Gavin Abo
May 1, 2013

wien2dfsdx

wien2dfsdx is a set of files for OpenDX, which was designed to plot contours of the 2D fermi surface from Wien2k data.

Background

OpenDX tutorial files “Isosurface2D.net” and “Isosurface2D.cfg” (in /usr/share/dx/samples/tutorial of the OpenDX installation) [http://opendx.informatics.jax.org/docs/html/pages/qikgu021.htm] were modified to create wien2dfsdx.

fort2dx was created using the following two file formats:

1) The fort.* file is based on the Wien2k fort file format [http://zeus.theochem.tuwien.ac.at/pipermail/wien/2012-December/018026.html].

2) The *.dx file is based on the OpenDX mulitgrid file format [http://www.poissonboltzmann.org/file-formats/mesh-and-data-formats/opendx-scalar-data].

Installation of OpenDX

OpenDX must be installed to use wien2dfsdx.

1. For Ubuntu or Debian, run in a terminal:

sudo apt-get install dx

Note: For other Linux distributions, refer to the OpenDX website [http://www.opendx.org/download.html]

Installing wien2dfsdx

1. Place “wien2dfsdx.tgz” in your home directory. The directory’s location should be given in a terminal by:

echo ~

2. Extract the wien2dfsdx files in a terminal:

tar -xvf wien2dfsdx.tgz

3. After extracting the files, you should find one script (fort2dx) in the “script” directory of the created “wien2dfsdx” directory (use the following terminal command to view it: ls

~/wien2dfsdx/script). Place the script in one of the PATH (echo $PATH) directories. The Wien2k directory should be a PATH directory, where the location can be given by:

echo $WIENROOT

4. After placing the script in $WIENROOT, make sure that it has executable file permission with the terminal command:

chmod +x fort2dx

5. The wien2dfsdx installation should now be complete.

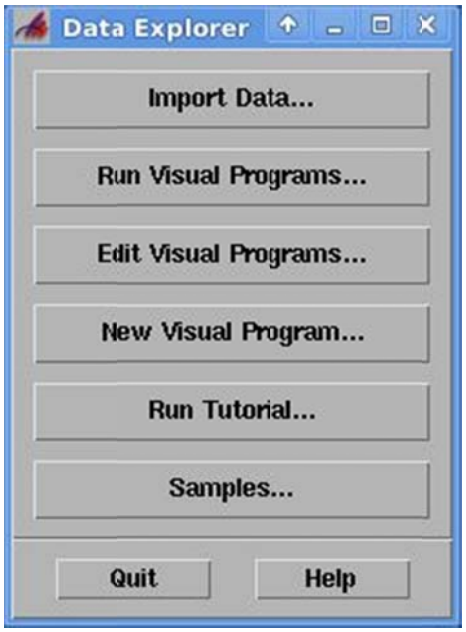
Running wien2dfsdx

Of note, you should be in a graphic user interface (GUI) environment. This means you have a desktop environment (gnome, kde, xfce, or etc).

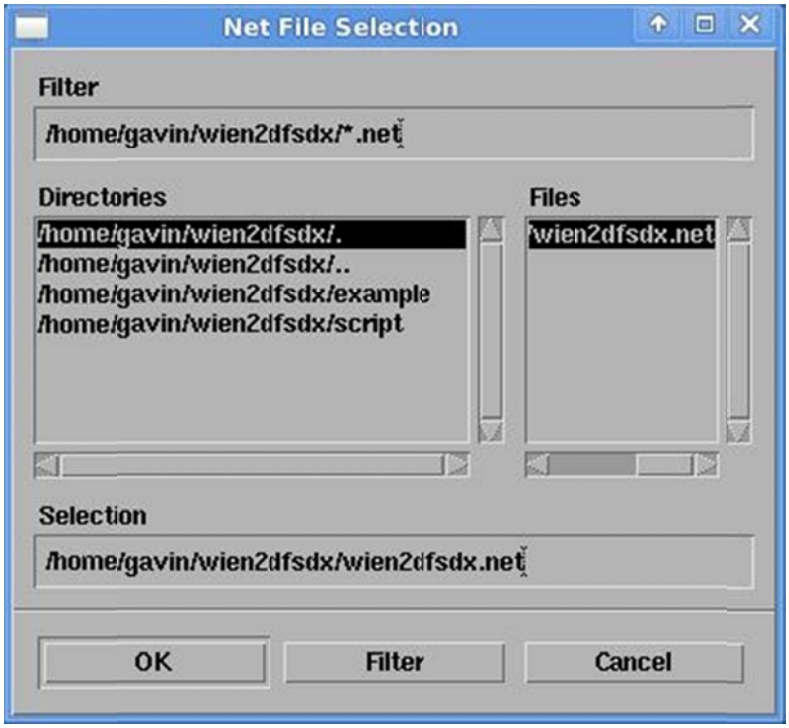
1. In a terminal, you can run OpenDX with the following commands:

cd ~/wien2dfsdx
dx

2. Click "Run Visual Programs…" in the window that appears:



3. Find and select the "wien2dfsdx.net" file, then click OK:



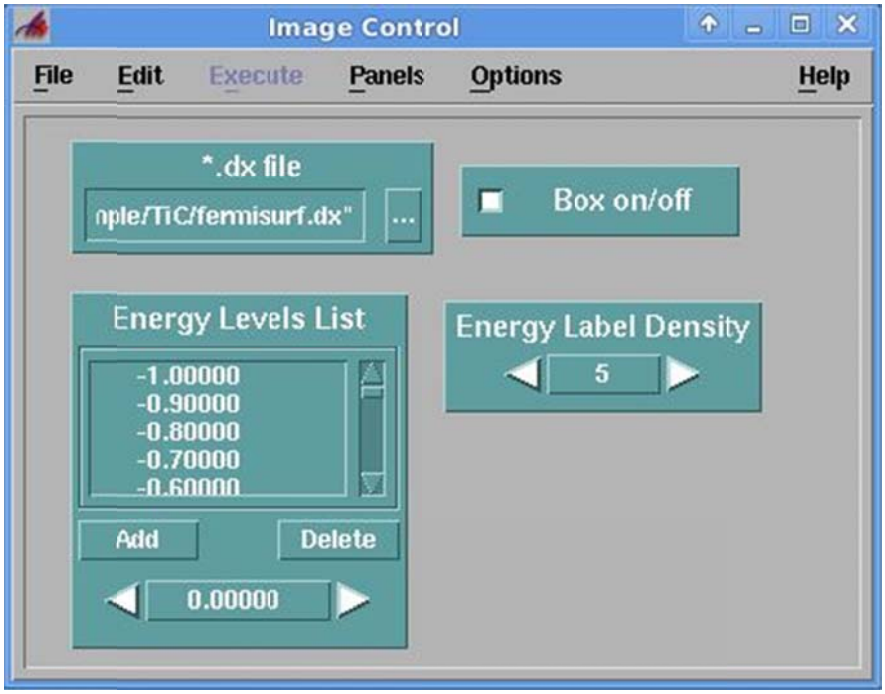
Note: “gavin” in the directory path is most likely replaced by your “username”.

4. Several windows should open.

5. Find the “Data Explorer” window:

6. Click “Windows”, then “Open All Control Panels”.

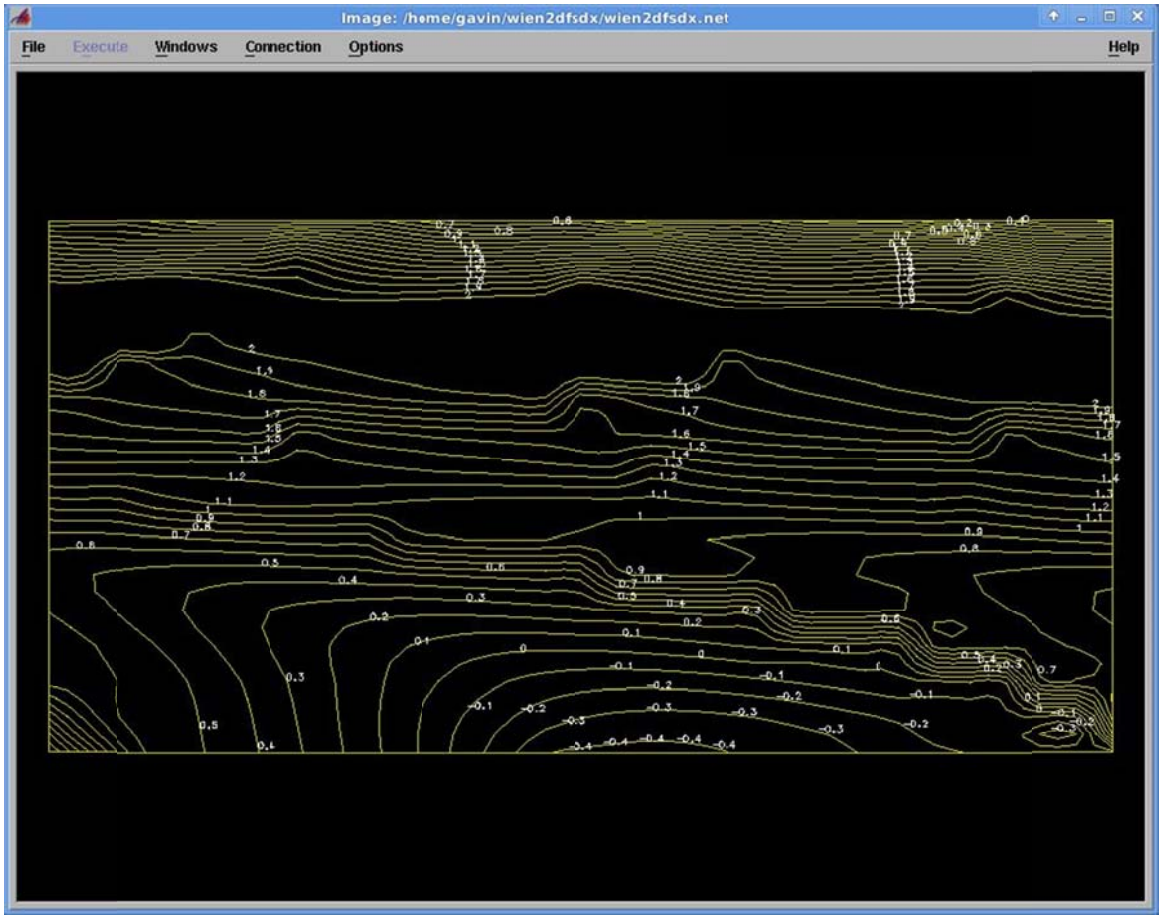
7. The “Image Control” window should appear:



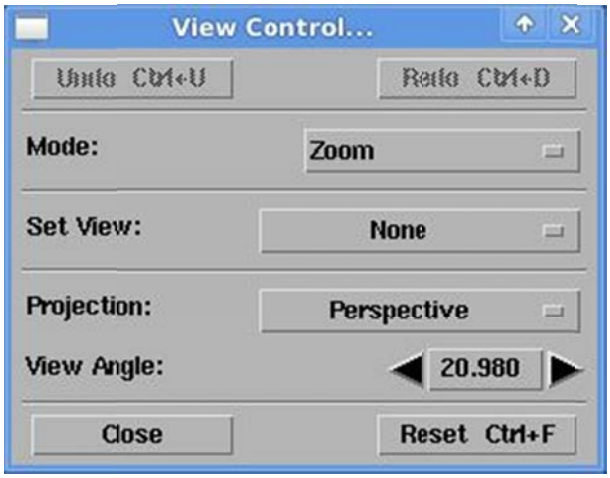
8. Use the "*.dx file" box to open the fermisurf.dx file in the TiC example directory (which should be at ~/wien2dfsdx/example/TiC). You could also open your own *.dx file, but you may have to create this file as described in later sections.

9. Click Execute, then Execute on Change. This will run the wien2dfsdx program, and the program should respond when your make any setting changes.

10. The user can make changes to in the "Image Control" window and observe the effects to the "Image" window:



If the "Image" window is blank, try the following. Click Options, View Control, and then a window similar to the following should appear:



Click Reset, the image should appear. The user can also change the other settings in the View Control to control the display of the image.

Comparison with Plotgenc

If we compare the plot below created with plotgenc to the plot created in OpenDX, the plotted data looks the same.

```
username@computername:~/wien/wiendata/TiC$ cp fort.14 fort.rho
username@computername:~/wien/wiendata/TiC$ plotgenc
 enter filename: (implies fn.plot, .input, .rho)
fort
...
   select 1 to rescale
          2 to change ilin
          3 to replot
          4 to label plot
        or 0 to end
1
 scale:
20
...
select 1 to rescale
          2 to change ilin
          3 to replot
          4 to label plot
        or 0 to end
2
 ilin=  1:    -1.0, 0.10, 2. <= These values were used in the “Energy Levels List” in OpenDX.
 ilin=  0:    -0.5, 0.05, 1.
 ilin= 999:   amin, adelta, amax
 ilin=   i:   specify i contour values
 ilin=  -i:   i lines with a0*sqrt( 2 )
 ilin= 888:   i lines with +-a0*sqrt( 2 )
1
...
select 1 to rescale
          2 to change ilin
          3 to replot
          4 to label plot
        or 0 to end
3
...
```

Create fort.* files

For example, for fort.14 of TiC using Wien2k 12.1 (with debian fftw3 library).

1. Complete the TiC scf cycle of the TiC example (in a terminal):

```
username@computername:~/wien/wiendata/TiC$ ls
TiC.struct
username@computername:~/wien/wiendata/TiC$ init_lapw -b -numk 1000
...
username@computername:~/wien/wiendata/TiC$ run_lapw -cc 0.0001
...
in cycle 12    ETEST: .0000029850000000   CTEST: .0000841
hup: Command not found.
 LAPW0 END
 LAPW1 END
 LAPW2 END
 CORE  END
 MIXER END
```

ec cc and fc_conv 1 1 1

> stop

2. Create fort.11 thru fort.14 (in a terminal):

username@computername:~/wien/wiendata/TiC$ fcc_fs_mesh
 generates fermi surface mesh in fcc case:
 plane Gamma-X-XP-K-Gamma: 1
 plane Gamma-X-U-L-Gamma: 2
 select 1-2:
1
 select mesh divisions: (even 30,...)
30
username@computername:~/wien/wiendata/TiC$ cp fort.2 TiC.klist
username@computername:~/wien/wiendata/TiC$ x lapw1
...
username@computername:~/wien/wiendata/TiC$ cp $WIENROOT/SRC_templates/case.insp TiC.insp
username@computername:~/wien/wiendata/TiC$ grepline_lapw :FER "*.scf" 1
in 1 files:
TiC.scf::FER : F E R M I - ENERGY(TETRAH.M.)= 0.6582138501
username@computername:~/wien/wiendata/TiC$ gedit TiC.insp
Replace "0.xxxx" with the fermi energy "0.6582138501".
Change number of bands "1 999" to "6 9". Note: An easy way to identify what bands intersect with the fermi level here is to use the BARGraph generated by xcrysden during 3D fermi surface plotting [http://www.xcrysden.org/doc/wien.html#fermi].
Save TiC.insp with these changes.
username@computername:~/wien/wiendata/TiC$ x spaghetti
 number of k-points read in case.vector= 496
...
username@computername:~/wien/wiendata/TiC$ gedit TiC.spaghetti_ene
Insert the following line at the top of this file:
31 16 0.74421 0.74421 61 31 0 0
This line is:
NX,NY,x-len,y-len,NXinter,NYinter,Invers,Flip as described in the Wien2k userguide.
NX: Count the number of 0 of band 7 in column 2.
NY: 496(from x spaghetti)/31(NX) = 16
x-len: Last value in column 1 of band 7
y-len: Last value in column 2 of band 7
NXinter: 2*NX-1 = 61
NYinter: 2*NY-1 = 31
Invers: Chosen to be 0 (use value suggested by *_fs_mesh or try different value if problem)
Flip: Chosen to be 0 (use value suggested by *_fs_mesh or try different value if problem)
Save TTiC.spaghetti_ene with this line.
username@computername:~/wien/wiendata/TiC$ spagh2rho < TiC.spaghetti_ene

3. The file fort.14 should now exist in the TiC directory

Example and Script

There is one example provided, which is for TiC. It should be found in ~/wien2dfsdx/example.

TiC Example

The "TiC.struct" file comes from "TiC.tar.gz" obtained from the Wien2k website [http://www.wien2k.at/reg_user/index.html]. The "fort.14" file was created as previously described in the section "Create fort.* files".

The "fermisurf.dx" file was created using the perl script "fort2dx". In other words, place "fort.14" in a directory where "fermisurf.dx" does not exist. Then in that directory in a terminal, run:

fort2dx fort.14 > fermisurf.dx

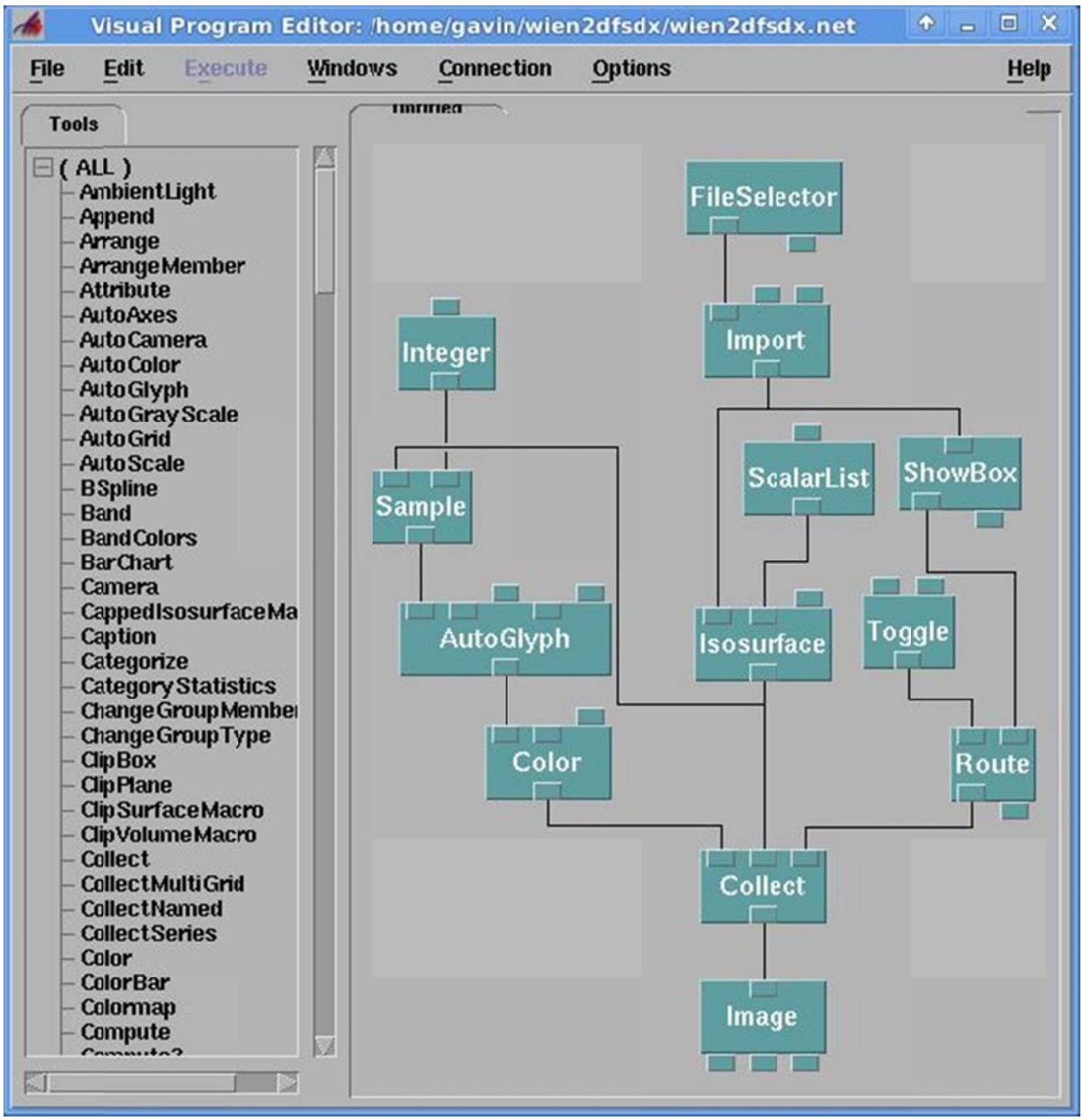
fort.14 can be replaced with any of the other fort.* files such as fort.11. The converted file can then be used for plotting in OpenDX. It is noted that fort2dx has not be test on other structures, so it might be necessary to edit fort2dx in a text editor for other structures.

OpenDX Programming

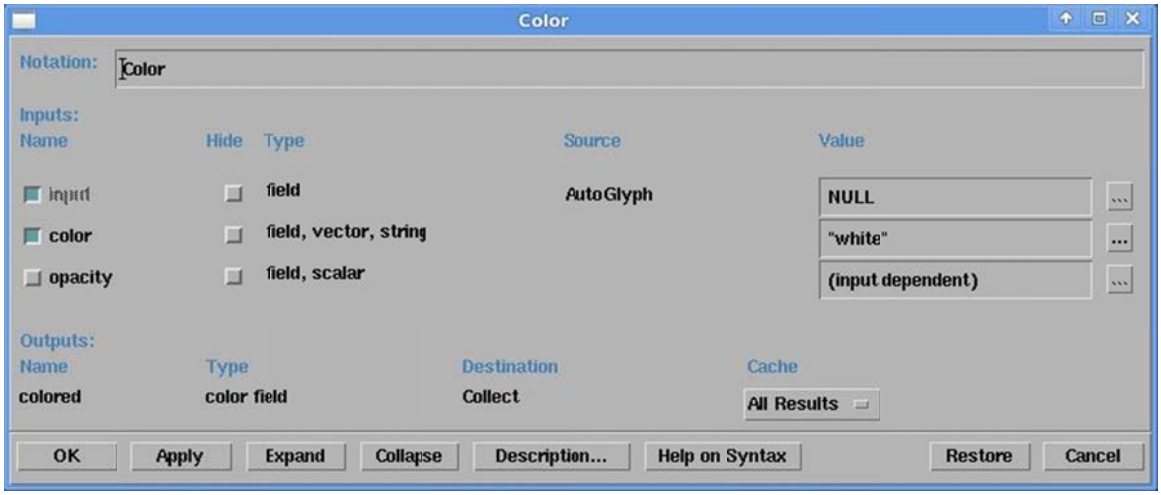
The "wien2dfsdx.net" file and its configuration file "wien2dfsdx.cfg" contain the code for wien2dfsdx. Control and functionality of the program can be adjusted by modifying the blocks with the "Visual Program Editor".

To access the "Visual Program Editor", click "Open Visual Program Editor" under "Windows" in the "Data Explorer" window.

For example, you should have a window that looks like the following:



Double left-click on the “Color” block, and the following window should appear:



Use the “Color” window to adjust parameters. For example, the Energy Label Density color in the image could be changed from “white” to “red”.

Use “Save Program As” under “File” in the “Data Explorer” window to save any programming changes to both “wien2dfsdx.net” and “wien2dfsdx.cfg”.

Future Work

Two future work possibilities for someone could be:

a) Improve plotting control and functionality of wien2dfsdx, such as try adding a title to the plot with a Caption block.
b) Create a separate OpenDX program for plotting 3D fermi surface and cutting of 2D Fermi surfaces.

Other information on fermi surface plotting

Xcrysden’s 3D fermi surface file format:

http://www.xcrysden.org/doc/XSF.html#bxsf

Elk’s OpenDX fermi surface program:

https://github.com/qsnake/elk/tree/master/examples/Al-Fermi-surface

Exciting’s OpenDX fermi surface program:

https://github.com/exciting/exciting/tree/master/src/src_fermisurfdx