

Information on the format 3 for pseudopotentials.

(Note: the implementation of format 3 was done by Fr. Detraux).

The format 3 for ABINIT pseudopotentials allows to use pseudopotentials from the table I in the Phys. Rev. B 58, 3641 (1998) paper by C. Hartwigsen, S. Goedecker and J. Hutter (HGH). This paper presents LDA pseudopotentials for all elements from H to Rn. Some of them are even presented twice, because of the possibility to include semi-core states. Their accuracy has been demonstrated in the HGH paper, but note that the energy cut-off needed to get this high accuracy might be larger than the one usually needed for Troullier-Martins or other pseudopotentials. So, convergence studies are very important !

A few lines must be added to the data mentioned in that table, and are described in the present file. ABINITv1.5 is able to read format 3 pseudopotential files, as well as later versions of ABINIT.

We will suppose that the user has the HGH table. For the description that follows, we will focus on the Sn pseudopotential. In the table (p. 3651), one finds:

```
Sn 4 0.605000 4.610912
    0.663544 1.648791 -.141974 -.576546
    0.745865 0.769355 -.445070
        0.103931 0.005057
    0.944459 0.225115
        0.007066
```

These data must be put in the following format to be read by ABINIT (this file is also found in the ~abinit/tests/Psps_for_tests directory, with the name 50sn.pspgh) :

```
Hartwigsen-Goedecker-Hutter psp for Tin, from PRB58, 3641 (1998) paper
50 4 980509 zatom,zion,pspdat
3 1 2 0 2001 0 pspcod,pspxc,lmax,lloc,mmax,r2well
0.605000 4.610912 0 0 0 rloc, c1, c2, c3, c4
0.663544 1.648791 -.141974 -.576546 rs, h11s, h22s, h33s
0.745865 0.769355 -.445070 0 rp, h11p, h22p, h33p
        0.103931 0.005057 0 k11p, k22p, k33p
0.944459 0.225115 0 0 rd, h11d, h23d, h33d
        0.007066 0 0 k11d, k22d, k33d
```

First, the following three lines have been added at the beginning of the data from the table :

```
Hartwigsen-Goedecker-Hutter psp for Tin, from PRB58, 3641 (1998) paper
50 4 980509 zatom,zion,pspdat
3 1 2 0 2001 0 pspcod,pspxc,lmax,lloc,mmax,r2well
```

Similar lines must be added to the data for other elements, in order to make them readable by ABINIT.

Line 1 is simply a header, that might include any information, and that will be printed without modification in the output of ABINIT.

Line 2 describes:

1. the atomic number (zatom);
2. the ionic charge (zion, number of valence electrons);
3. the date of pseudopotential generation.

The two first information are crucial, the third one is not really important. The atomic number is 1 for Hydrogen, 8 for Oxygen, and so on. The ionic charge should be the same number as the second number mentioned in the data table (described as 'Zion' in section VI of the paper)

Line 3 describes:

1. the format of the pseudopotential (pspcod ; must be 3 for this format);
2. the XC functional used to generate the pseudopotential (pspxc ; here, must be 1)
3. the maximal angular momentum of the wavefunctions described

in the pseudopotential file

```
lmax=0 if purely local pseudopotential: H, He, Lisc, Besc ;
lmax=1 for s and p projectors : Li, B ... Ar, Ksc, Au ;
lmax=2 for s, p and d projectors : K, Ca, ... Cs, Ba, Hfsc ...
Ptsc, Ausc ... Rn ;
lmax=3 for s, p, d and f projectors : Cssc, Basc, Lasc ... Lusc
- lloc has no meaning, and is set to 0
- mmax has no meaning, and is set to 2001
- the last number can be set to 0 .
```

The lines that follow these three lines are generated from the data in the table, though the name of the element and Zion are not reproduced. Note also that each line has to be completed with zeroes, to give the format presented at the beginning of the section VI of the HGH paper : five columns for the first of these lines, then 4 columns for each projector, and 3 columns for the spin-orbit splitting. For readability, the meaning of each number has also been added in our example pseudopotential file (for example, 'rloc, c1, c2, c3, c4') but these are NOT read by ABINIT. Thus, unlike the zeroes, it is not important to add them to the data from the table.

Inside ABINIT, the pseudopotential with format 1 will be treated by the routine psp2in.f, that calls psp2lo.f (local part) and psp2nl.f (non-local part).

As a matter of numerical accuracy, note that the integral of $(V@+Zion/r) r^2$ in psp2lo.f is performed analytically without cut-off.

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