

The Guide 1.1 (addendum 1) to CASTEP 3.9

Phil Lindan

Computational Materials Science Group,
Daresbury Laboratory, Warrington WA4 4AD, UK

`ukcp@dl.ac.uk`
<http://www.cse.clrc.ac.uk/Activity/UKCP>

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This revision makes more clear the procedure for constructing `.recpot` files when using norm-conserving pseudopotentials.

0.0.1 Preparing `.recpot` when using norm-conserving potentials

The norm-conserving potentials are in the `.recpot` files in the `POTENTIALS_NC/` directory. (Remember, both the `CASTEP` input file `.recpot` and the norm-conserving potential files share the same suffix.) Broadly, the foregoing description relating to constructing the `CASTEP` input file `.recpot` when using ultrasoft pseudopotentials carries over to norm-conserving ones. There are three differences. Firstly, an extra line should be inserted in the file containing information about nonlinear core corrections. Secondly, the norm-conserving potentials do not contain the Core Charge line. Thirdly, each norm-conserving pseudopotential must be terminated by a line containing the integer 1000

After the Comments Section, the first few lines of the norm-conserving pseudopotential files in the `POTENTIALS_NC/` directory have the following format:

```

3 5
 100.0000000000
   2.9612498283   -217140.6718750000   -54282.9492187500
-24124.1113281250   -13568.5205078125   -8682.7910156250

```

Line one is the version line, line two is the value of `PSGMAX`, the maximum wavevector of the pseudopotential in $1/\text{\AA}$, and subsequent lines define the local part of the potential. The nonlinear core correction line is inserted after `PSGMAX`, so that the file becomes:

```

3 5
 100.0000000000
   0.0000000000         0.0000000000
   2.9612498283   -217140.6718750000   -54282.9492187500
-24124.1113281250   -13568.5205078125   -8682.7910156250

```

The two numbers are read into the variables `fcharg` and `rcharg`, the prefactor and core radius for the nonlinear core charge respectively. For all the norm-conserving potentials in `POTENTIALS_NC/` these numbers should be zero.

Since there is no Core Charge Line you need to find the core charges for the pseudopotentials by other means. Usually the Comments Section of the potential file contains enough information to deduce the core charge. The configurations used in generating the potential indicate which states were treated as valence states. Subtraction of the number of core states from the atomic number gives the core charge.

A second method, which is always reliable, is based on the nature of the local

potential V . As the magnitude of the wavevector $q \rightarrow 0$, corresponding to large distances, V tends to that of a point charge, given by

$$V = Z/q^2. \quad (1)$$

For a norm-conserving pseudopotential we can find the smallest wavevector and the corresponding local potential. The line after the Version Line contains the radial grid maximum `PSGMAX` (in $1/\text{\AA}$), with the potential tabulated on a grid of `(NPSPTN-1)` points. `NPSPTN` is almost always 2001, though some very early potentials used a value of 501. The smallest wavevector is therefore `(PSGMAX/(NPSPTN-1))`. The value of the V at the smallest wavevector is second number in the following line. Including the necessary conversion factors, the pseudopotential core charge is given by the nearest integer to

$$\text{ICHARG} = \frac{|V|}{180.95263} \left(\frac{\text{PSGMAX}}{\text{NPSPTN} - 1} \right)^2 \quad (2)$$

For the boron norm-conserving pseudopotential `POTENTIALS_NC/B_00.recpot` this becomes:

$$\text{ICHARG} = \frac{217140.671875}{180.95263} \left(\frac{100}{2000} \right)^2, \quad (3)$$

yielding `ICHARG = 3`.

The steps in preparing `.recpot` with norm-conserving pseudopotentials are thus:

1. Determine the highest version number of the potentials you are using from the Version Lines and insert it as the first line of `.recpot`
2. Set the `ICHARG` parameters in `.rundat` to the core charges as calculated or read from the potential files.
3. Remove the Comments Section and Version Line from all the potentials, insert the Nonlinear Core Correction line and append a line with the integer "1000" to them.
4. Insert all the potentials into the `.rundat` file, in the same order as the species appear in the other input files.

0.0.2 Using both ultrasoft and norm-conserving pseudopotentials together

CASTEP will run with a mixture of ultrasoft and norm-conserving pseudopotentials. The steps in preparing the `.recpot` file are an obvious merge of the instructions given in the previous two sections.