Chapter 7.1

FOURIER MAPS & MAPVIEW

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7.3.1 Introduction

There are two Fourier programs available in the *WinGX* package, the **SLANT PLANE** and **FFT** options. The former is a more general program and allows the user to calculate a Fourier map in a general plane, while program **FFT** always calculates a full unit cell map.

MAPVIEW is used to visualise the electron-density maps written by **SLANT PLANE** and **FFT.** Drawings are either vector (*i.e.* line) drawings or bitmap plots. It is an updated version of **CONTOUR,** with many more features and styles of plots. It is a generally featured program, which allows input from several map file formats other than the *WinGX* format (XD grd files, Gaussian cube files, *etc*), *i.e.* functions other than electron density may be read in

- Map files may now be read dynamically into the program. Map files are direct-access binary files with the file structure outlined in Section 7.3.6.
- All screen illustrations may be saved as PostScript files (either monochrome or colour), or as Windows BMP files, or copied to the clipboard (from where they may be inserted into word processor or graphics programs). The vector illustrations may also be directly printed to a local printer.
- Illustrations are automatically scaled according to the axial lengths and non-orthogonal axes.
- Display colours (foreground, background, text colour *etc*) are user-selectable.
- Six different plot-styles are available. Five of these styles may be used with any MapFile, but the 3D-IsoSurface option requires a Mapfile containing more than one plane.

The available plot-styles are :
1. **2D-Contour**. This option draws a contour plot of a single map-section. No interpolation is used. The foreground colour is used for both negative and positive contours, negative contours being drawn with dashed lines and positive contours with solid lines.
2. **2D-PixelMap**. This option draws a single map-section with each discrete grid-point shown as a colour-coded rectangular "pixel". Since the number of "pixels" corresponds to the actual digital resolution of the MapFile, this is a scientifically accurate representation of the data. The colour-scheme is fixed, with blue representing the lowest density levels and yellow the highest levels.
3. **2D-BitMap**. This option draws a single map-section as a bitmapped image. The electron-density is interpolated between grid-points and colour-coded according to the currently selected colour-table. There are five available colour-tables, GRAY-SCALE, HEAT, RAINBOW, BGYRW and SERPENT, the default being BGYRW. The image is calculated on a pixel-by-pixel basis, so the drawing time is longer than for options 1 & 2.

4. **3D-Relief**. This option draws a single map-section as a relief-plot with the Z-axis representing the magnitude of the density at that point. Each grid-point is connected to neighbouring points to give the familiar "net-like" appearance. The orientation of the plot may be altered by the standard "mouse dragging" operation.

5. **3D-Surface**. This option is similar to 4, except that the height-field surface is rendered. This bitmapped surface may be rendered in a single colour, or a colour-table may be used to emphasise the height. This option gives a more photo-realistic view of the surface than option 4, but as the image is calculated on a pixel-by-pixel basis, it takes considerably longer to draw.

6. **3D-IsoSurface**. This option is only available if the Mapfile contains more than one plane. A bitmapped iso-surface at the selected level is drawn either as a single colour or as a colour-coded height-field. It is possible to select either negative or positive levels for the iso-surface.

7.3.2 General information

For all the 2D-options, when the mouse cursor lies over the map image, a continuous display of the current cursor position (map x- and y-coordinates) and function density at that point is given. In this mode the cursor changes from the normal arrow-cursor to a cross-hair cursor. Maps containing more than one section may be advanced or retraced using the **Frame>>** or **Frame<<** buttons and a particular section may be selected with the **Select Section** button. If the map contains more than one section, it may be quickly visualised with the **StartMovie** button which moves continuously, section by section up and down the map until any key is hit or the mouse-cursor is moved over the canvas. The **StartMovie** option is only available for the vector-illustrations (styles 1,2 & 5), since the other styles are too time-consuming to draw. Parameters relating to the currently loaded map and currently selected section is given in a panel to the side of the graphics window.
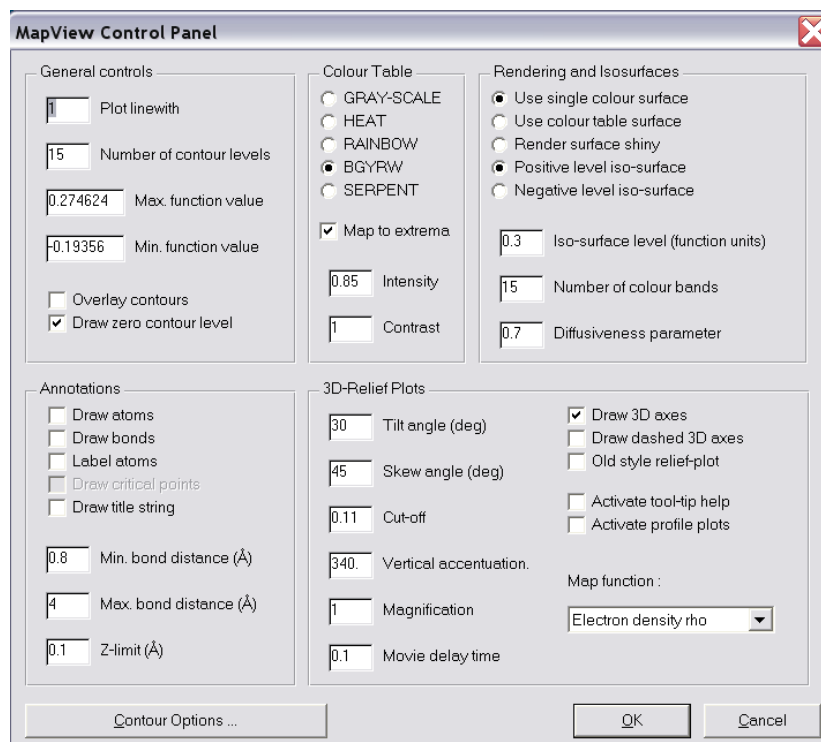
A number of program options may be set using the dialog window shown above. This dialog box is activated by a right mouse click on the drawing canvas. Most items are self-explanatory. If the "Activate profile plot" option is selected, then draging a line across the map causes a secondary window to display the 2D-profile along that line.
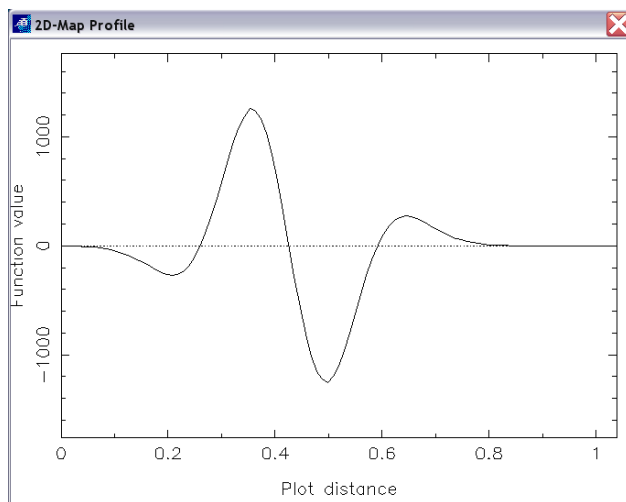
The "map to extrema" option fits the colour table used for the bitmap plots to the actual extrema of the map. If this option is switched off, then the extrema are given as $\pm$ the absolute maximum, so that the centre of the colour map always corresponds to zero function value.

7.3.2.1 Contours
No interpolation is used to generate the contours, so if smoother sections are required, the map must be recalculated using a finer grid. The *contour interval* may be explicitly set using the **Options[Set Contours]** menu item, and the contour colours and line styles may also be set.

7.3.2.2 Maximum/minumum density
The maximum density is by default the highest point in the MapFile, the minimum density the lowest point. Different values may be selected for either parameter. This has the effect of truncating the density at these level(s), a feature which is useful in examining weak features in the presence of intense peaks.

7.3.2.3 Atoms, bonds and atom labels
Atoms, bonds and atom-labels may be overlaid in the 2D-options only. The bond-distance calculation is unsophisticated - a bond will be drawn between every pair of atoms whose *distance* fulfils the criterion.

Min. bond distance < *distance* < **Max. bond distance**

7.3.2.4 Colour-tables
The colours for the colour-tables are taken from PGXTAL and are stored internally. It is possible to modify these colours in two ways. The colour-intensity may be reduced from the normal level of 1.0 (which gives the pure colour-map) since these pure colours are quite garish and difficult to look at. The default colour intensity of 0.75 gives a more reasonable colour scheme. The contrast may also be changed from the default value. A value smaller than 1.0 emphasises the lower intensities, while a value larger than 1.0 emphasises the higher intensities. The user needs to experiment to find the optimum settings.

7.3.2.5 Axial scaling
If the angle between the two projected axes (given as ANGLE in the display) differs from 90° or the axial lengths are unequal, then axial scaling is automatically chosen if options 1 or 3 are selected (axial scaling cannot be used for option 2). This action may be deselected using the **Options[Use axial scaling]** menu item.

7.3.3 Menu Options

7.3.3.1 Open Mapfile...
Reads in a new MapFile. MAPVIEW can read its own format (called *name*.**MPF**), XD grid files (**XD_*.grd**) , Gaussian style CUBE files (***.cube**) and some AIMPAC grid files (***.grid**). On startup, MAPVIEW will load the file **MapFile** if it finds it in the current working directory. Axial scaling is set automatically if non-equal or non-orthogonal axes are read from the MapFile.

7.3.3.2 Save as PostScript
The current image will be saved as a colour or monochrome PostScript file. It is named automatically as MAPVxxx.PS where xxx = 001-999. Previously written PostScript files will not be overwritten.

7.3.3.3 Save as BMP
The current image will be saved as a Window BMP file. It is named automatically as MAPVxxx.BMP where xxx = 001-999. Previously written BMP files will not be overwritten. The size will depend on the graphical resolution and colour-depth of your monitor.

7.3.3.4 Copy To Clipboard
The current image is copied to the clip-board, form where it may be inserted as a graphical object into other programs.

7.3.3.5 Print...
The current image is sent to the local printer. The current colour scheme will be used (except that the background is always printed as white).

7.3.3.6 Select Colours/Load Default Colours
The display colours may be individually selected. The foreground colours is used for the contours. The colour tables are unaffected by this option. Load Default Colours returns all individually selected colours to their default values

7.3.7 Options
This opens the above-shown dialog box which allows the user to set a number of parameters.

7.3.4 Program limitations
1. The previous maximum number of grid points allowed in the x- and y-directions (NX and NY), which was 200, is now lifted, as storage for all maps is now assigned dynamically.
2. The continuous electron-density read-out only functions for the 2D-options. If PostScript hardcopy is selected, this function is temporarily switched off until a new image is drawn (simply reselect the appropriate menu item).

7.3.6 MapFile structure
For reasons of efficiency, the WinGX MapFile format **(*.mpf)** is a *binary direct-access* file. Each record is one word (4 bytes) in length. The file starts with a header of 19 records containing the information shown in Table 1. This is followed by NX*NY*NPLANES records which give the function values F(I,J,K) in the FORTRAN format :

$$(((F(I,J,K),\ J=1,NY),\ I=1,NX),\ K=1,NPLANES)$$

The file ends with the atom co-ordinates starting with record number XX = (20 + NX*NY*NPLANES) which gives the number of atoms NAT, followed by NAT*5 records for these NAT atoms as detailed in Table 1.

Table 1. Record structure of MapFile

NREC	VARIABLE	TYPE	MEANING
1	NX	INTEGER*4	number of grid-points along x
2	NY	INTEGER*4	number of grid-points along y
3	NPLANES	INTEGER*4	number of map sections
4	DX	REAL*4	increment in x-direction
5	DY	REAL*4	increment in y-direction
6	DZ	REAL*4	increment in z-direction
7	CELL(1)	REAL*4	real-space unit vector length along x
8	CELL(2)	REAL*4	real-space unit vector length along y
9	CELL(3)	REAL*4	real-space unit vector length along z
10	CELL(4)	REAL*4	angle between y and z vectors
11	CELL(5)	REAL*4	angle between x and z vectors
12	CELL(6)	REAL*4	angle between x and y vectors
13	XSTART	REAL*4	starting value along x-direction
14	YSTART	REAL*4	starting value along y-direction
15	ZSTART	REAL*4	starting value along z-direction
16	IAXIS	INTEGER*4	projection axis(A*=1,B*=2,C*=3)
17	IMODE	INTEGER*4	1 = 3D-Fourier, 2=Slant plane
18	RMIN	REAL*4	minimum function value in map
19	RMAX	REAL*4	maximum function value in map
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			followed by NX*NY*NPLANES records giving the function values in the running order (((F(I,J,K),J=1,NY),I=1,NX),K=1,NPLANES)
.			
XX	NAT	INTEGER*4	number of atoms. Record number XX here indicates (20+NX*NY*NPLANES)
			followed by NAT*5 records for the NAT atoms. The coordinates are in the appropriate units, i.e cell fractions for IMODE=1 and Angstroms for IMODE=2
XX+1	LAB1(I)	CHARACTER*4	first four characters of atomlabel(I)
XX+2	LAB2(I)	CHARACTER*4	second four characters of atomlabel(I)
XX+3	X(I)	REAL*4	x coordinate of atom(I)
XX+4	Y(I)	REAL*4	y coordinate of atom(I)
XX+5	Z(I)	REAL*4	z coordinate of atom(I)

7.3.7 Graphics acknowledgement

The graphics in this program use the PGPLOT library (version 5.2.0) of Tim Pearson (http://astro.caltech.edu/@tjp/pgplot/index.html) and a heavily modified version of the PGXTAL library of Devinder Sivia (http://www.isis.rl.ac.uk/dataanalysis /dsplot/).