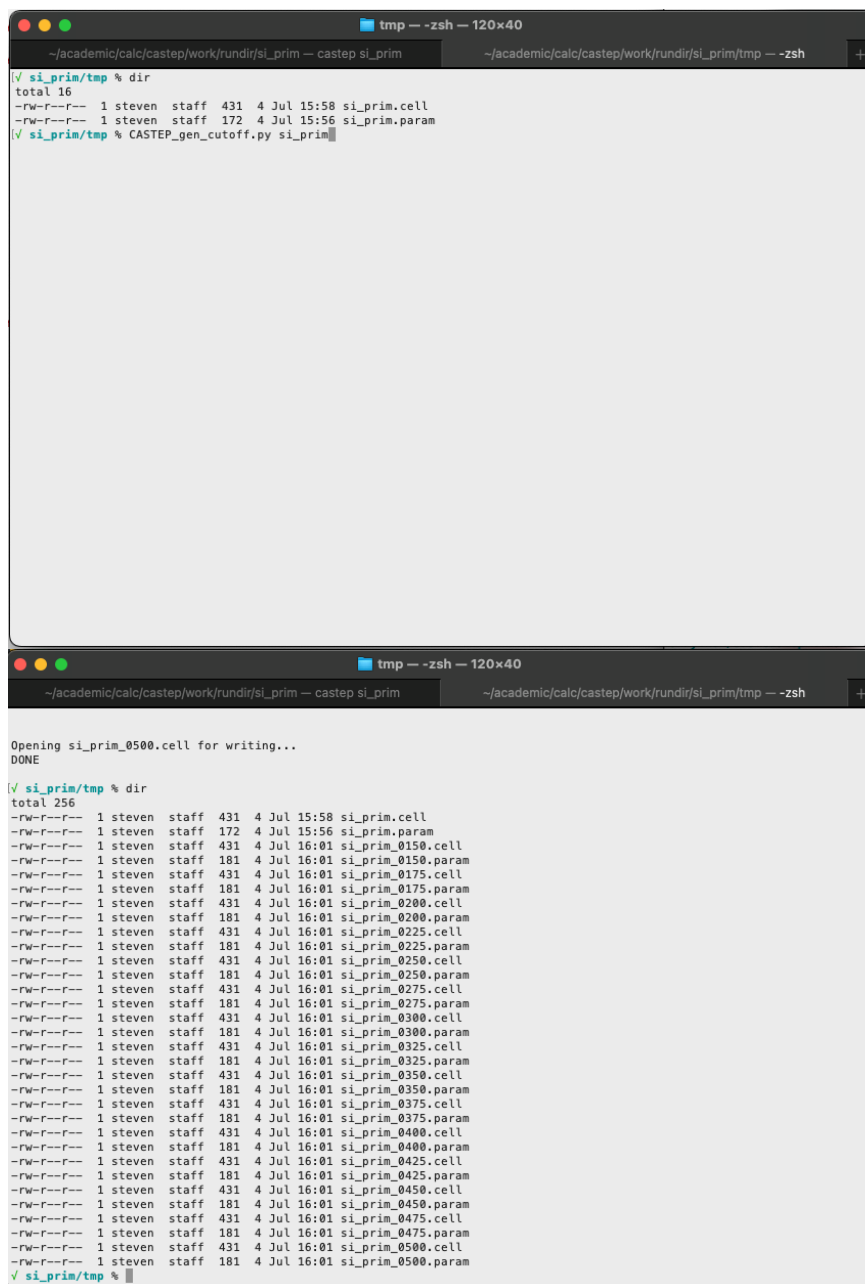


The programme CASTEP_gen_cutoff.py will take a .cell and .param input and generate a set of inputs for different plane wave energy cutoff. The range of cutoff values can be set by editing the CASTEP_gen_curoff.py file.

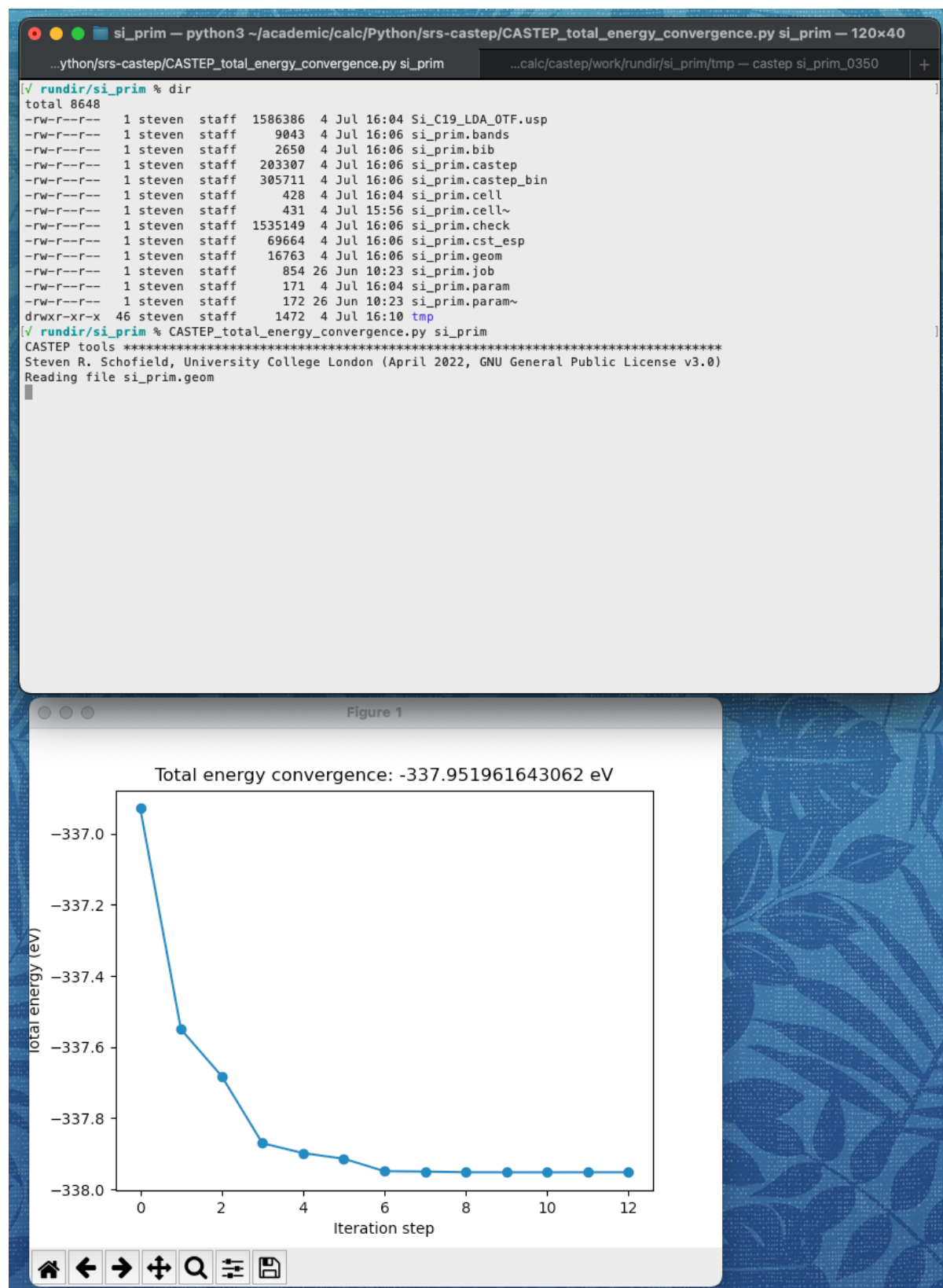


```
tmp -- -zsh -- 120x40
~/academic/calc/castep/work/rundir/si_prim -- castep si_prim
~/academic/calc/castep/work/rundir/si_prim/tmp -- -zsh

√ si_prim/tmp % dir
total 16
-rw-r--r--  1 steven  staff   431  4 Jul 15:58  si_prim.cell
-rw-r--r--  1 steven  staff   172  4 Jul 15:56  si_prim.param
√ si_prim/tmp % CASTEP_gen_cutoff.py si_prim

Opening si_prim_0500.cell for writing...
DONE
√ si_prim/tmp % dir
total 256
-rw-r--r--  1 steven  staff   431  4 Jul 15:58  si_prim.cell
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0150.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0150.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0175.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0175.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0200.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0200.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0225.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0225.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0250.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0250.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0275.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0275.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0300.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0300.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0325.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0325.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0350.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0350.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0375.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0375.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0400.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0400.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0425.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0425.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0450.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0450.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0475.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0475.param
-rw-r--r--  1 steven  staff   431  4 Jul 16:01  si_prim_0500.cell
-rw-r--r--  1 steven  staff   181  4 Jul 16:01  si_prim_0500.param
√ si_prim/tmp %
```

The file CASTEP_total_energy_convergence.py will read a single geometry optimisation .castep output file and plot the SCF convergence per geometry optimisation step. This is mainly a sanity check the calculation has run correctly.



The CASTEP_multiple_file_convergence.py will read the total energy and bond length from a series of .castep files and generate a text file for plotting with some programme. The .castep files should first all be copied to a single directory and CASTEP_multiple_file_convergence.py should be run from in that directory. The energy should work for any calculation, but the bond-length probably only works properly for the primitive unit cell. This could be modified also to extract other parameters.

```

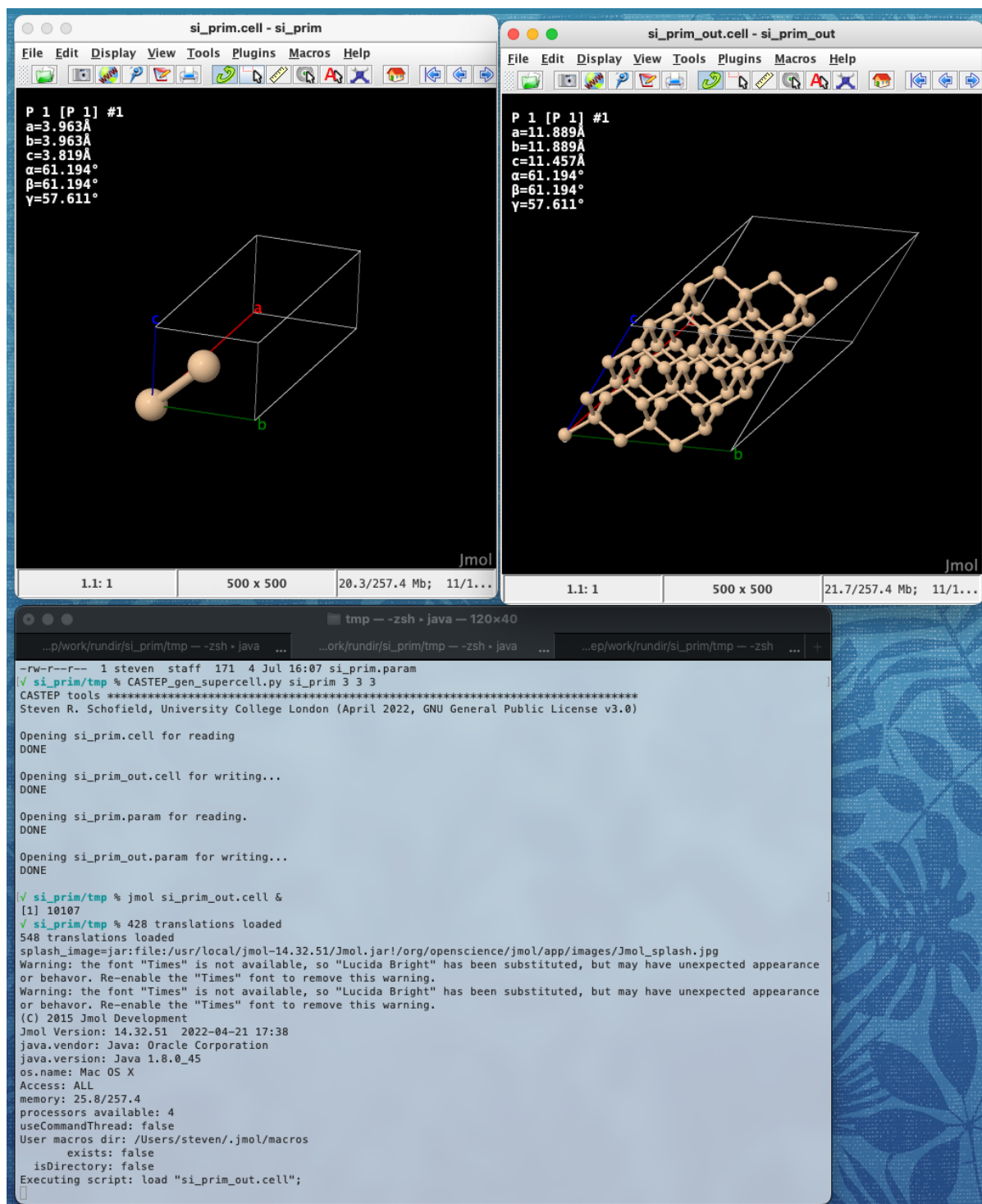
tmp -- -zsh -- 120x40
~/academic/calc/castep/work/rundir/si_prim/tmp/tmp -- -zsh
[✓ tmp/tmp % dir
total 664
-rw-r--r-- 1 steven staff 57560 4 Jul 16:13 si_prim_0250.castep
-rw-r--r-- 1 steven staff 57560 4 Jul 16:13 si_prim_0300.castep
-rw-r--r-- 1 steven staff 57398 4 Jul 16:13 si_prim_0350.castep
-rw-r--r-- 1 steven staff 57398 4 Jul 16:13 si_prim_0400.castep
-rw-r--r-- 1 steven staff 57398 4 Jul 16:13 si_prim_0450.castep
-rw-r--r-- 1 steven staff 31468 4 Jul 16:13 si_prim_0500.castep
[✓ tmp/tmp % CASTEP_multiple_file_convergence.py
CASTEP tools *****
Steven R. Schofield, University College London (April 2022, GNU General Public License v3.0)

Wrote output file multiple_file_output.txt :

Filename      Cutoff      TotalE      Bondlength      Warnings
si_prim_0250  250.0      -337.977783  2.34081         --
si_prim_0300  300.0      -337.982543  2.34068         --
si_prim_0350  350.0      -337.982898  2.34047         --
si_prim_0400  400.0      -337.983032  2.34045         --
si_prim_0450  450.0      -337.983166  2.34045         --
si_prim_0500  500.0      --          --             --
[✓ tmp/tmp % dir
total 672
-rw-r--r-- 1 steven staff 567 4 Jul 16:13 multiple_file_output.txt
-rw-r--r-- 1 steven staff 57560 4 Jul 16:13 si_prim_0250.castep
-rw-r--r-- 1 steven staff 57560 4 Jul 16:13 si_prim_0300.castep
-rw-r--r-- 1 steven staff 57398 4 Jul 16:13 si_prim_0350.castep
-rw-r--r-- 1 steven staff 57398 4 Jul 16:13 si_prim_0400.castep
-rw-r--r-- 1 steven staff 57398 4 Jul 16:13 si_prim_0450.castep
-rw-r--r-- 1 steven staff 31468 4 Jul 16:13 si_prim_0500.castep
[✓ tmp/tmp %

```

The programme CASTEP_gen_supercell.py reads in a unit cell and generates a new larger one depending on the integers supplied in the input:



The file CASTEP_reorder_coords.py reorders the cell coordinates by z, then y, then z. This is useful after generating a larger cell from a smaller one, for example, and will be useful when working with surfaces.

```

tmp -- -zsh -- 98x73
...rk/rundir/si_prim/tmp -- -zsh ...
/tmp -- -zsh -- 98x73
...rk/rundir/si_prim/tmp -- -zsh ...
/tmp -- -zsh -- 98x73
...rk/rundir/si_prim/tmp -- -zsh ...
DONE
tmp -- -zsh -- 106x75
...rk/rundir/si_prim/tmp -- -zsh ...
/tmp -- -zsh -- 106x75
...rk/rundir/si_prim/tmp -- -zsh ...
/tmp -- -zsh -- 106x75
...rk/rundir/si_prim/tmp -- -zsh ...

```