

Parallel Materials Modelling Packages

CASTEP Exercises

1 Introduction

This handout contains specific instructions for running CASTEP calculations on ARCHER. Detailed descriptions of the practical exercises are available on the web at:

<http://www.castep.org/CASTEP/OnlineTutorials>

We recommend exercises 2, 3, 5 and 7, although feel free to work on other exercises if these suit your experience and/or interests better.

Please note that the nano editor is now available on ARCHER by loading the nano module:

```
guest01@eslogin008:~> module load nano
```

2 Running CASTEP

To run a CASTEP 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 castep.pbs
#!/bin/bash --login

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

cd $PBS_O_WORKDIR

module load castep
export PSPOT_DIR=/work/y07/y07/castep/7.0.2-phase1/tests/Pseudopotentials

aprun -n 24 $CASTEP_EXE <castep_args>
```

The arguments passed to CASTEP 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 CASTEP tools

CASTEP also comes with a set of helpful programs (`castep2cube` etc.), which are used to work with the output files generated by CASTEP. These are available to run on the front-end nodes (i.e. without a

batch script), as they are not typically compute intensive. To use these tools, do:

```
module load castep-serial
```

And the tools directory will be added to you \$PATH.

4 Post-processing scripts

The CASTEP post processing scripts can be downloaded from:

```
http://ccpforge.cse.rl.ac.uk/gf/download/frsrelease/259/4636/scripts-7.0.2.tar.gz
```

You can either install these scripts on your local system or in your directory on ARCHER.