HOWTO generate the same PAW atomic data with USPP and AtomPAW

Example on Iron

Keywords in **bold** *<u>do not</u> have to be changed for a comparison with AtomPAW*

fe_ae_d7s1.adat USPP file

```
1  0  0  0  3                ifae,ifpsp,ifprt,ifplw,ilogd
2.0 -5.0 5.0  200             rlogd,emin,emax,nnt
1.0d-10 1.0d-09 0.2  0        thresh,tol,damp,maxit
iron                          title
26.0  0.00  5.0               z,xion,exfact
200.0  5.11  165.45           rmax,aasf,bbsf
8    2                        ncspvs,irel
100  2.000  -515.0            nnlz,wwnl,ee
200  2.000   -60.5            nnlz,wwnl,ee
210  6.000   -51.5            nnlz,wwnl,ee
300  2.000    -7.0            nnlz,wwnl,ee
310  6.000    -4.5            nnlz,wwnl,ee
320  7.000    -1.0            nnlz,wwnl,ee
400  1.000    -0.5            nnlz,wwnl,ee
410  0.000    -0.2            nnlz,wwnl,ee
```

- r_{PAW}
- $1+l_{max}$
- Z
- *These are hidden values in AtomPAW*
- r_{max}
- 0 for LDA-PW, 5 for GGA-PBE
- Total nb of states
- $1/(r_0.Z)$
- 0 for nonrelativistic, 2 for scalarrelativistic
- $-\ln(r_0.Z)$
- Electronic configuration
- *Where r_0 is printed in AtomPAW output file*

fe_ps.adat USPP file

```
0  2  1  1  3                 ifae,ifpsp,ifprt,ifplw,ilogd
2.0 -5.0 5.0  200             rlogd,emin,emax,nnt
1.0d-10 1.0d-09 0.2  0        thresh,tol,damp,maxit
iron                          title
3    5    3                   ncores,nvales,nang
10.0  20.0  40.0  10.0        besrmax,besemin,besemax,besde
3  1  2.0  1.95               keyps,ifpcor,rinner,rpcore
6  1.9                        nbeta,rcloc
2.0  2.0  2.0                 rc

0  1  0.0  2                  lll,keyee,eeread,iptype
0  4  0.0  2                  lll,keyee,eeread,iptype
1  2  0.0  2                  lll,keyee,eeread,iptype
1  5  0.0  2                  lll,keyee,eeread,iptype
2  3  0.0  2                  lll,keyee,eeread,iptype
2  0  2.0  2                  lll,keyee,eeread,iptype
8  10.0                       npf,ptryc
3  0  0.0  1                  lloc,keyee,eloc,iploctype
3  8  10.0                    ifqopt,nqf,qtryc
```

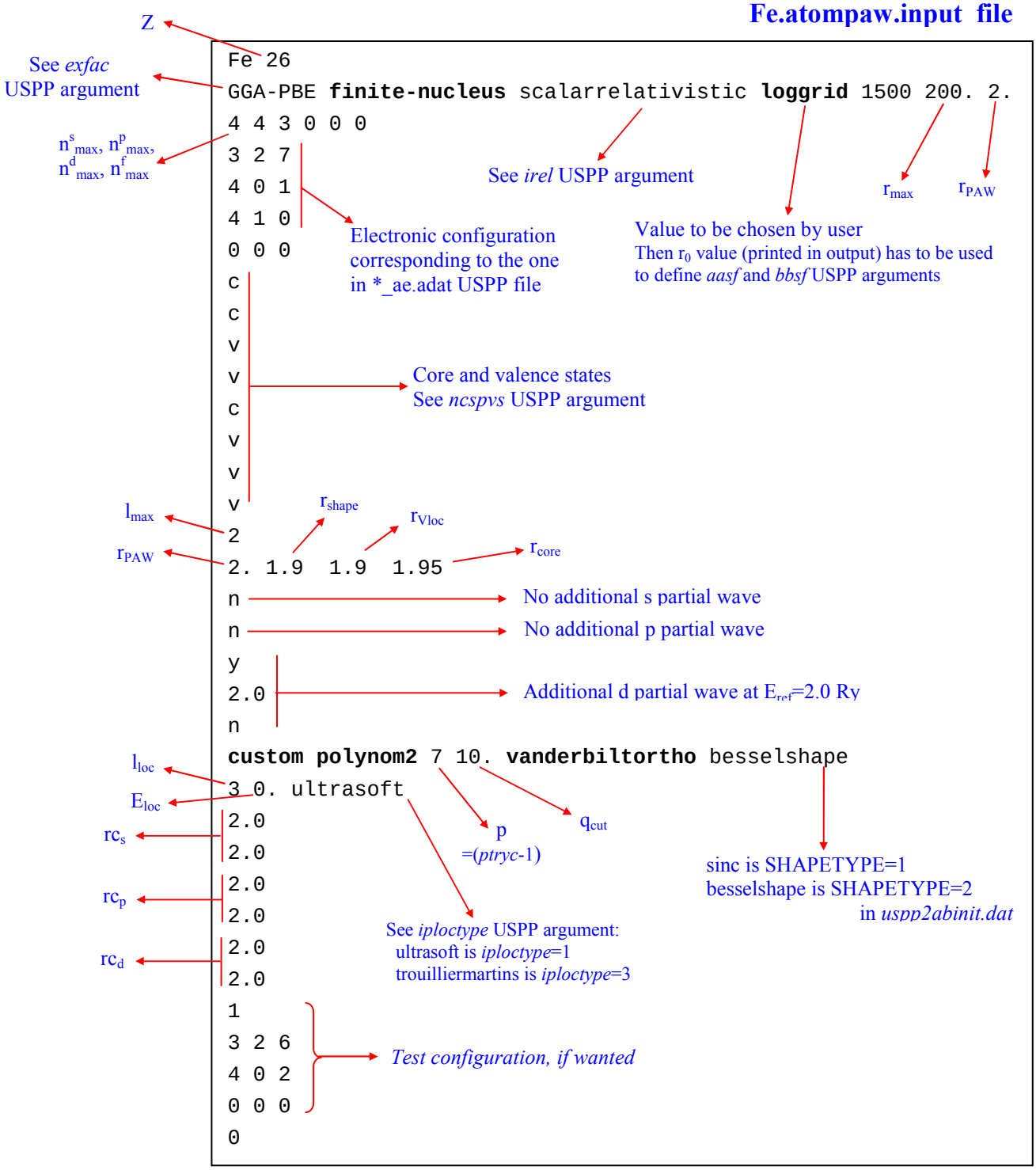
- r_{PAW}
- $1+l_{max}$
- Nb of core states *(nb of "c" in AtomPAW)*
- Nb of valence states *(nb of "v" in AtomPAW)*
- $1+l_{max}$
- r_{core}
- rc_s, rc_p, rc_d, rc_f
- r_{Vloc}
- Total number of partial waves = Nb of valence states + Nb of additional partial waves
- First s partial wave (valence state #1)
- 2nd s partial wave (valence state #4)
- First p partial wave (valence state #2)
- 2nd p partial wave (valence state #5)
- First d partial wave (valence state #3)
- 2nd d partial wave (additional) at E_{ref}=2.0 Ry
- 1+p
- q_{cut}
- 1 for ultrasoft, 3 for trouilliermartins
- l_{loc}
- E_{loc}
- Change only if necessary !

Uspp2abinit.dat USPP

```
SHAPETYPE= 2
RCOMPFACT= 0.95
OPT_TCORE=1
USE_XC_NHAT=0
ECUT_RSO=  10.
WERROR_RSO= 0.0005
GAMMAFACT_RSO= 2.
```

- 1 for sinc, 2 for besselshape
- RCOMPFACT= r_{shape}/r_{PAW}
- Mandatory for the comparison with AtomPAW
- This is asked by AtomPAW2Abinit (*include compensation in XC or not ?*)
- Real Space Optimization: Same values as those asked by AtomPAW2Abinit (Comment for no real space optimization)

Fe.atompaw.input file




```
Fe 26
GGA-PBE finite-nucleus scalarrelativistic loggrid 1500 200. 2.
4 4 3 0 0 0
3 2 7
4 0 1
4 1 0
0 0 0
c
c
v
v
c
v
v
v
2
2. 1.9  1.9  1.95
n
n
y
2.0
n
custom polynom2 7 10. vanderbiltortho besselshape
3 0. ultrasoft
2.0
2.0
2.0
2.0
2.0
2.0
1
3 2 6
4 0 2
0 0 0
0
```

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