FPLO14.00-45

Getting Started

Manuel Richter & Klaus Koepernik
Oleg Janson & Helge Rosner

March 31, 2014
m.richter@ifw-dresden.de
janson@cpfs.mpg.de

In this little primer, you will be explained how to run FPLO14.00-45 on one of the simplest possible systems, *fcc* aluminum.

It is presumed that you have installed FPLO14.00-45 in a UNIX-derived environment. All necessary keystrokes are given, together with a short explanation. Moreover, screenshots are included every now and then. They should give you the doubtlessness that everything is correct when you go through the exercise on your own platform.

In the present example, we will hardly change the default input settings. Even the element and the lattice structure are pre-defined. Nonetheless, you should be reminded of our recommendation to include all changes of the default input settings and the version number in any publication of FPLO results. In many cases, this will only be the chemical composition, the lattice structure and the chosen lattice parameters. Such information is usually given in the publication anyway. You may also choose to work with another **k**-mesh or change the numerics. If you enter such information in your publication, everybody who has FPLO14.00-45 at hand will be able to repeat your calculation and convince himself of the result. This is what one may understand as a **reproducible computer experiment**.

Now, open a terminal at your computer and go ahead! What we learn in this getting started lesson is to calculate the density of states (DOS) and band structure, and finally how to evaluate the theoretical equilibrium volume.

Remark: ⟨CR⟩ stands for carriage return and simply corresponds to pressing the "Enter" key

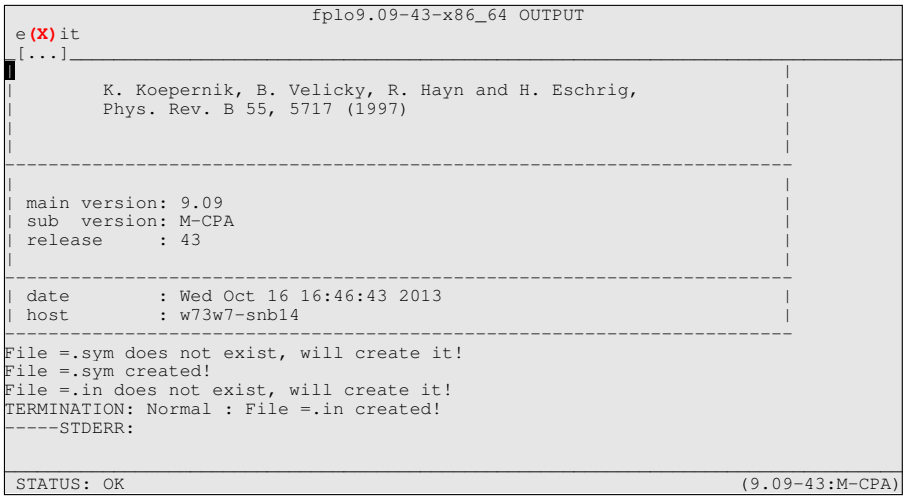
Key sequence	Explanation
`mkdir Al` ⟨CR⟩	create directory `Al`
`cd Al` ⟨CR⟩	change into directory `Al`

Well, everybody who is experienced in computers knows that a tidy organization of the directory tree will keep away (almost) all troubles! We start our course with a very straight calculation. Usually, for a new compound or for the evaluation of sensitive quantities one needs to start with some initial calculations. We run the calculation in a directory called "`SC`". Here, "`SC`" stands for self consistent.

Key sequence	Explanation
`mkdir SC` ⟨CR⟩	create directory `SC`
`cd SC` ⟨CR⟩	change into directory `SC`
`ls` ⟨CR⟩	list all files (directory is empty)
`fedit14.00-45-x86_64` ⟨CR⟩	call input editor

Remark: The coexistence of different computer architectures makes it necessary to build individual executables for each architecture. This in turn requires a naming convention to tell the executables apart.

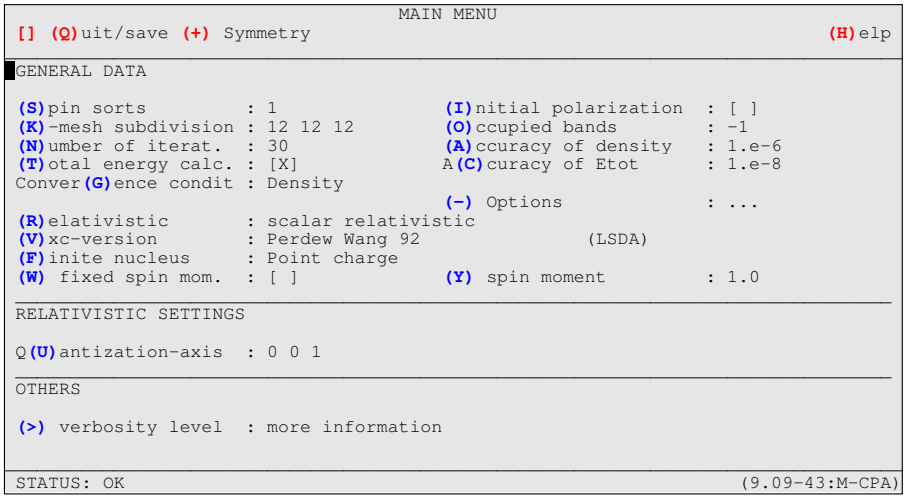
The actual executable of FPLO14.00-45 will then have a suffix, which in the version used for this manual results in the executable name `fplo14.00-45-x86_64`. The same holds for other executables like `fedit14.00-45-x86_64`.[1].



The input editor, `fedit14.00-45-x86_64`, has called, upon invoking, the executable `fplo14.00-45-x86_64`. Several default input files have automatically been created by the code. (To avoid mistakes if various versions are installed, the version number is written in the lower right corner. [2])

Key sequence	Explanation
x	exit initialization information

This brings us to the main input menu:

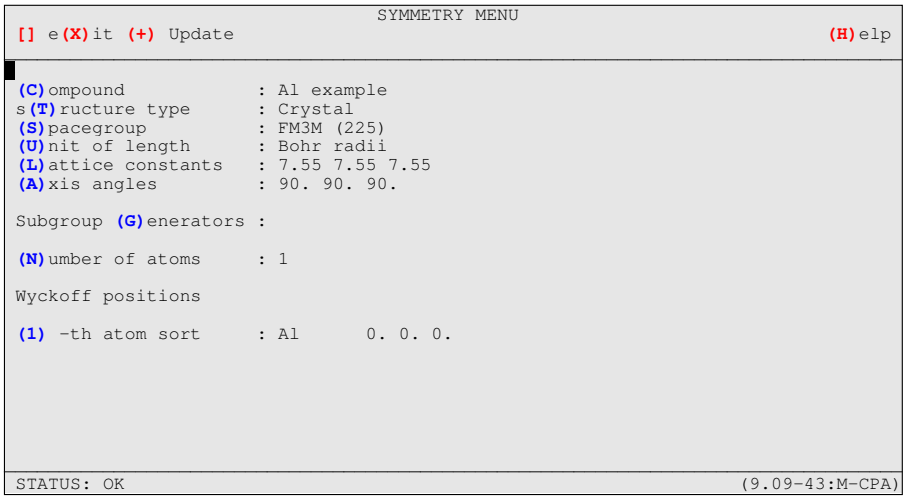


[1] In older FPLO versions symbolic links with the generic names `fplo` and `fedit` were generated. In order to avoid confusion with an increasing number of code updates, this practice has been discontinued. From now on only the full names are used.

[2] The version number consists of the main version (14.00 in our case), followed by a minus and the release number (45). The string after the colon is a subversion, which is important for developers only.

The input editor is operated by hot-keys (not case sensitive), indicated in red or blue on the screen. The blue keys are used for selecting entries of the present menu. The red keys (in our case the '+') select another menu or exit the input editor. Typing 'h' opens a help screen. Note, that keys of the right-hand (numerical) part of some keyboards do not work. Use only the keys of the central (main) part.

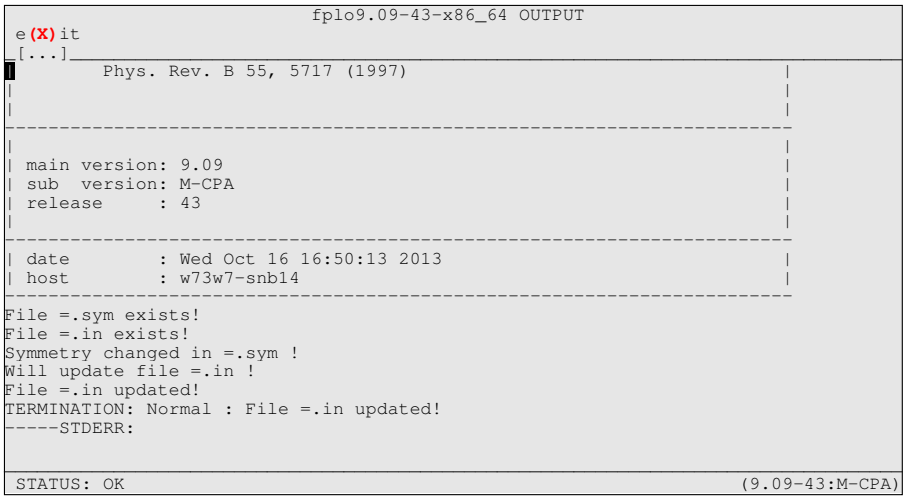
Key sequence	Explanation
+	select symmetry menu



The lattice structure and chemical composition have to be defined in every calculation. Looking at the screen, we find that everything is already fine for our example, aluminum. The space group is correctly 225, the lattice parameter is reasonable (7.55 Bohr radii), and the only atom of the elementary cell is in the position (0,0,0).

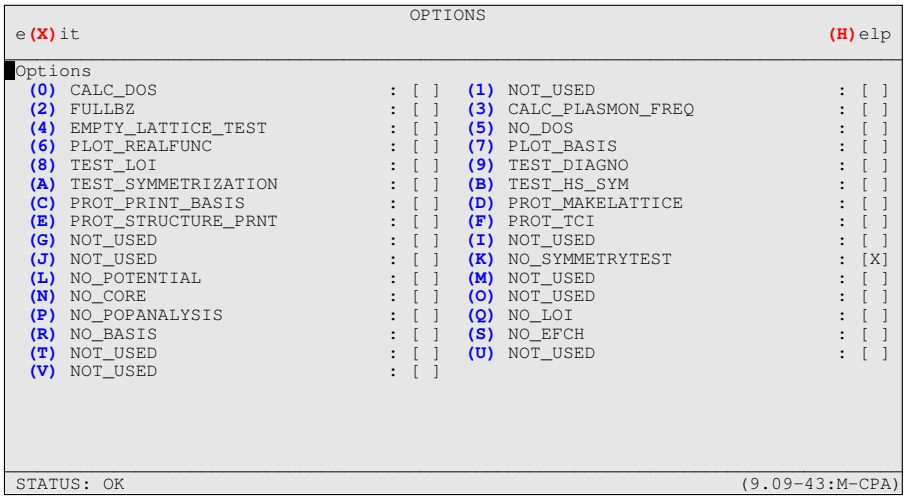
Whenever you have changed any detail in the symmetry menu, you need to update the structure (using the '+' sign again). If you forget this action, a warning message will remind you to do it. For training purposes, we will carry out the update now, even though we have not changed anything.

Key sequence	Explanation
+	update crystal structure



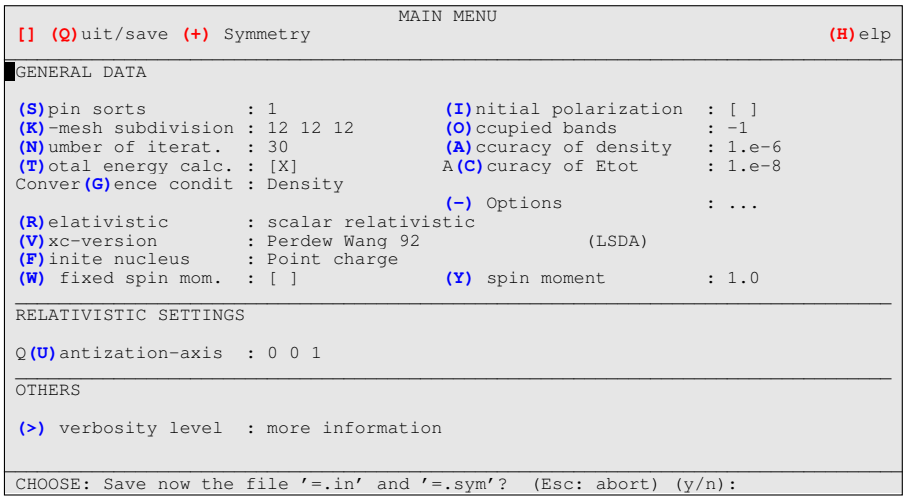
The editor invokes `fplo14.00-45-x86_64`, and the code updates the input files. The `fplo14.00-45-x86_64` output is printed on the screen. (You can scroll all screens which are only partially displayed using control and cursor keys as explained in the help screen of the main menu.) We leave this information screen by typing 'x' and proceed further to the main menu. This menu is already known to us (second screenshot).

Key sequence	Explanation
x	exit update information
x	exit symmetry menu
–	select options menu



There are many options available, and only a few will be used by the routine user. Only one of them is switched on by default, namely the symmetry test is skipped. We do not make any changes and proceed.

Key sequence	Explanation
x	exit options menu
q	quit input editor and save input files



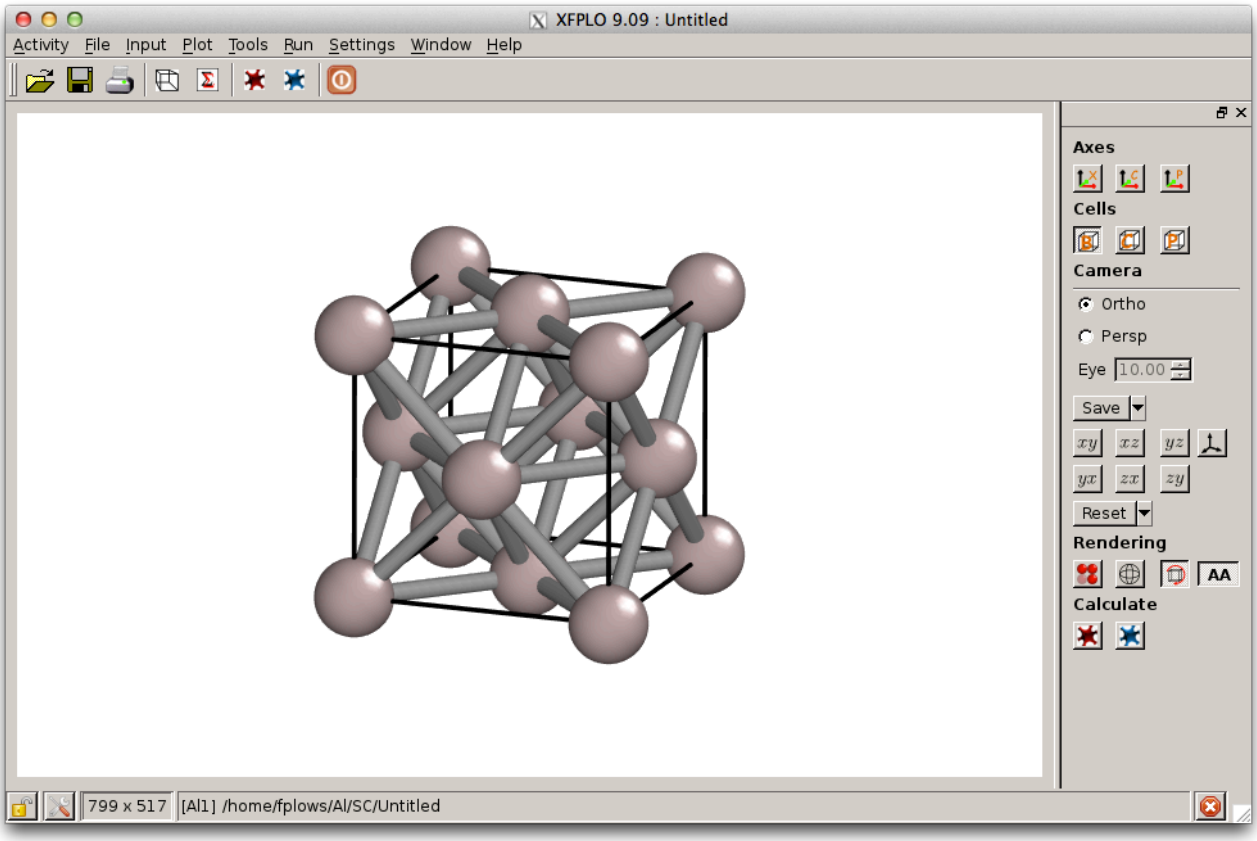
Now, we are done with the input preparation. Well, there were no changes of the default settings. In fact, we only had a look at the menus, which contain the data most often altered in practical applications. (Reminder: If you would publish the results of a calculation, you are recommended to tell all essential changes of the default values like **k**-mesh, xc-version, etc.)

Key sequence	Explanation
`y`	confirm saving
`ls` ⟨CR⟩	list all created files

This is how your terminal may look like now:

```
fplows@w73w7-snb14:~$ mkdir Al
fplows@w73w7-snb14:~$ cd Al/
fplows@w73w7-snb14:~/Al$ mkdir SC
fplows@w73w7-snb14:~/Al$ cd SC/
fplows@w73w7-snb14:~/Al/SC$ ls
fplows@w73w7-snb14:~/Al/SC$ fedit9.09-43-x86_64
FEDIT Version 9.09:M-CPA Release 43 Platform -x86_64
Program       fplo9.09-43-x86_64

Will create directory '/home/fplows/Al/SC/+tmp'.
Directory '/home/fplows/Al/SC/+tmp' created.


fplows@w73w7-snb14:~/Al/SC$ ls
+fedit  +fedithelp  +symminfo  +tmp  =.in  =.in.bak  =.str_template  =.sym
=.sym.bak
fplows@w73w7-snb14:~/Al/SC$
```

Key sequence	Explanation
`fplo14.00-45-x86_64 > out` ⟨CR⟩	run `fplo14.00-45-x86_64` and save output **wait till finished (on modern machines a few seconds)**
`ls` ⟨CR⟩	list all created files
`xfplo =.in` ⟨CR⟩	look at the crystal structure using `xfplo`



Key sequence	Explanation
⟨Crtl⟩ + w (on the xfplo screen)	quit xfplo

Key sequence	Explanation
view out ⟨CR⟩	inspect output file
?Population ⟨CR⟩	search last population analysis (What we really do here is to search for the population analysis from the end of the output. Another viewer will have a different hotkey for this)

```
------------------------------------------------------------------------
                          Population Analysis
                    (valence electron numbers)

      El Site                                                    SUM       Excess electrons
                  2s        2p        3s        4s        3p        4p        3d
N_net  Al   1    2.00299   6.01070   1.00634   0.00200   0.67697   0.00309   0.04126   9.74335
N_gros Al   1    1.99994   6.00076   1.21254  -0.01842   1.55011  -0.04580   0.30087  11.00000   0.00000


total net   electron number:                                      9.74335
total gross electron number:                                     11.00000   0.00000


------------------------------------------------------------------------
```

This is the final population analysis. The 3*d* orbitals contribute almost exclusively to the overlap population (difference between gross and net). This behavior is typical for polarization states. To check the validity of a calculation, one should always look at the population analysis. As a rule of thumb, the gross population should be larger or not much smaller than the net population. Furthermore, the net population should not

be negative. For semi core states (i.e. filled shells that are included in the valence basis) the full electron number (s: 2, p: 6, d: 10, f: 14) should come out within a range of a few hundreds of electrons for both gross and net population. (For very heavy atoms the deviation from the integer occupation can be of the order of a few tens of electrons.) In spin polarized calculations there will be four lines per atom. The first two (marked `N_`) are the populations and the second two (marked `M_`) are the magnetic moments of the orbitals.

Key sequence	Explanation
`:q` ⟨CR⟩	quit inspection of output file
`grep "last deviation" out` ⟨CR⟩	check iteration
or shorter: `grep "st de" out` ⟨CR⟩	

```
fplows@w73w7-snb14:~/Al/SC$ grep "st de" out
SCF: iteration  0  dimension  0  last deviation u=  0.00E+00
SCF: iteration  1  dimension  1  last deviation u=  0.11E+00
SCF: iteration  2  dimension  1  last deviation u=  0.10E+00
SCF: iteration  3  dimension  2  last deviation u=  0.14E-01
SCF: iteration  4  dimension  1  last deviation u=  0.99E-02
SCF: iteration  5  dimension  2  last deviation u=  0.19E-03
SCF: iteration  6  dimension  1  last deviation u=  0.11E-03
SCF: iteration  7  dimension  2  last deviation u=  0.12E-04
SCF: iteration  8  dimension  3  last deviation u=  0.78E-05
SCF: iteration  9  dimension  1  last deviation u=  0.15E-05
SCF: iteration 10  dimension  1  last deviation u=  0.46E-08 CONVERGED
fplows@w73w7-snb14:~/Al/SC$
```

Each line shows the information about the iteration progress of one SCF cycle. The real number u to the right is a measure for the convergence of the calculation. The standard criterion to consider a calculation to be converged is if u falls below a certain threshold (default 10^{-6}). However, there are further things to be checked. The values of total energy (of the last step!) can be output using the script `grEE`:

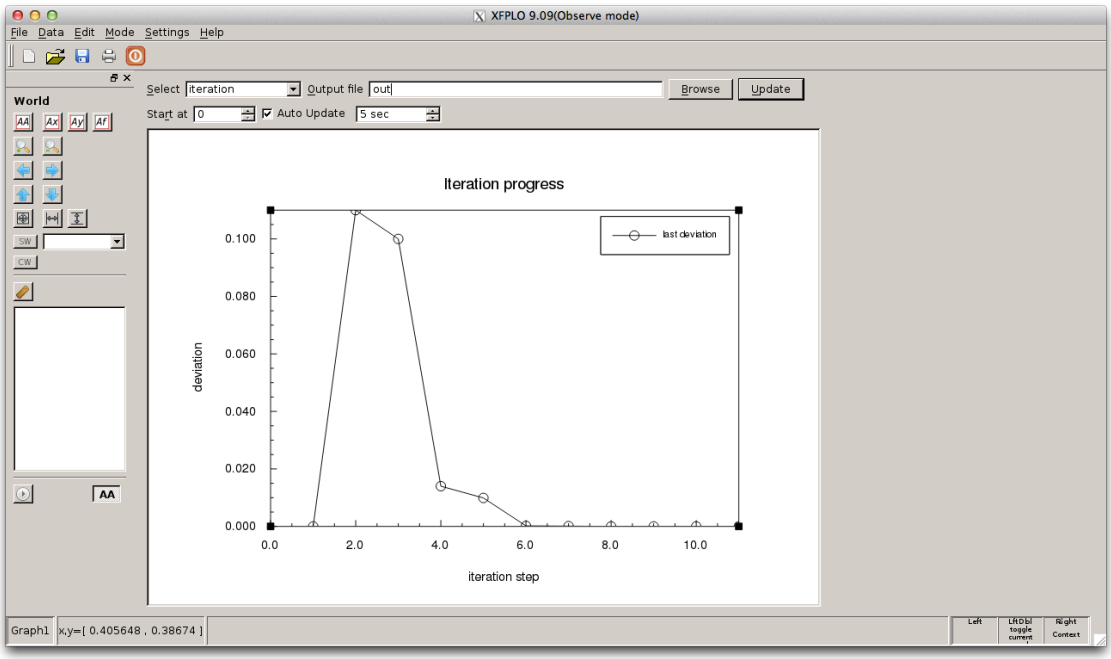
Key sequence	Explanation
`grEE` ⟨CR⟩	print total energy values

```
fplows@w73w7-snb14:~/Al/SC$ grEE
 -241.9194604174 242.17167366 -466.38219031 -17.70894377
fplows@w73w7-snb14:~/Al/SC$
```

The first value is the total energy followed by the kinetic energy, the Coulomb energy and the xc-energy. If DFT+U is used a column with the additional DFT+U energy contribution is added at the end.

You can visualize the data by calling the `xfbp` program.

Key sequence	Explanation
`xfbp` ⟨CR⟩	start `xfbp`
menu “Mode” ⟶ “Observe” ⟶ “Iteration progress”	show the iteration progress



The evolution of the total energy values with the number of iterations is displayed.

Key sequence	Explanation
⟨Crtl⟩ + q (on the xfbp screen)	quit xfbp

Key sequence	Explanation
fedit14.00-45-x86_64 ⟨CR⟩	call input editor
<SPACE>	select more menus (if the (red) symbol [] is shown in the upper menu, then there are further submenus accessible in this way)
b	select bandplot menu

The bandplot menu allows you to define a band structure calculation on symmetry lines. The DOS is provided as well. The latter can also be obtained by switching on the appropriate option in the option menu.

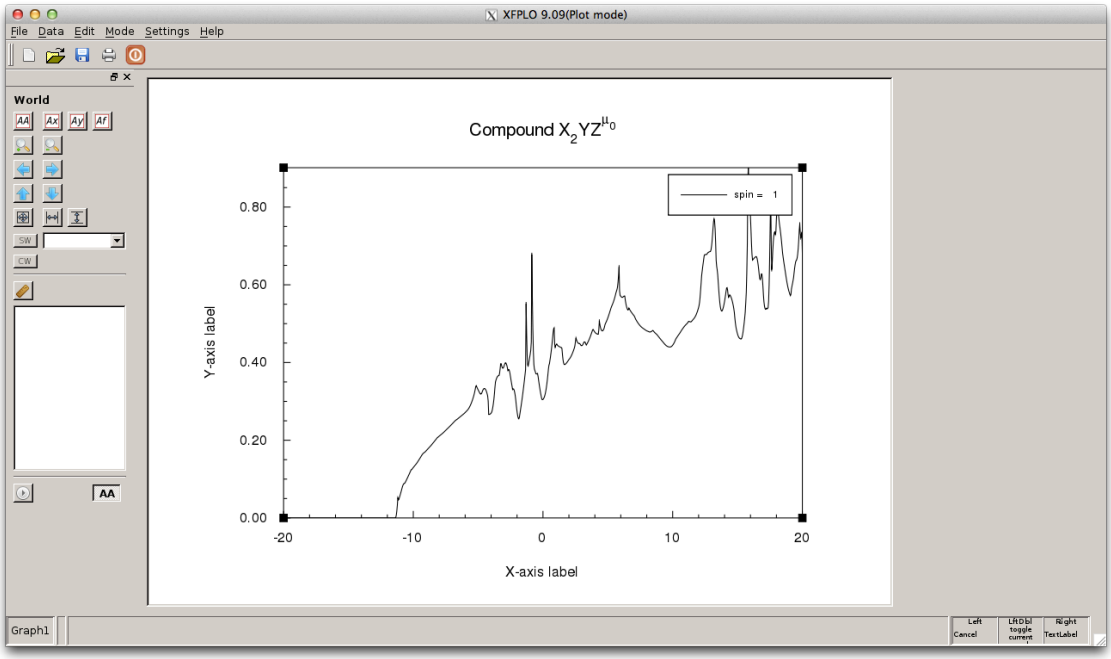
```
                                    BANDPLOT
e(X)it                                                                  (H)elp
 (B)andstructure plot        : [ ]
 (R)ead sym-points           : [X]
 (S)teps between sym-points  : 50
 DOS/AKBL/BANDS

 Number of e(-)pts (non-CPA) : 1000              (P)lot IDOS      : [ ]
                                                 plot n(E)t DOS   : [ ]

 (L)ower energy bound [eV] relative to E_f : -20.0
 (U)pper energy bound [eV] relative to E_f : 20.0

 Restr(I)ct bands to window  : [ ]

 Local (D)OS sites    :

 FREL pro(J)ection    : jmu
 BAND WEIGHTS/FAT BANDS

 Weights def (F)ile          :

 (W)eights                   : [ ]
 (T)ransform quant. axis     : [ ]
 X-(A)xis                    : 1.0 0.0 0.0
 (Z)-axis                    : 0.0 0.0 1.0


 (N)umber of sym-points      : 9
 No.    Label                 k-point

 (1)    : $~G                 : 0 0 0
 (2)    : X                   : 1 0 0
 (3)    : W                   : 1 1/2 0
 (4)    : K                   : 3/4 3/4 0
 (5)    : $~G                 : 0 0 0
 (6)    : L                   : 1/2 1/2 1/2
 (7)    : W                   : 1 1/2 0
 (8)    : U                   : 1 1/4 1/4
 (9)    : X                   : 1 0 0
STATUS: OK                                                  (9.09-43:M-CPA)
```

Key sequence	Explanation
`b`	select band structure plot
`x`	exit bandplot menu
`q`	quit input editor and save input files
`y`	confirm saving
`fplo14.00-45-x86_64 > out.bs &` ⟨CR⟩	run `fplo14.00-45-x86_64` in background **wait for finishing (few seconds)**
`ls` ⟨CR⟩	list all files

```
fplows@w73w7-snb14:~/Al/SC$ fedit9.09-43-x86_64
FEDIT Version 9.09:M-CPA Release 43 Platform -x86_64
Program       fplo9.09-43-x86_64

Temporary directory '/home/fplows/Al/SC/+tmp' exists.


fplows@w73w7-snb14:~/Al/SC$ fplo9.09-43-x86_64 > out.bs &
[1] 3641
fplows@w73w7-snb14:~/Al/SC$
[1]+  Done                    fplo9.09-43-x86_64 > out.bs
fplows@w73w7-snb14:~/Al/SC$ ls
+band               +dos.sort001.nl004  +dos.total.l001  +fedit      +symminfo  =.str_template  out.bs
+dos.sort001        +dos.sort001.nl005  +dos.total.l002  +fedithelp  +tmp       =.sym           primitive.ps
+dos.sort001.nl001  +dos.sort001.nl006  +dos.total.l003  +points     =.dens     =.sym.bak
+dos.sort001.nl002  +dos.sort001.nl007  +dos.total.l004  +run        =.in       bravais.ps
+dos.sort001.nl003  +dos.total          +dos.total.l005  +symmetry   =.in.bak   out
fplows@w73w7-snb14:~/Al/SC$
```

The number of created files is already considerable. The DOS is given in sort- (Wyckoff position) (`+dos...sort001...`) and basis-state projection (`+dos...nl001` etc.) We have a look at the total DOS:

Key sequence	Explanation
`xfbp +dos.total` ⟨CR⟩	display total DOS



Key sequence	Explanation
⟨Crtl⟩ + `q` (on the `xfbp` screen)	quit `xfbp`

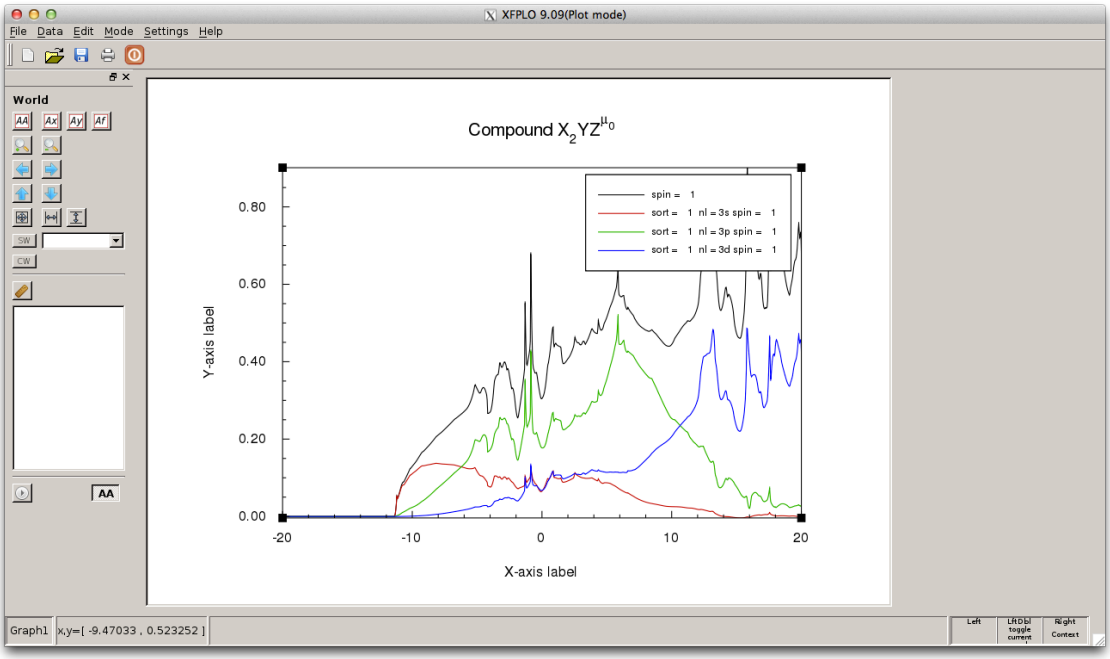
In many cases, the partial density of states is a subject of interest: one can see which states contribute to the total density of states at a certain energy. The partial (Wyckoff/sort averaged) DOS is stored in the `+dos.sort00...nl00...` files. The first line of each file contains the information about the basis state:

Key sequence	Explanation
`head -n 1 +dos.sort001.nl00[1-7]` ⟨CR⟩	print the first lines of the partial DOS files

```
fplows@w73w7-snb14:~/Al/SC$ head -n 1 +dos.sort001.nl00[1-7]
==> +dos.sort001.nl001 <==
# sort =    1  nl = 2s spin =    1

==> +dos.sort001.nl002 <==
# sort =    1  nl = 2p spin =    1

==> +dos.sort001.nl003 <==
# sort =    1  nl = 3s spin =    1

==> +dos.sort001.nl004 <==
# sort =    1  nl = 4s spin =    1

==> +dos.sort001.nl005 <==
# sort =    1  nl = 3p spin =    1

==> +dos.sort001.nl006 <==
# sort =    1  nl = 4p spin =    1

==> +dos.sort001.nl007 <==
# sort =    1  nl = 3d spin =    1
fplows@w73w7-snb14:~/Al/SC$
```

Let's print the partial DOS for 3*s*, 3*p* and 3*d* orbitals together with the total DOS:

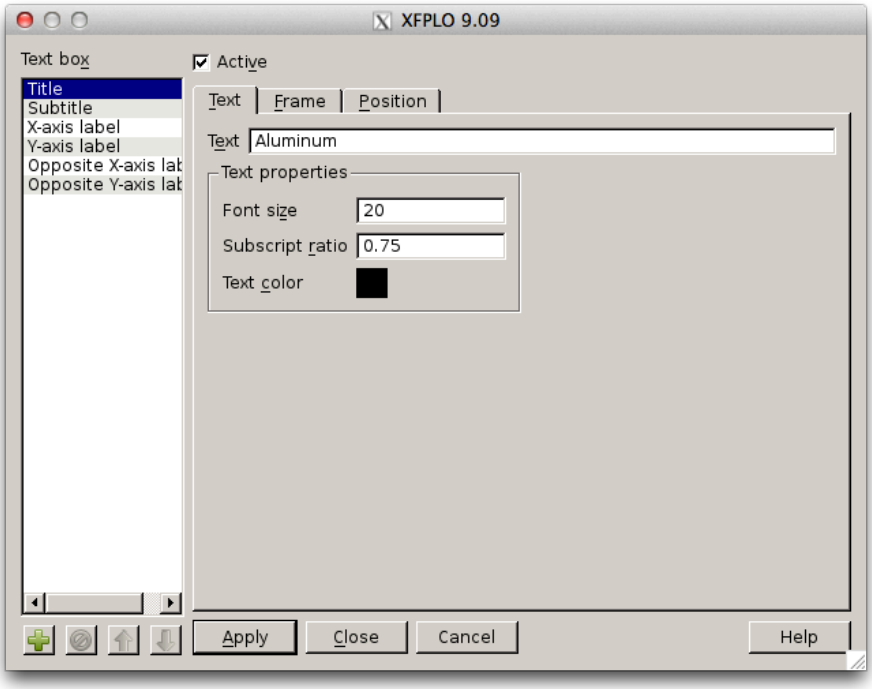
Key sequence	Explanation
`xfbp +dos.total +dos.sort001.nl00[3,5,7]` ⟨CR⟩	display total and partial DOS



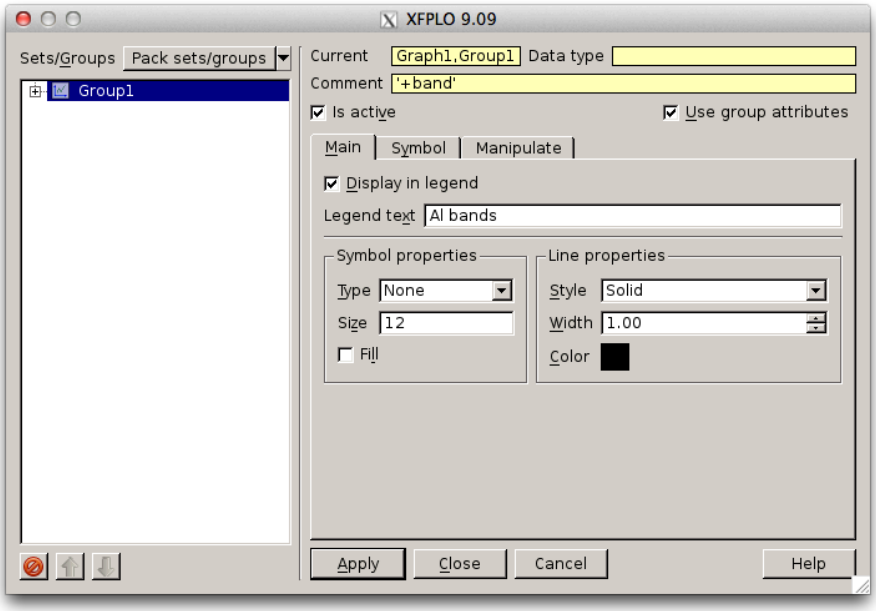
The 3*s* states are lowest in energy, and at Fermi level 3*p* states dominate, while 3*s* and 3*d* have almost the same contribution to the total DOS.

Now we are going to plot the band structure using the same tool, `xfbp`.

Key sequence	Explanation
`xfbp +band`	open the band structure file
right-click on the title ⟶ “properties”	show title properties
change the content of the `Text` field to “Aluminum”	modify the title

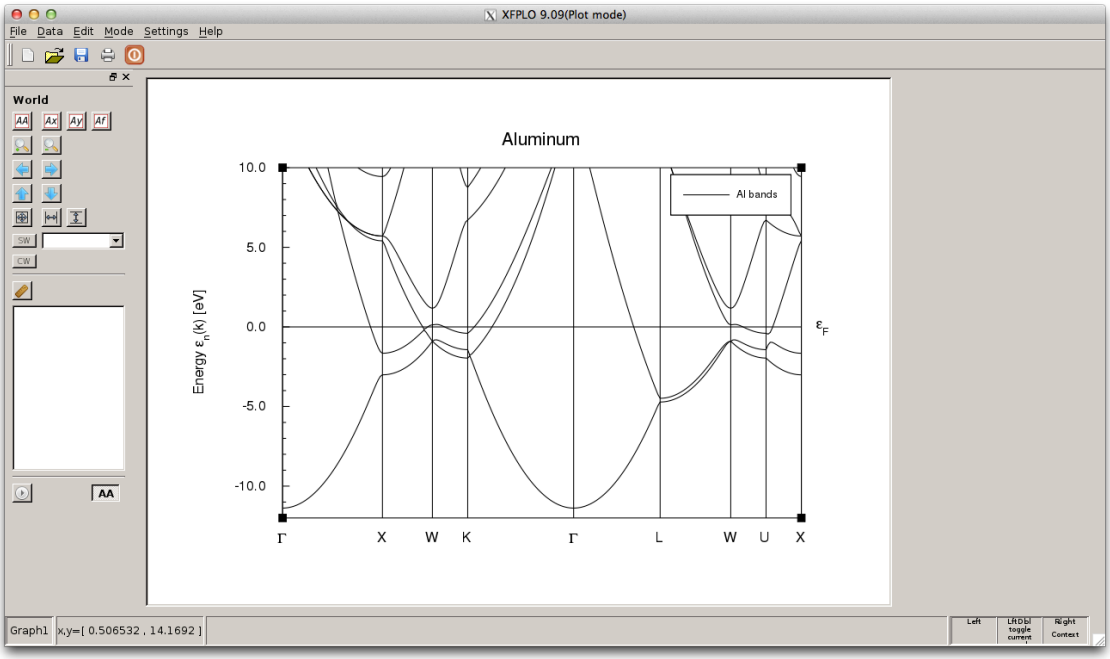


Key sequence	Explanation
click the “Apply” button	apply changes
click the “Close” button	close the dialog
right-click on one of the bands ⟶ “group”	open group properties
change the content of the `Legend text` field to “Al bands”	modify the legend text



Key sequence	Explanation
click the "Apply" button	apply changes
click the "Close" button	close the dialog

Your screen should look like this:



What you see is valence bands of Al. You can change the energy window by clicking the menu "Edit" $\longrightarrow$ "World" $\longrightarrow$ "Properties", and modifying "Min" and "Max" fields, but lets continue for now.

Key sequence	Explanation
⟨`Crtl`⟩ + `q` (on the `xfbp` screen)	quit `xfbp`

We now proceed to the final goal, the calculation of the total energy in dependence of the lattice parameter.

Key sequence	Explanation
`cd ..`	goto parent directory "`Al`"
`mkdir a0=7.55` ⟨CR⟩	create directory for present a_0
`cp SC/* a0=7.55` ⟨CR⟩	copy all files into `a0=7.55`
`mkdir a0=7.50` ⟨CR⟩	create directory for another a_0
`mkdir a0=7.60` ⟨CR⟩	create directory for another a_0
`ls` ⟨CR⟩	just to look
`cp a0=7.55/=* a0=7.50` ⟨CR⟩	copy input files into the new directory
`cp a0=7.55/=* a0=7.60` ⟨CR⟩	copy input files into the new directory
`cd a0=7.50` ⟨CR⟩	change into directory `a0=7.50`
`fedit14.00-45-x86_64` ⟨CR⟩	call `fedit14.00-45-x86_64`
+	select symmetry menu
`L7.50 , ,` ⟨CR⟩	change lattice constant
+	update lattice geometry

```
                                fplo9.09-43-x86_64 OUTPUT
 e(X)it
 [...]
                                                                              |
| main version: 9.09                                                        |
| sub  version: M-CPA                                                       |
| release     : 43                                                          |
|                                                                           |
-----------------------------------------------------------------------------
| date        : Fri Oct 18 08:41:59 2013                                    |
| host        : w73w7-snb14                                                 |
-----------------------------------------------------------------------------
File =.sym exists!
File =.in exists!
Symmetry changed in =.sym !
Will update file =.in !
WARNING in MODULE IO(fplo_io):
 lattice type or lattice constants changed!
 Will take default values for special bandplot symmetry points!
File =.in updated!
TERMINATION: Normal : File =.in updated!
-----STDERR:

 STATUS: OK                                                    (9.09-43:M-CPA)
```

The warning message refers to possibly user-defined points for the band structure plot, that are overwritten now with the default settings.

Key sequence	Explanation
x	exit update information
x	exit symmetry menu
q	quit fedit14.00-45-x86_64
y	confirm saving
fplo14.00-45-x86_64 > out & ⟨CR⟩	run fplo14.00-45-x86_64 in background
cd ../a0=7.60 ⟨CR⟩	change into directory a0=7.60
fedit14.00-45-x86_64 ⟨CR⟩	call fedit14.00-45-x86_64
+	select symmetry menu
L7.60 , , ⟨CR⟩	change lattice constant
+	update lattice geometry
x	exit update information
x	exit symmetry menu
q	quit fedit14.00-45-x86_64
y	confirm saving
fplo14.00-45-x86_64 > out & ⟨CR⟩	run fplo14.00-45-x86_64 in background
ps ⟨CR⟩	check the running jobs
cd .. ⟨CR⟩	change into parent directory
grit a0= ⟨CR⟩	check convergence

What you see now depends on the moment when you look at the progress...

```
fplows@w73w7-snb14:~/Al$ grit a0=
a0=7.50/out SCF: iteration 5 dimension 1 last deviation u= 0.50E-06 CONVERGED
a0=7.55/out SCF: iteration 1 dimension 0 last deviation u= 0.46E-08 CONVERGED
a0=7.60/out SCF: iteration 5 dimension 1 last deviation u= 0.55E-06 CONVERGED
fplows@w73w7-snb14:~/Al$
```

When both calculations are **finished** after a minute, you may compare the total energies and estimate the theoretical lattice constant.

Key sequence	Explanation
grEE a0= | tee ea0 ⟨CR⟩	print energies and save to file 'ea0'

```
fplows@w73w7-snb14:~/Al$ grEE a0= | tee ea0
7.50 -241.9194426350 242.19211517 -466.39637611 -17.71518170
7.55 -241.9194604174 242.17167366 -466.38219031 -17.70894377
7.60 -241.9193607411 242.15229278 -466.36879406 -17.70285946
fplows@w73w7-snb14:~/Al$
```

In the left column, you see the lattice parameter, the next column gives the related total energies. The minimum of the total energy is close to $a = 7.55$ Bohr radii.

Take a rest!