Test Report on Electron Localization Function (ELF) Implementation in Norm-Conserving Plane-Waves Formalism.

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Chapter 1

Test on an isolated H atom.

We use the Fermi-Amaldi exchange-correlation functional ($ixc = 20$) and no spin polarization (not available with this functional).
For single H atom we have the wavefunction which is $1s$ atomic orbital. For analytical approach[1] we thus use the spherical harmonic formulation which is given by:

$$\psi = \varphi_{1s}(r,\theta,\phi) = \sqrt{\frac{Z^3}{\pi a_0^3}} e^{-Z\frac{|\mathbf{r}|}{a_0}} \tag{1.1}$$

with Z the atomic number and a_0 the Bohr constant.
We obtain for H atom ($Z = 1$):

- the electronic density

$$n(\mathbf{r}) = |\psi|^2 = |\varphi_{1s}(r,\theta,\phi)|^2 = \frac{1}{\pi a_0^3} e^{-\frac{2|\mathbf{r}|}{a_0}} \tag{1.2}$$

- the kinetic energy density

$$\tau(\mathbf{r}) = \frac{1}{2}|\nabla\psi|^2 = \frac{1}{2}|\nabla\varphi_{1s}(r,\theta,\phi)|^2 = \frac{1}{2\pi a_0^5} e^{-\frac{2|\mathbf{r}|}{a_0}} \tag{1.3}$$

- the square norm of the gradient of the electronic density

$$|\nabla n(\mathbf{r})|^2 = \left|\nabla|\psi|^2\right|^2 = \left|\nabla|\varphi_{1s}(r,\theta,\phi)|^2\right|^2 = \left|\frac{-2}{\pi a_0^4} e^{-\frac{2|\mathbf{r}|}{a_0}}\right|^2 = \frac{4}{\pi^2 a_0^8} e^{-\frac{4|\mathbf{r}|}{a_0}} \tag{1.4}$$

[1] For theoritical and implementation details see chap. 3 in /doc/theory/ELF/

- the Weizsäcker kinetic energy density

$$\frac{1}{8}\frac{|\nabla n(\mathbf{r})|^2}{n(\mathbf{r})} = \frac{1}{8}\frac{\frac{4}{\pi^2 a_0^8}e^{-\frac{4|\mathbf{r}|}{a_0}}}{\frac{1}{\pi a_0^3}e^{-\frac{2|\mathbf{r}|}{a_0}}} = \frac{1}{2\pi a_0^5}e^{-\frac{2|\mathbf{r}|}{a_0}} \tag{1.5}$$

- the Thomas-Fermi kinetic energy density

$$\frac{3}{10}\left(3\pi^2\right)^{2/3} n^{5/3}(\mathbf{r}) = 2.871 \times \left(\frac{1}{\pi a_0^3}e^{-\frac{2|\mathbf{r}|}{a_0}}\right)^{5/3} \tag{1.6}$$

- the ELF

$$ELF(\mathbf{r}) = \frac{1}{1+\left(\frac{\tau(\mathbf{r})-\frac{1}{8}\frac{|\nabla n(\mathbf{r})|^2}{n(\mathbf{r})}}{2.871\times n^{5/3}(\mathbf{r})}\right)} = \frac{1}{1+\left(\frac{0}{2.871\times n^{5/3}(\mathbf{r})}\right)} = 1 \tag{1.7}$$

As we can see the ELF should be 1 everywhere for the single hydrogen atom because the kinetic energy density and the Weizsäcker kinetic energy density are equal in that case[2] (see Eq. **??** and **??**).

[2]the ELF is also equal to 1 everywhere for an isolated helium atom.

1.1 Standard test.

The standard input file used is the following:

```
acell 3*30
ecut 100
diemac 1.0d0
diemix 0.5d0
iscf 3
ixc 20
kpt 3*0.25
natom 1
nband 1
nkpt 1
nline 3
nsppol 1
nstep 6
nsym 8
ntypat 1
occ 1
rprim 100 010 001
symrel
1 0 0   0 1 0   0 0 1
-1 0 0   0 1 0   0 0 1
1 0 0   0-1 0   0 0 1
-1 0 0   0-1 0   0 0 1
1 0 0   0 1 0   0 0-1
-1 0 0   0 1 0   0 0-1
1 0 0   0-1 0   0 0-1
-1 0 0   0-1 0   0 0-1
tnons 24*0
tolwfr 1.0d-14
typat 1
wtk 1
znucl 1
xred 3*0
prtelf 1 #output a _ELF file.
```

We observe on the following pictures the result of ABINIT compared to previous analytical formula.
First the convergence with the acell parameter (Fig.(**??**)).

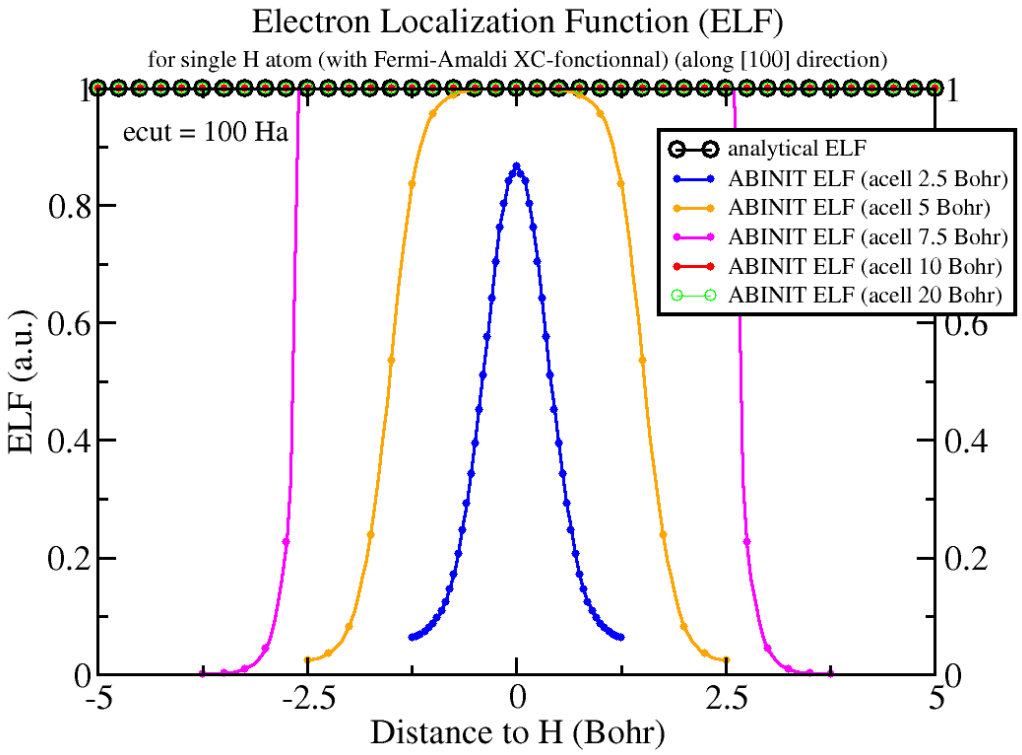

Figure 1.1: Comparison between analytical ELF and ABINIT ELF for an isolated H atom.

Then the convergence with ecut parameter (Fig.(**??**)). The thing is that the convergence of ELF seems to be more sensitive to the acell parameter than the ecut parameter, at least here for the hydrogen atom. For instance with only an ecut of 10 Ha but with a 10 Bohr box we already obtain 1 everywhere.

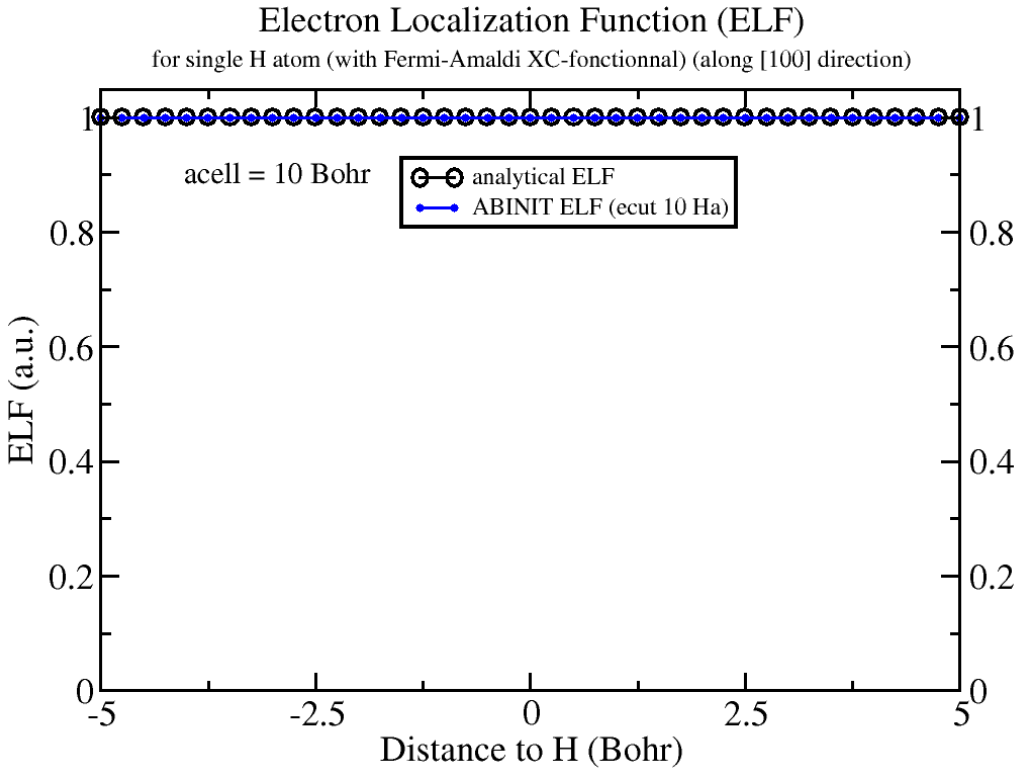

Figure 1.2: Comparison between analytical ELF and ABINIT ELF for an isolated H atom.

Chapter 2

Test on an isolated Li atom.

Since the hydrogen atom is a bit peculiar for test of ELF we have also performed a test with another isolated atom. We use here lithium (Li) because ELF which can be used to show up the shell structure of isolated atoms, is very simple fo Li. Actually for Li this is just a single s shell. We use for that an all electron calculation[1].

First with a bare pseudopotential (Fig.(**??**) and Fig.(**??**)):

Then with **fhi** pseudopotential (Fig.(**??**) and Fig.(**??**)):

[1] the pseudopotential used is 03li.pspfhi and also a by-hand constructed bare pseudopotential 03li.bare

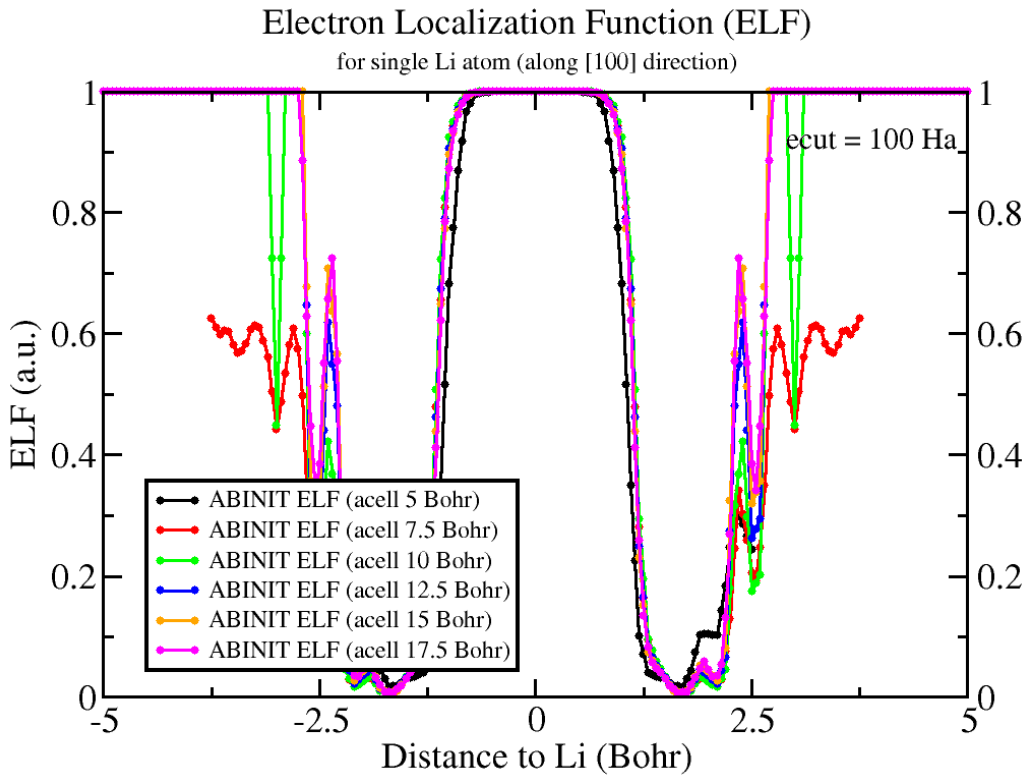

Figure 2.1: ABINIT *ELF* for an isolated Li atom with a bare pseudo.

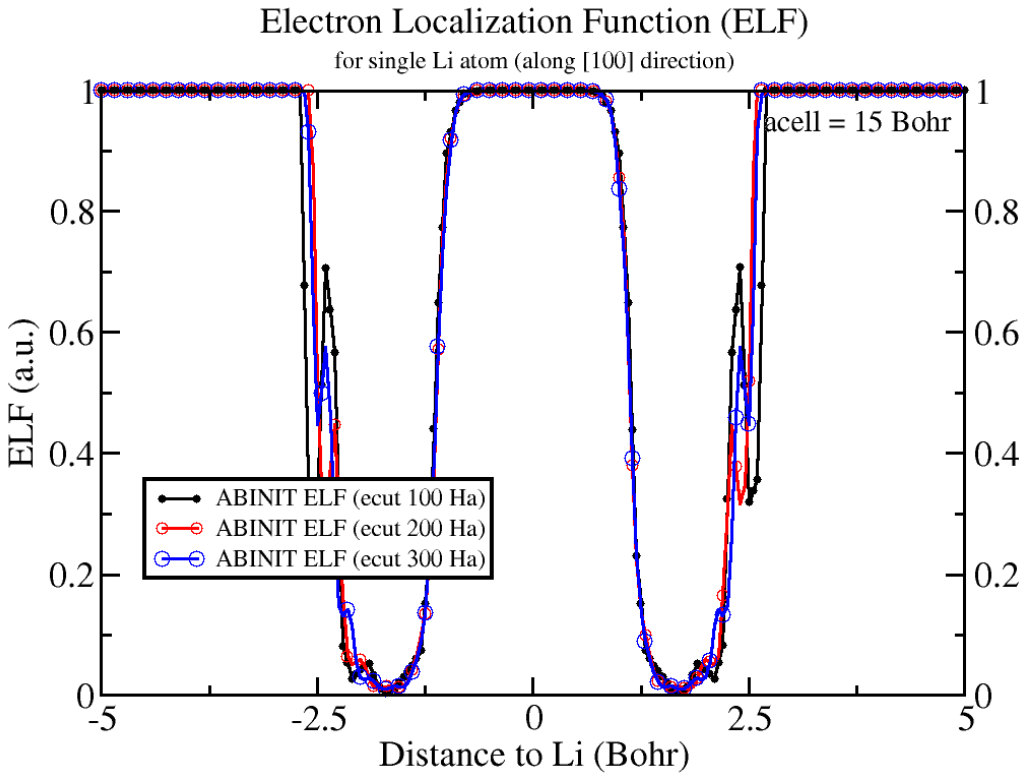

Figure 2.2: ABINIT *ELF* for an isolated Li atom with a bare pseudo.

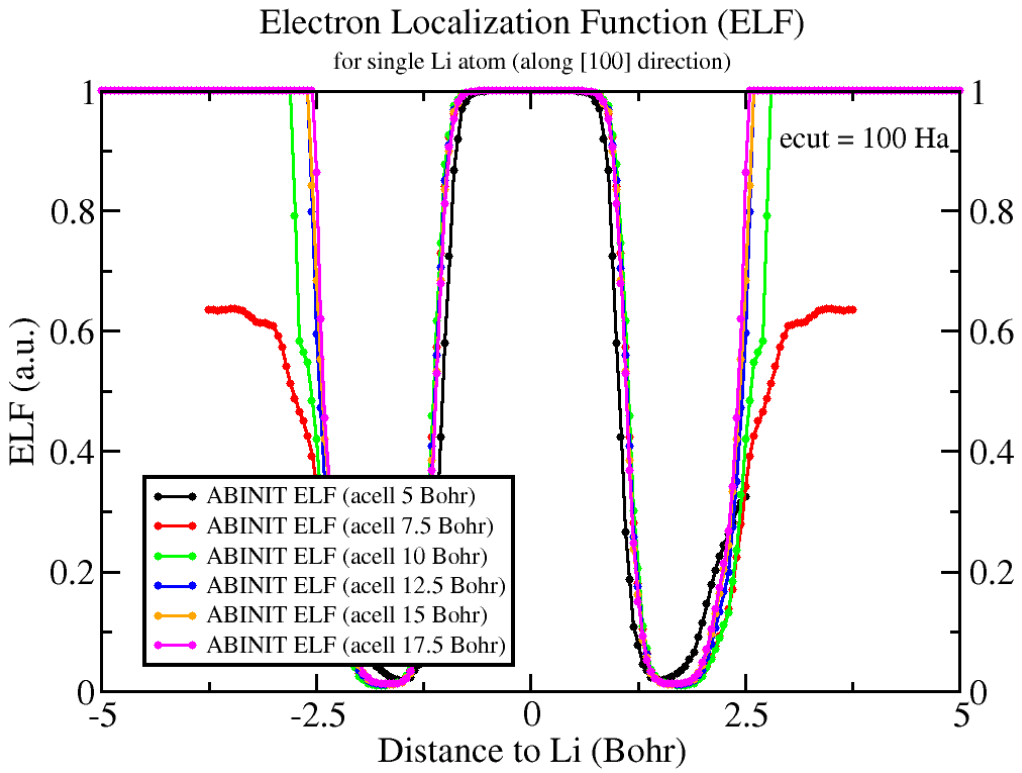

Figure 2.3: ABINIT *ELF* for an isolated Li atom with a **fhi** pseudo.

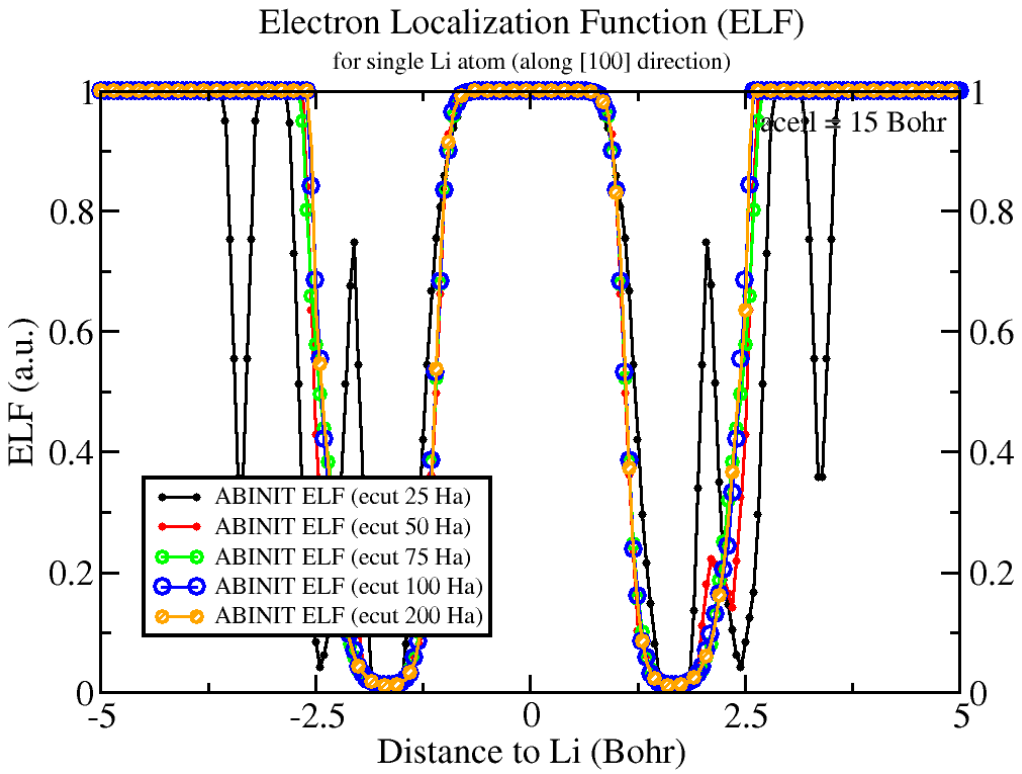

Figure 2.4: ABINIT *ELF* for an isolated Li atom with a **fhi** pseudo.