduction to doing classical calculations using CP2K, ‘Lecture 4’ covers Molecular Dynamics in NVE and NVT ensembles, and ‘Lecture 6’ introduces DFT calculations with Quickstep.

Some more detailed tutorials can also be found at:

<http://www.cp2k.org/tutorials>

These take a closer look at the fundamental tasks needed to set up a reliable, well-converged Quickstep calculation.

Look through both pages and choose some exercises that match your level of experience and interest. Please work through the exercises at your own pace, referring to the instructions below for details specific to ARCHER.

Course staff will also be available to discuss issues relating to your own calculations if you wish.

### 2 Running CP2K

To run a CP2K 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 cp2k.pbs
#!/bin/bash --login

#PBS -N test_cp2k
#PBS -l select=1
#PBS -l walltime=0:5:0
#PBS -A y14

cd $PBS_O_WORKDIR

module load cp2k

aprun -n 24 cp2k.popt -i energy.inp -o energy.out
```

The arguments passed to CP2K will need to be modified as you follow the different exercises. You might consider running each exercise in a different directory to keep the output files separate.

### 3 Visualisation & Analysis

Some exercises require the use of VMD for visualise the psystem (e.g. Exercise 2: Geometry Optimization). To use VMD on ARCHER you will need to enabled X11 forwarding in your SSH connection. With OpenSSH this is done by adding the `-X` flag. You will also need to load the `vmd` module before running VMD:

```
iains-mbp:~ ibethune$ ssh -X guest02@login.archer.ac.uk
Password:
Last login: Mon Apr 21 09:56:27 2014 from <snip>
=====
login.archer.ac.uk
-----
<snip>
=====
guest02@eslogin005:~> cd /work/y14/y14/guest02
guest02@eslogin005:/work/y14/y14/guest02> module load vmd
guest02@eslogin005:/work/y14/y14/guest02> vmd geopt-pos-1.xyz
```

For plotting data, ARCHER has the following tools installed:

- **GNUplot**: simply type `gnuplot`
- **XMGrace**: first load the `xmgrace` module then run `xmgrace`