How to test a norm-conserving pseudopotential

```
$ grep "&d" OUT
 ATM3.3    26-NOV-12   N Test -- GS 2s2 2p3                                &v&d
 ATM3.3    26-NOV-12   N Test -- 2s1.8 2p3.2                              &v&d
 ATM3.3    26-NOV-12   N Test -- 2s1.6 2p3.4                              &v&d
 ATM3.3    26-NOV-12   N Test -- 2s2.0 2p3.7 (ionic configuration -0.7)   &v&d
 &d total energy differences in series
 &d          1        2        3        4
 &d  1    0.0000
 &d  2    0.1640   0.0000
 &d  3    0.3281   0.1641   0.0000
 &d  4   -0.1815  -0.3455  -0.5096   0.0000
*----- End of series ----* spdfg &d&v
 ATM3.3    26-NOV-12   N Test -- GS 2s2 2p3                                &v&d
 ATM3.3    26-NOV-12   N Test -- 2s1.8 2p3.2                              &v&d
 ATM3.3    26-NOV-12   N Test -- 2s1.6 2p3.4                              &v&d
 ATM3.3    26-NOV-12   N Test -- 2s2.0 2p3.7 (ionic configuration -0.7)   &v&d
 &d total energy differences in series
 &d          1        2        3        4
 &d  1    0.0000
 &d  2    0.1640   0.0000
 &d  3    0.3280   0.1640   0.0000
 &d  4   -0.1815  -0.3454  -0.5094   0.0000
*----- End of series ----* spdfg &d&v
```

Objectives

Test a norm-conserving pseudopotential using ATOM

Description of the input file of the ATOM code for a pseudopotential test

```
#
# All-electron calculations for a series of N configurations
#
   ae N Test -- GS 2s2 2p3
   N    ca
       0.0
    1    2
    2    0      2.00
    2    1      3.00
   ae N Test -- 2s1.8 2p3.2
   N    ca
       0.0
    1    2
    2    0      1.80
    2    1      3.20
   ae N Test -- 2s1.6 2p3.4
   N    ca
       0.0
    1    2
    2    0      1.60
    2    1      3.40
   ae N Test -- 2s2.0 2p3.7 (ionic configuration -0.7)
   N    ca
       0.0
    1    2
    2    0      2.00
    2    1      3.70
#
#  Test
#
   pt N Test -- GS 2s2 2p3
   N    ca
       0.0
    1    2
    2    0      2.00
    2    1      3.00
   pt N Test -- 2s1.8 2p3.2
   N    ca
       0.0
    1    2
    2    0      1.80
    2    1      3.20
   pt N Test -- 2s1.6 2p3.4
   N    ca
       0.0
    1    2
    2    0      1.60
    2    1      3.40
   pt N Test -- 2s2.0 2p3.7 (ionic configuration -0.7)
   N    ca
       0.0
    1    2
    2    0      2.00
    2    1      3.70
```

N $1s^2$ $2s^2\ 2p^3\ 3d^0\ 4f^0$

core — valence

Concatenations of **all electron**

For each configuration, the block is the same as for an all electron calculations, replacing **pt instead of ae**

And **pseudopotential tests for the same configurations and in the same order**

How to run a pseudopotential test with ATOM

```
$ ../../Utils/pt.sh N.test.inp N.tm2.vps
==> Output data in directory N.test-N.tm2



$ cd N.test-N.tm2
$ ls
AECHARGE AEWFNR2 ECONF_DIFFS PTCHARGE PTWFNR2 VPSIN pt.gplot vcharge.gps
AEWFNR0 AE_ECONF INP PTWFNR0 PT_ECONF charge.gplot pt.gps vspin.gplot
AEWFNR1 CHARGE OUT PTWFNR1 RHO charge.gps vcharge.gplot vspin.gps
```

Run the script

First, the name of the input
Second, the name of the pseudopotential in .vps (unformatted) format

Different output files in a new directory

The name of the directory is the concatenation of the name of the input file and the name of the pseudopotential file, both without the .inp and the .vps extensions

An explanation of the different files can be found in the ATOM User's Guide (page 6)

How to compare the AE and PS eigenvalues for different configurations

```
$ grep '&v' OUT | grep s
 ATM3.3    26-NOV-12   N Test -- GS 2s2 2p3                                  &v&d
 2s   0.0    2.0000      -1.35223895       4.72576386     -15.36854475  &v
 ATM3.3    26-NOV-12   N Test -- 2s1.8 2p3.2                                &v&d
 2s   0.0    1.8000      -1.35891385       4.72972423     -15.37523266  &v
 ATM3.3    26-NOV-12   N Test -- 2s1.6 2p3.4                                &v&d
 2s   0.0    1.6000      -1.36547758       4.73353731     -15.38169011  &v
 ATM3.3    26-NOV-12   N Test -- 2s2.0 2p3.7 (ionic configuration -0.7)  &v&d
 2s   0.0    2.0000      -0.81353235       4.49656286     -14.98792667  &v
*----- End of series ----* spdfg &d&v
 ATM3.3    26-NOV-12   N Test -- GS 2s2 2p3                                  &v&d
 1s   0.0    2.0000      -1.35223540       1.17006955      -8.02041752  &v
 ATM3.3    26-NOV-12   N Test -- 2s1.8 2p3.2                                &v&d
 1s   0.0    1.8000      -1.35867311       1.17125438      -8.02276479  &v
 ATM3.3    26-NOV-12   N Test -- 2s1.6 2p3.4                                &v&d
 1s   0.0    1.6000      -1.36497481       1.17239512      -8.02501762  &v
 ATM3.3    26-NOV-12   N Test -- 2s2.0 2p3.7 (ionic configuration -0.7)  &v&d
 1s   0.0    2.0000      -0.81324485       1.10746390      -7.88685310  &v
*----- End of series ----* spdfg &d&v
```

Repeat for the p, d, anf f shells

Units in Ry

The typical difference should be of around 1 mRyd for a ``good'' pseudopotential

The real proof of good transferability, remember, can only come from a molecular or solid-state calculation

Note that the PT levels are labeled starting from principal quantum number 1

How to compare the differences in total energies between different configurations

All electron

Pseudoatom

```
$ grep "&d" OUT
 ATM3.3    26-NOV-12   N Test -- GS 2s2 2p3                                  &v&d
 ATM3.3    26-NOV-12   N Test -- 2s1.8 2p3.2                                 &v&d
 ATM3.3    26-NOV-12   N Test -- 2s1.6 2p3.4                                 &v&d
 ATM3.3    26-NOV-12   N Test -- 2s2.0 2p3.7 (ionic configuration -0.7)      &v&d
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 &d          1        2        3        4
 &d  1    0.0000
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 &d  3    0.3281   0.1641   0.0000
 &d  4   -0.1815  -0.3455  -0.5096   0.0000
*----- End of series ----* spdfg &d&v
 ATM3.3    26-NOV-12   N Test -- GS 2s2 2p3                                  &v&d
 ATM3.3    26-NOV-12   N Test -- 2s1.8 2p3.2                                 &v&d
 ATM3.3    26-NOV-12   N Test -- 2s1.6 2p3.4                                 &v&d
 ATM3.3    26-NOV-12   N Test -- 2s2.0 2p3.7 (ionic configuration -0.7)      &v&d
 &d total energy differences in series
 &d          1        2        3        4
 &d  1    0.0000
 &d  2    0.1640   0.0000
 &d  3    0.3280   0.1640   0.0000
 &d  4   -0.1815  -0.3454  -0.5094   0.0000
*----- End of series ----* spdfg &d&v
```

Cross excitations between different configurations

The typical difference should be of around 1 mRyd for a “good” pseudopotential