ESRF

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Last revision: 9 August 2001

Xop/Xplot User's Guide

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1

Getting started: plotting your data (visualization)

Xplot is general package for creating X-Y graphics which also allows sophisticated data visualization, processing, manipulation and analysis. It is part of the XOP packege (http://www.esrf.fr/computing/scientific/xop). It is fully interactive, permitting also a large number of manipulation and presentation of the data.
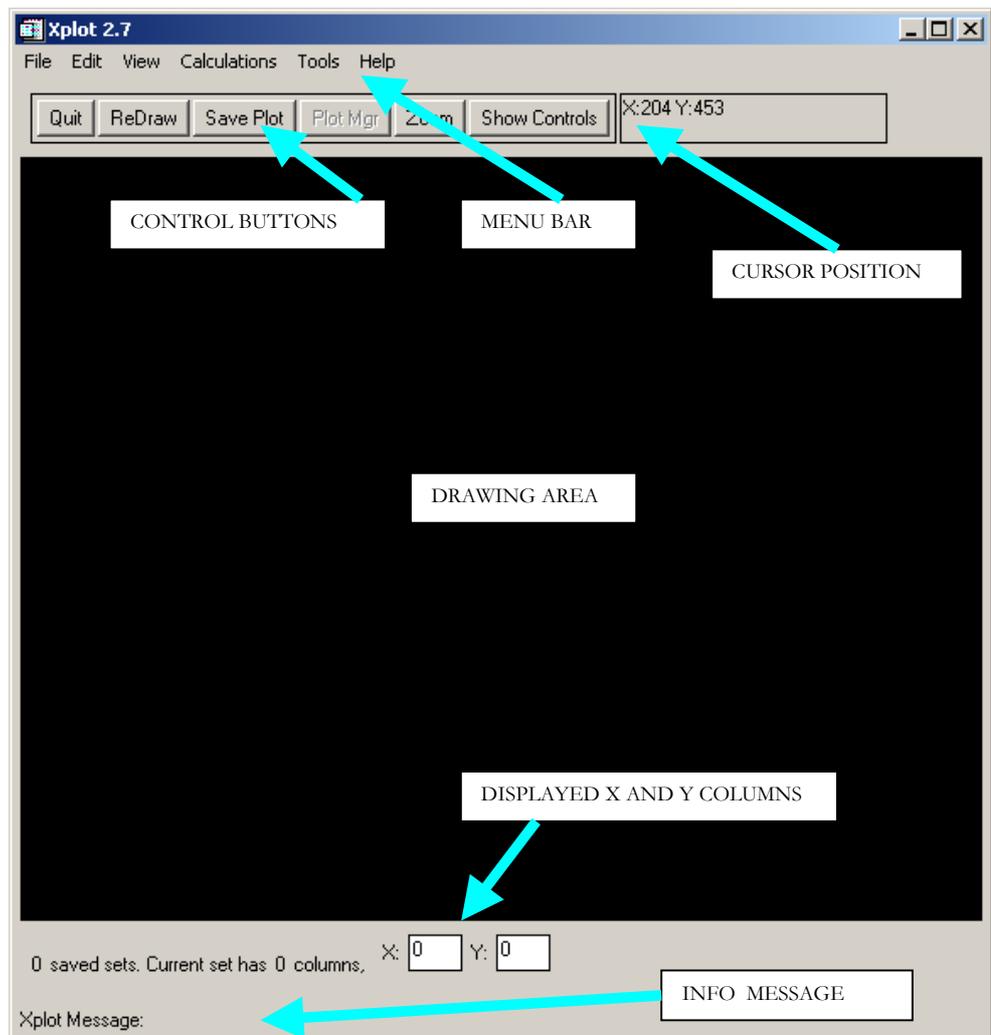
Few of its capabilities are summarized here:

- Direct loading of data from multicolumn ASCII data files. Access and merge multiple sets of data.

- Access to SPEC data files.

- Direct printing from workstations and PCs. PostScript and Encapsulated PostScript outputs.

- Linear and logarithmic X- and Y-axes.

- Apply and change symbols, line styles, colors, thickness, fonts, etc.

- Label, annotate, add legends, titles, etc. to the plots.

- Zoom, shift, switch columns, and over-plot data.

- Save and restore plots and attributes in a XPLOT backup file.

- Data analysis: extrema, moments, integrals, derivatives, CDFs, smoothing, user-defined operations, interactive Fourier Filtering, interpolations, convolutions and correlations.

- Fitting: linear regression, polynomial fit, Gaussian fit and non-linear fit (Levenberg-Marquardt and others) whith an on-line user-defined function.)

These features will be discussed in more detail later

Launch Xplot. Window overview

There are several ways to start Xplot. One of them is to start Xplot from the Xop main window: go to Tools menu and select Xplot(Plotting tool). Other typical ways are: from applications inside Xop, from Start|Xop|Xplot menu under Windows, entering "xop xplot" at the command prompt under Unix. A new window like this one appears:

The different areas in this window are

- Menu bar: Contains the menus to access all the features in Xplot

- Control buttons: Used to invoke the most commonly used functions

- Drawing area: The zone where your graph will appear

- Displayed X and Y columns: The X and Y data displayed in the Drawing area are two columns from a multicolumn table called "data set".

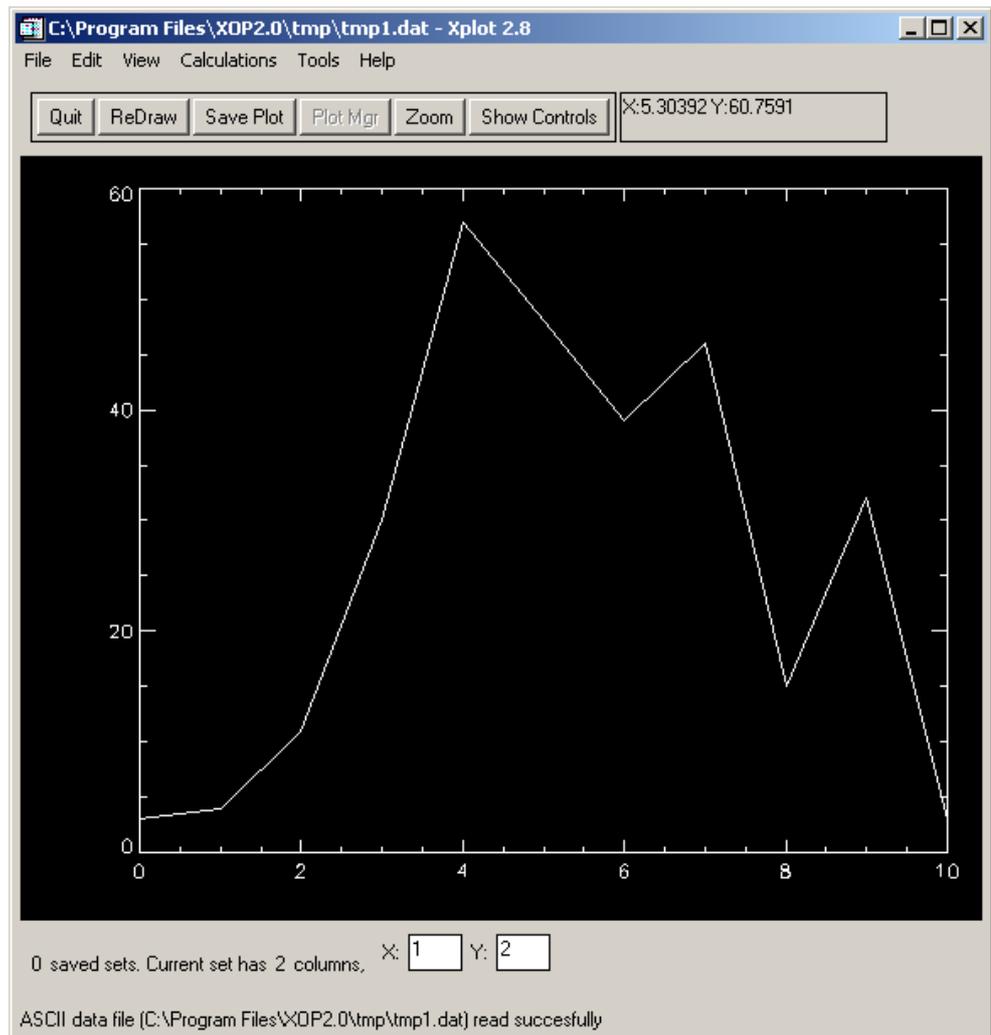- Info message: You can read here some on-going information from Xplot

Create a line plot

Create or locate a file with the data you want to plot. For example, write a file called tmp1.dat with your favorite editor, or with the Xop file editor available in Xop|Tools|IDL file editor… I entered the following data in two columns, using a simple blank character as a separator. Note that I also wrote a comment section. You can write any text as comment. Xplot will ignore it.

Important: if you are creating an ASCII data file, do not user the dash (#) symbol for starting the comment. This is the standard header symbol for SPEC files and Xplot will get confused.

; this is a comment:
; example of data to test Xplot
0 3
1 4
2 11
3 30
4 57
5 48
6 39
7 46
8 15
9 32
10 3

Now your can use Xplot|File|Load Data File… to get the data in Xplot. Now your Xplot window looks like this:
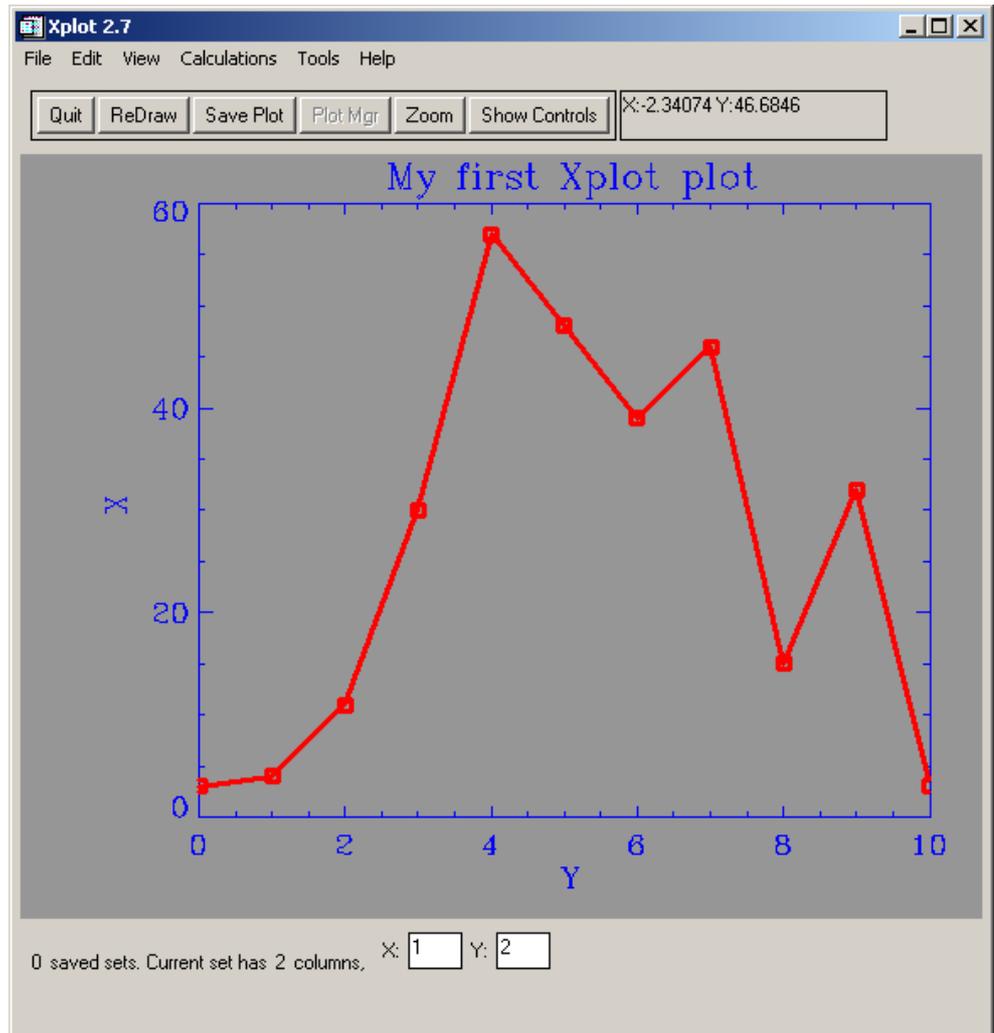
You can:

- See data numerical values using Xplot|View|Show Data
- Edit some numbers using Xplot|Edit|Data
- Save numerical data to a file using Xplot|File|Write ASCII file with current set…
- Print it using: File|Print Plot…

You may notice that when you move the mouse on the display, you get the coordinates in the top of the window. You are now invited to press the Show Controls button, and you will get an additional window with several controls. Play a little with the controls and you will be able to change the plotting symbol, the line style, display the data in logarithmic scale, change font, thickness, character size, and colors. The default color table is just black and white. If your started Xplot from the Xop window, you see at the bottom of the colortable some predefined useful colors. Click on one of these colors to change, for example, the lines color. If clicking is difficult, just enter the cumber of the color (between 0 and 31) and validate with <enter>. You can scan colors using the ">>" or "<<"

buttons. For playing with colors, you may want to load a nicer color table by using the `Change color table` button. This button pops-up a new window, click for example the line `16 LEVEL` and then the button `done`. You will see that a multicolored table appears in the bottom of the Xplot controls window. Now click in the desired color for selecting your background, line and axis colors. For example, after few manipulation and adding titles with Xplot|Edit|Titles and you can get something like:

Overplotting and printing

One of the most important features of Xplot is the capability to display multi-line graphs with data coming from different origins. Data in Xplot is structured in the so-called sets.

A set is an array or matrix containing N points (or rows) and M columns.

A typical X/Y plot data as described in the `tmp1.dat` file is a set with 11 points and two columns, the first one for the X points and the second one for Y. Xplot stores the data in multiple sets, and each set may hold a different number of points or columns. Xplot allows multi-line plots, in which the data for each line is a couple of columns from a given set. Xplot options `Calculations` and `File/ Load Data File...` allows to create new columns in defined sets and new sets from files or from operations between existing sets.

You can change the X and Y columns for the plot in the current set of data by just typing the column numbers in the bottom of the Xplot window:

Try for example to write a 1 in the Y column, then type <Enter> and you will see in your display a straight line, in other words the first column of the set plotted against itself. You can invert the X and one axis by typing 2 and 1 in the X and Y columns, respectively.

It is very important to type <Enter> after modifying any text widget in Xplot. That permits Xplot to understand you have finished with the editing, and process the event.

You can connect and disconnect the plot symbols with lines by using the first control in the Xplot Controls window.
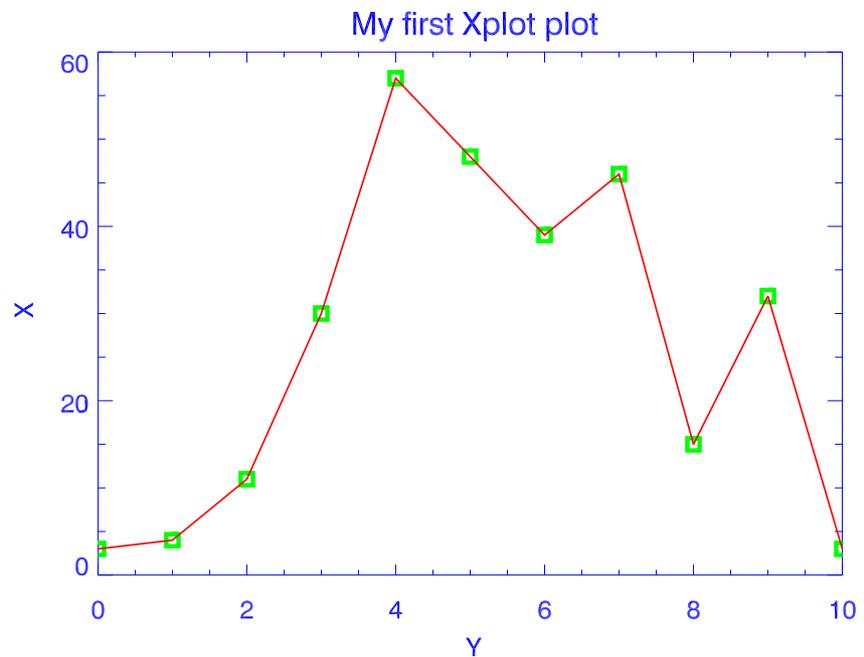
But it is also possible to do it by overplotting twice the same data points, the first plot points are connected with solid line, and the second plot uses disconnected symbols. This is, for example, the only way to display the line with a given color (i.e. red) and the symbols with another one (i.e. green). We are going to do that to learn an important feature of Xplot, the possibility of creating multi-line plots. Follow the next steps:

•   Display your points with `Symbol Connection: Connected` and `Plot Symbol: 0:Line` (Xplot defaults). Color the lines in Red (using color index 2 if you started Xplot from Xop). Change if you want the thickness to a thicker value (i.e. 3).

•   Press the button `Save Current`. You may notice that nothing happened, but in fact, if you see at the Xplot message at the bottom of the Xplot window, you can read that "`Current set saved and now the current set is a copy of the saved one`". You have now two lines on your display, but as both are the same data with the same attributes, they look like a single one.

•   From the Xplot controls window, change the `Plot Symbol` to, for example, `6: Square`, change the Symbol connection to Disconnected, and change also the `Line/Symbol thickness` to 8 (for doing that, you can use the slider, or directly enter an 8 plus <Enter> in the text widget on the top of the slider). Select now in the `Lines` color green (index 3). You will see the square symbol points (current set) and an overplotted red line which is the saved set.

Now, controls apply to the current set of data, and the saved set's attributes are not affected by controls.

The current set can be overwritten by using the `File/Load Data File...` option. This option allows to load a set in a multi column ASCII file to the current set, without affecting the saved sets. The ASCII multicolumn file can also contain any number of text lines, which are interpreted as comments and ignored by Xplot. Thus, by using the `Save Current` button, one may build complicated multi-line plots, with data coming from one or different files.

You can print the result. Often, you do not want to print, but to use the graph in a paper or other document. Here, you need the maximum of resolution and a bitmap (screen capture) is not desirable. I usually print to en encapsulated PostScript file and import it in Word. For example, for obtaining this graph

I did the following:

- In Xplot, print to a PS file. I set "encapsulated", "color" and "TrueType" PS font.
- I opened the resulting file.eps with GhostView in my PC. I added a preview bitmap using Edit|Add EPS Preview|Windows metafile. Save it with another name. This preview will allow you to see the plot in your screen when you import it in word. Otherwise, it will print on a PS printer, but you cannot see it on the screen
- In Word, import the eps file using the Insert|Picture|From File… You can easily resize and operate on it by double clicking on it.

Operating with data
(data analysis)

This section will show you how to focus attention on a subset of your data and how to manipulate it with mathematical tools to obtain new data or improve the existing one.

Activate the data for analysis

In general, when you import a data set in Xplot, what you see in the drawing area is a subset of the imported data. When you apply a tool from the Xplot window (like, for example, Xplot|Calculations|Derivative), it is applied to the *active data* , which, in many cases, is the data you see in the drawing area, but not always. Let us define some terminology that will help us in further explaining Xplot actions:

Definitions
Xplot data is all data that is already available or will be available to Xplot. Xplot data may be in a single file or in multiple files. For example, our file tmp1.dat is Xplot data. If I create another similar file tmp2.dat to be used in Xplot (to overplot data to tmp2.dat), the Xplot data is everything contained in both files. A typical SPEC file usually contains many blocks of data (called *scans*). All data in one (or many) SPEC file are Xplot data. Xplot data is structured in data sets, or simply sets.

A *set* is an array or matrix containing N points (or rows) and M columns. Our file tmp1.dat contains a single set, with two columns. A SPEC file usually contains many sets (or scans). When a set is loaded in Xplot (usually by Xplot|File|Load data file you can manipulate it using the Xplot controls. It is called *current set*. The current set has at least two columns, but may have more. You can display X-Y graphs of the current set by assigning a column to X and another column to Y. This is done with the display column boxes (or pulldown menus) at the bottom of the Xplot window. If you change the column number, which index starts with one, you must press <enter> to validate and tell Xplot to update. However, you can restrict the view of the X and Y data of your current set. For example, you can change the limits of the plot (using Xplot|Edit|Limits|Set Limits and Styles…) or simply by selecting part of the plot and applying the zoon button (click ReDraw to unzoom). Sets are important to create compound plots of several curves. For that you should use the Save Plot button.

Plot attributes: they are characteristics of the plot that are not included in the data itself, like color, thickness, plot limits, etc.

Selected data: Click and drag the mouse over the wanted region in the drawing area. You selected an X and Y interval in the plotted data. The selected limits appear in the Xplot message. We call "selected data" the points of the current set with X values in that interval.
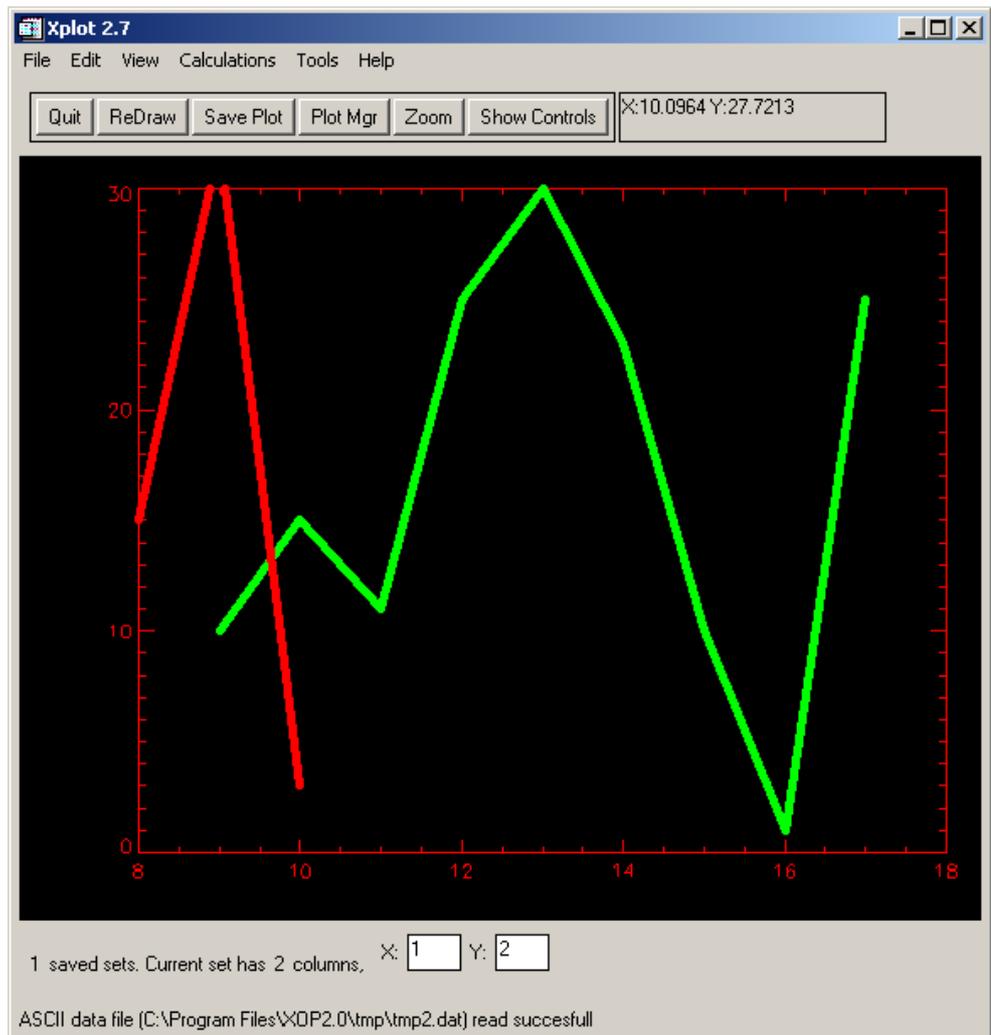
Active data: they are the data to be used for the data analysis operations. The active data contains the points included in the X limits defined in the Xplot|Edit|Limits section. The default is that all points are active data. However, you can define manually your limits using Xplot|edit|Limits|Set limits and Styles… In some cases, it is easier to set the limits by *selecting* data and then using Xplot|edit|Limits|Set Limits as Selection Area. You can always go back to default limits by using Xplot|edit|Limits|Set Defaults

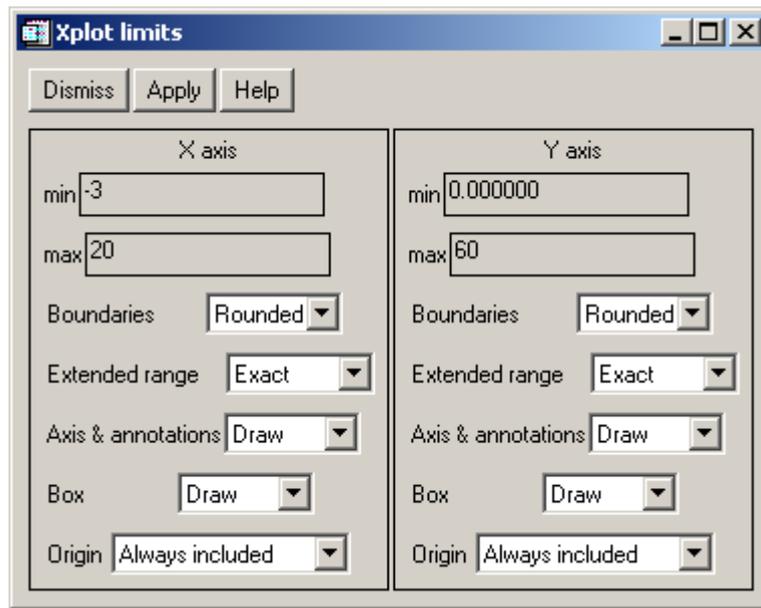### Overplotting sets (creating compound plots)

For example, to create a plot from data in two different files tmp1.dat and tmp2.dat, load first tmp1.dat. The current set now is the two-column data in tmp1.dat. Manipulate it if you want (change color to red, line thickness to 5, etc) and then press "Save Plot" button. Apparently nothing happened. You only see at the message line: "1 Saved sets". This means that the set you manipulated is saved to some kind of background state, becoming present, but inactive. So, what is the current set now? The answer is: an identical copy of the saved one. Now, create the next file tmp2.dat like:

```
; this is a comment:
; example of data to test Xplot
9 10
10 15
11 11
12 25
13 30
14 23
15 10
16 1
17 25
```
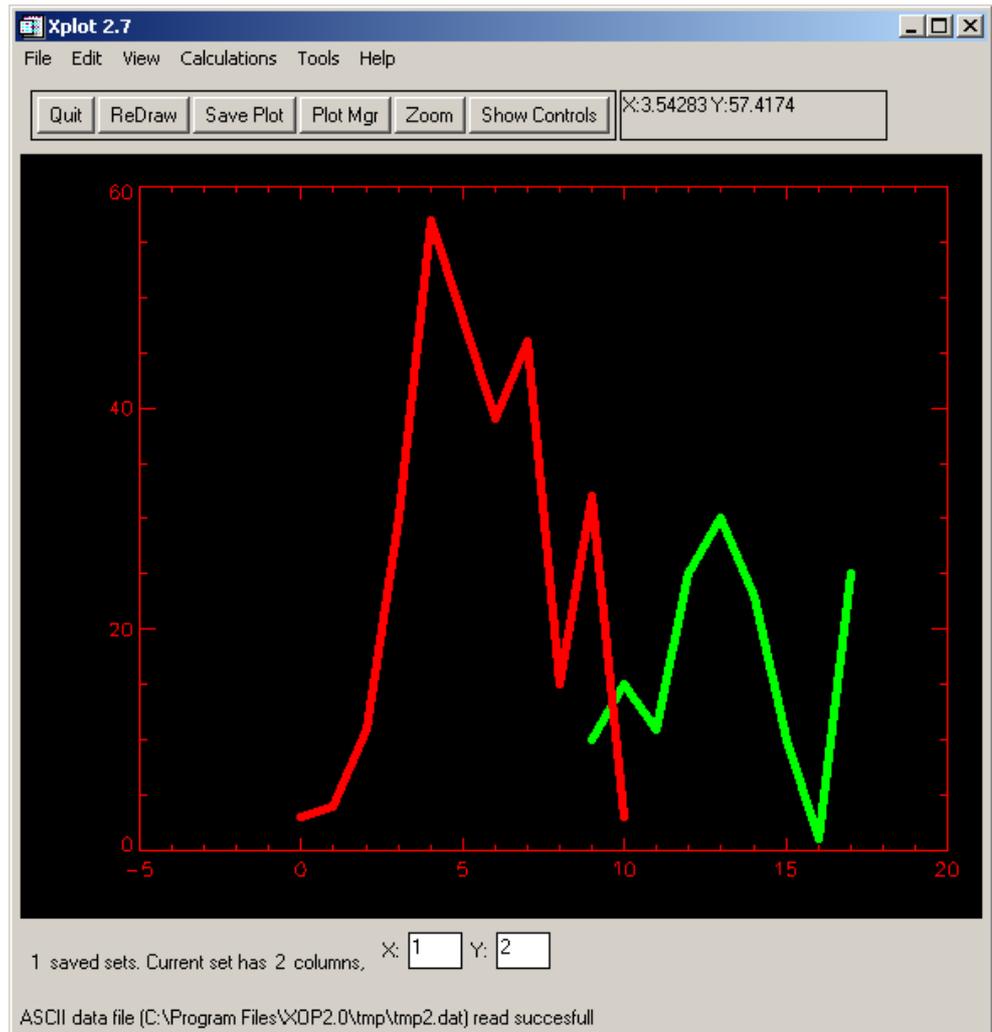and load it in Xplot using Xplot|File|Load Data File… What happened? To see more clearly what happened, change the line color to green (index 3). You obtain:

You see in green the new loaded file. You see in red the old saved set (only part of it, because Xplot automatically sets the plot limits adapted to the current set). Any operation you do in Xplot will be applied to the current set (green). May be this resulting plot is not what you wanted. You can change the limits by hand to make both sets appear in the drawing area, by using Xplot|Edit|Limits|Set Limits and Styles…I changed the limits to:

and this is what I get:

Note that I entered the X axis min value to –3 and got –5 in the plot. This is because Xplot rounds the limits in order to present a better looking plot. If you really want to start the plot at the X value of –3, just set "Boundaries: exact" in the Limits window.

With Xplot, you can overplot many curves by iteratively loading and then using the "Save Plot" button to keep them. Attributes for a saved curve cannot be modified. To modify them you should pass the saved curve to the current set, using the Plot Manager (Plot Mgr button). The plot manager also permits to delete saved sets.

Selecting, zooming and setting plot limis

To focus the attention in some part of the plot, first *select* it. For that, click and drag the mouse over the wanted region. The selected limits appear in the Xplot message line. The selected area is useful for three things

- Zoom it. Press the Zoom button to adjust the plot boundaries to the selected area. Press "ReDraw" to go back the original plot. Note that although you pressed the "ReDraw" the selection is not lost: click "Zoom" button again, and you will see again the zoomed plot.

- You can define the limits of the plot to the selected area, by choosing Xplot|Edit|Limits|Set Limits as Selection Area. The limits are then fixed and even if you load a new data set, they will not change. To change manually the limits, use Xplot|Edit|Limits|Set Limits and Styles… To tell Xplot to adjust the limits automatically to the current set, select Xplot|Edit|Limits|Set Defaults.

- Information of selected area is passed to two "Edit" operations: i) Xplot|Edit|Data… allows you to modify and remove points. When you select this option, the selected points will be highlighted. ii) Xplot|Edit|Cut… allows you to remove undesirable parts of your current set. The default limits presented here are adjusted to the selection area.

Note that the defaut limits (automatic limits adjustment) is manifested in the Xplot|Edit|Limits|Set Limits and Styles… window with the same numerical value for the min and max (usually zero).

The active data for the data analysis (most operations in the Xplot|Calculations menu) is the selected X and Y columns in the current set, in the interval selected by the plot limits (check them with Xplot|Edit|Limits|Set Limits and Styles…). This means that a typical operation (e.g., derivative) will be applied only to the X-Y data in the current set in the [xmin, xmax] interval set in Xplot|Edit|Limits|Set Limits and Styles…

Data analysis

There are many operations that can be applied to the active data in Xplot. There are under the Xplot|Calculations menu.

Remember that:

The *active* data for the data analysis (most operations in the Xplot|Calculations menu) is the selected X and Y columns in the current set, in the interval selected by the plot limits (check them with Xplot|Edit|Limits|Set Limits and Styles…).

Statistics

- Xplot|Calculations|Width/Integral/MinMax: Calculates the full width at half-maximum (FWHM), extrema and integral of the active data. You can optionally write some of these values as a plot Legend. Integration is done by using the INT_TABULATED IDL routine.

- Moments: Calculate the moments (mean, variance, skewness, kurtosis, mean absolute deviation and standard deviation) of the current data. It uses the MOMENT function

Data manipulation (creating and combining data)

- Create data set…Allows to easily create a set of data by definging the abscissas interval and a formula for the ordinates.

- New window with current set. Allows to export the current set to another Xplot window. This is useful when we want to perform some operations conserving the original look in the main window.

- Operations with columns… & Operations with sets…These options, because of their importance, are explained in detail in the next sections.

Derivative/Integral-based operations

- Derivative: This options created a new Xplot window with the derivative of the current data. It uses the DERIV function of IDL.

- CDF… This options created a new Xplot window with the Cumulative Distribution Function (CDF) of the current data. This function is the inverse function of the derivative. For example, applying first the derivative and then CDF to your data you should go back to the original data. The calculation is done calling the INT_TABULATED function a number of times equal to the number of abscissa points. The CDF function of a given signal *f(x)* is defined as:

$$CDF(x) = \int_{-\infty}^{x} f(y)dy \qquad (1.1)$$

- Powel Spectral Density…This option computes the power-spectral-density function from the active data. It is defined as: PSD=(Xmax-Xmin)*ABS(FFT(Y),-1)^2. Note that the use of FFT implies that the abscissa points must be equi-spaced.

- Fourier Filtering… This option permits interactive Fourier filtering of the current data. It uses a slightly modified version of the IDL filtering example, which permits Input/Output of users values. When you call this option, a new window appears, showing three displays: one with the original signal, one with the filtered signal and another one with the filtering window used. You can select different `Filter Functions`, `Filter Order`, `Filter Type` and values of `Frequency cutoff` and `Bandwidth`. Open for example these option from Xplot holding the sinusoidal data from last section. Play with the `Frequency Cutoff` function and you will see how you can filter the high frequency component (with cutoff values below 20, approximately). You can save the displayed values to file(s) by using the `File/ Save as (New ASCII FIle)...` option from the menu bar, and then the filtered data can be re-injected in Xplot for further manipulation.

- Convolution and Correlation…This option permits to calculate convolution and correlation between two data sets, A (the current set) and B. The set B can be one of the following cases: 1) B=A autoconvolution/autocorrelation cases. 2) B from an external file. 3) B a Gaussian, Lorentzian or a liner combination of both (the so-called pseudo-Voigt function: $v(x)=r*L(x)+(1-r)G(x)$, with r the ratio or linear coefficient between Lorentzian and Gaussian). The Convolution and correlation are calculated from: $CONV(x) = $ integral$(A(y) B(x-y) dy)$; $CORR(x) = $ integral$(A(y) B(y-x) dy)$. Of course, $CONV(x) = CORR(x)$ if $B(y)$ is symmetrical. The program interpolate both curves (using INTERPOL) to the biggest interval and smallest step between both abscissas and convolute/correlate them).The result may be normalized. The program uses the FFT method to perform the calculations

Interpolation/Smooth

- Smooth… The Xplot smooth option smooths the Y data of the active graph. Two methods are available: i) Boxcar average: the results are a current set smoothed with a boxcar average of the specified width. ii) Least Squares: the results are a current set smoothed applying a least squares smoothing polynomial filter also called Savitzky-Golay smoothing filter. Xplot uses the SMOOTH function of IDL for the Boxcar method and the POLY_SMOOTH routine of Frank Varosi for the Savitzky-Golay one.

- Interpolation/Spline… This options creates a new Xplot window with interpolated data. This option is normally used to create a new set of data with the same look than the original, but with a different number of points. Three possible interpolations are possible: i) Linear Interpolation (using INTERPOL from IDL). ii) Spline interpolation (using SPLINE from IDL). This option asks for the TENSION value. The default value is 1.0. If TENSION is close to 0, (e.g., .01), then effectively there is a cubic spline fit. If TENSION is large, (e.g.,greater than 10), then the fit will be like a polynomial interpolation. iii) Parametric Spline (using SPLINE_P from

IDL). Here the number of points of the result is defined by the program itself.

Miscellaneous

- Find peaks. It uses a original algorithm to find peaks in a curve. For more information, please read the on-line documentation.

- Histogram… Makes histograms from the displayed data.

Operations with columns…

This option allows you to calculate a new column data in the current set as a function of the existing ones. The result can:

- Be appended to the set, thus substituting the current set by a new one with one more column.

- Substitute an existing column in the current set.

- Be exported to a new Xplot window.

The user has to type in the pop-up window the expression in IDL syntax to create the new column data. This expression has variables names named as `col1`, `col2`, etc. for referring to the existing columns in the current set. After the column operation the old X and Y columns are still displayed. You have to change manually the Y column to visualize newly created data (in the case that data is not overwritten to the same column).

This option allows you to do a lot of data analysis and data reduction operation on your data. For example, you can try with the data of tmp1.dat some column expressions (supposing currently display X is `col1` and Y is `col2`) (consider the new created column as a new Y column, unless specified otherwise)

- Normalization of the peak value to 10: col2/max(col2)*10

- Normalization of Y column data between in the Y interval [0,1]: `(col2-min(col2))/(max(col2)-min(col2))`

- Substract a straighth line Y=2X+3: `col2 – (2*col1+3)`

- Shift data vertically 10 units (vertical translation): col2+10

- Shift data horizontally 5 units: col1+5 (the new created column is now X)

- Average columns 2 to 4: (col2+col3+col4)/3

- Square of column X: `col1^2`

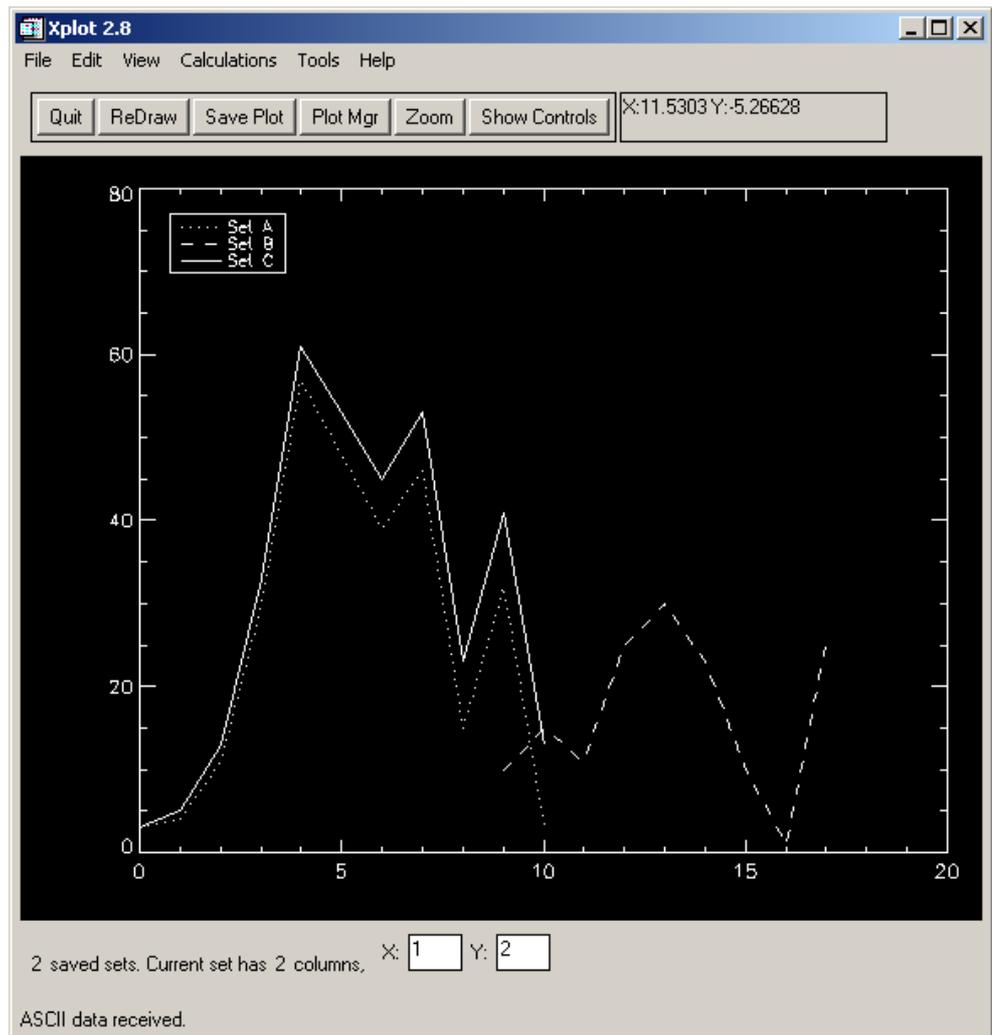- Natural logarithmic of column 1: `alog(col1)`

You can also type your expression as a function of other IDL functions.

Operations with sets...

This option allows you to create a new two-column set of data (which will be named C), as a function of the X and Y columns of the current set (that we call set A), and an optional two-column set (called B) that is sitting in a disk file. The user must provide an expression to create the abscissas and ordinates of the new set C (named Cx and Cy, respectively). This expression has to be written in IDL syntax, and is a function of the abscissas and ordinates of the data sets A and B (with abscissas Ax and Bx and ordinates Ax and Ay).

In the case that the abscissas of the A set (Ax) is different from the newly created Cx, then the A data set is interpolated to fit in the new grid Cx. The same happens for B, if two sets are selected.

An example: load the file tmp1.dat in Xplot, call Operations with sets... option and type in the input data window the following parameters: `Cx = Ax*1.0, Cy = Ay+By, Number of data sets: 2, A data set: current set, B data file: tmp2.dat, Write output to file: No, Overplot original data: Yes.` These inputs means that we want to create a new set C with abscissas values the same as the original one (Cx=Ax), and the ordinates value is Ax plus 2 times Bx, there B is a set defined in the tmp.dat file (in this example the sets A and B are the same, but is evident that B may be a file with any data). The input data window and the resulting new window with the resulting data (after clicking the `Accept` button) looks like:

In the new window you can see three data lines: The resulting one plus the original ones (as requested). Some values of set C are a bit different from the originals (set A) due to the contribution of the extrapolated set B.

You can merge the abscissas values of two data sets using the XOP MergeArrays library function: Cx=MergeArrays(Ax,Bx). The "Operations with data set" option can also be used to create data from scratch in Xplot. For that you may use the IDL function FINDGEN(N), that creates an array of N points starting from 0 and ending in N-1. You may operate with that in order to define the abscissas values (Cx), and then define the ordinates (Cy) as a function of Cx. However, it is simpler to use the option: Xplot|Calculations|Create data set…

Advanced features: XOP macros

You can do sophisticated analysis by creating an XOP macro. This is a sort of program that is interpreted line by line. You can use it to create and manipulate your data, to make iterative data analysis, etc. You can call XOP macro from Xplot|Tools|XOP Macro and optionally you can input the current plot in Xplot. You can also call Xplot from an XOP Macro.

Chapter

3

Modeling data (curve fitting)

Once one has the experimental data cleaned in some way (after doing some manipulation of data analysis or data reduction), one will probably want if the data agrees with some "model" which is expressed in terms of a mathematical function that depends on some parameters. The goal of the fitting process is to adjust this parameters to the data itself.

Fitting data to a polymonial

It is possible to develop methods which allow to fit data to a straight line or to a polynomial without any "a priori" estimation of the parameters. Xplot includes the following algorithms in the Xplot|Calculations|Fit – Polymomial&Gaussian… entry:

1) Chi-Square Linear Regression. It uses the IDL LINFIT function, which fits the paired data {xi, yi} to the linear model, y = A + Bx, by minimizing the chi-square error statistic.

2) Robust Estimation Linear Regressionv. It uses the IDL LADFIT function, which fits the paired data {xi, yi} to the linear model, y = A + Bx, using a "robust" least absolute deviation method.

3) Least Square Polynomial Fit. It uses the IDL POLYFITW, which performs a least-square polynomial using matrix inversion to determine the coefficients.

4) Singular Value Decomposition Polynomial Fit. It uses the IDL SVDFIT, which performs a least squares fit using singular value decomposition (SVD) It is based on the routine with the same name of Numerical Recipes in C: The Art of Scientific Computing (Second Edition), published by Cambridge University Press.

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Non-linear fitting (predefined functions)

Fitting data with a Gaussian with a polymonial background

Use Xplot|Calculations| Fit – Polymomial&Gaussian… option and select entry 5) Gaussian + polynomial background. Then select the wanted polymonial degree (up to a 2). It uses the IDL GAUSSFIT function which performs a non-linear least-squares fit.

Fitting data to to multiple peaks (Gaussians and/or Lorentzian)

Select the oprion Xplot|Calculations|Fit – Multiple peaks… It will ask you the maximum number of peaks wanted. An independet application (XpeakFit) appears that allows you to interactive define your peaks and background and then make the fit. It performs non-linear fit using the MPFit routine of Craig B. Markwardt.

Remember the formula for the Gaussian:

$$G(x) = A_0 e^{-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2} \tag{1.2}$$

with $FWHM = 2\sqrt{2\ln(2)}\sigma$. The lorentzian is:

$$L(x) = \frac{A_0}{1 + \left(\frac{FWHM}{2}\right)^2} \tag{1.3}$$

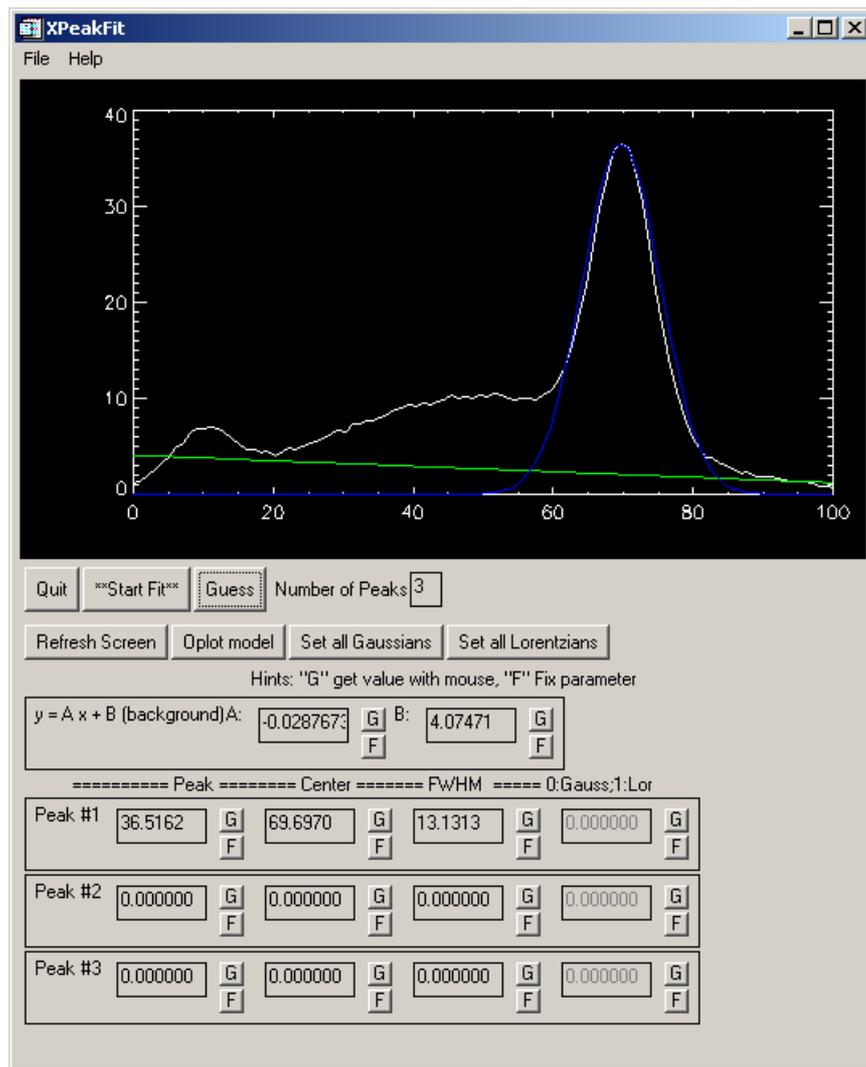And the psuudo-Voigt is defined as $C\,L(x) + (1-C)\,G(x)$

Example:

Create some fake data consisting in three Gaussians plus a noise. For that you can use an XOP macro, enter and run the following text:
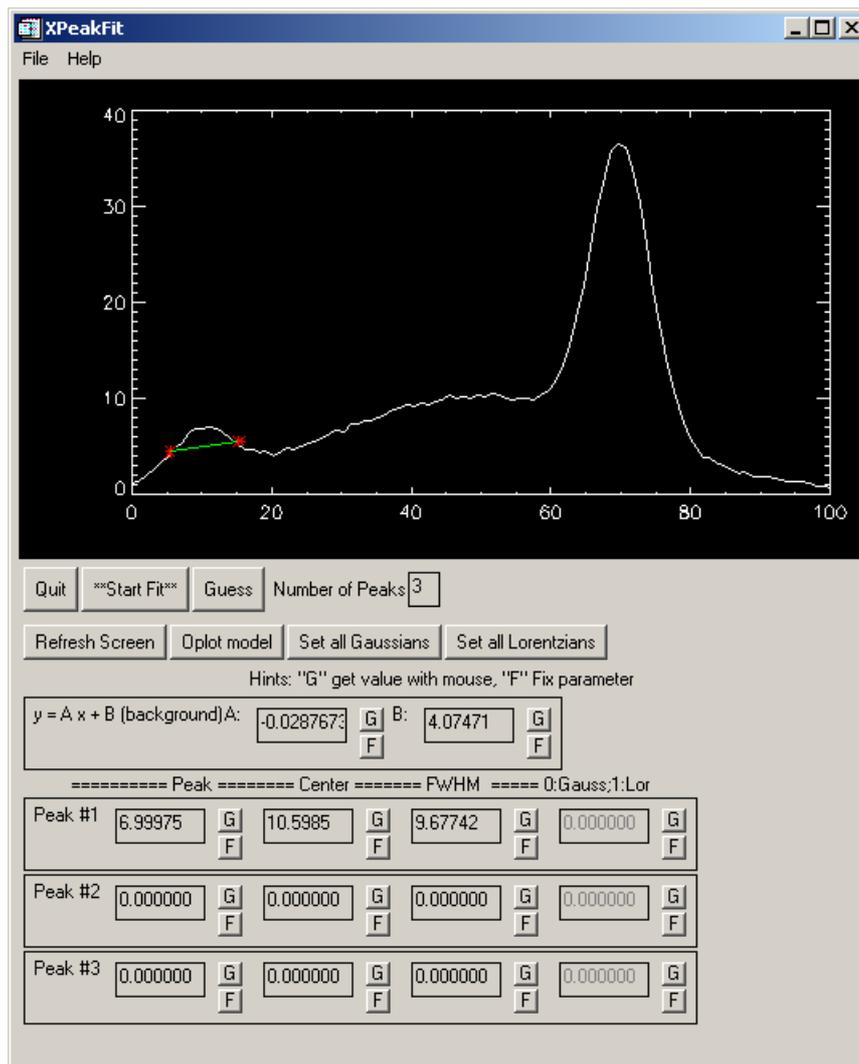
```
;
; create data set ( 3 gaussian + noise)
;
sigmas = [10.0, 50, 10.0]/(
2.0*sqrt(2*alog(2)) )
x=makeArray1(100,0,100)
y1= 5.*exp( -0.5*( (x-10.)/sigmas[0] )^2 )
y2= 10.*exp( -0.5*( (x-50.)/sigmas[1] )^2 )
y3= 30.*exp( -0.5*( (x-70.)/sigmas[2] )^2 )
ynoise =  0.5*randomu(seed,100)
y=y1+y2+y3+ynoise
;
; write data to a file (not needed)
;
OpenW,unit,'fakedata.dat',/Get_Lun
FOR i=0,99 DO printf,unit,x[i],y[i]
Free_Lun,unit
itmp = Dialog_Message('File fakedata.dat
written to disk.')
```

Open the resulting file (fakedata.dat) with Xplot and call Xplot|Calculations|Fit – Multiple Peaks… Enter 3 at the maximum number of peaks (we created three peaks). You will get the application window with the data loaded. We know that there is no background,.so we want to fix the background coefficients to zero. Click the "F" button close to the A and B coefficients of the background. They become inactive, meaning that they are "fixed", i.e., the fitting procedure will not change them. We know that the peaks are Gaussian and not Lorentzian, so we fix the last column parameter labelled as "0=Gauss,1=Lor". Cleck in the corresponding "F" buttons. Then click the "Guess" button to see what is the proposed starting solution. I got:
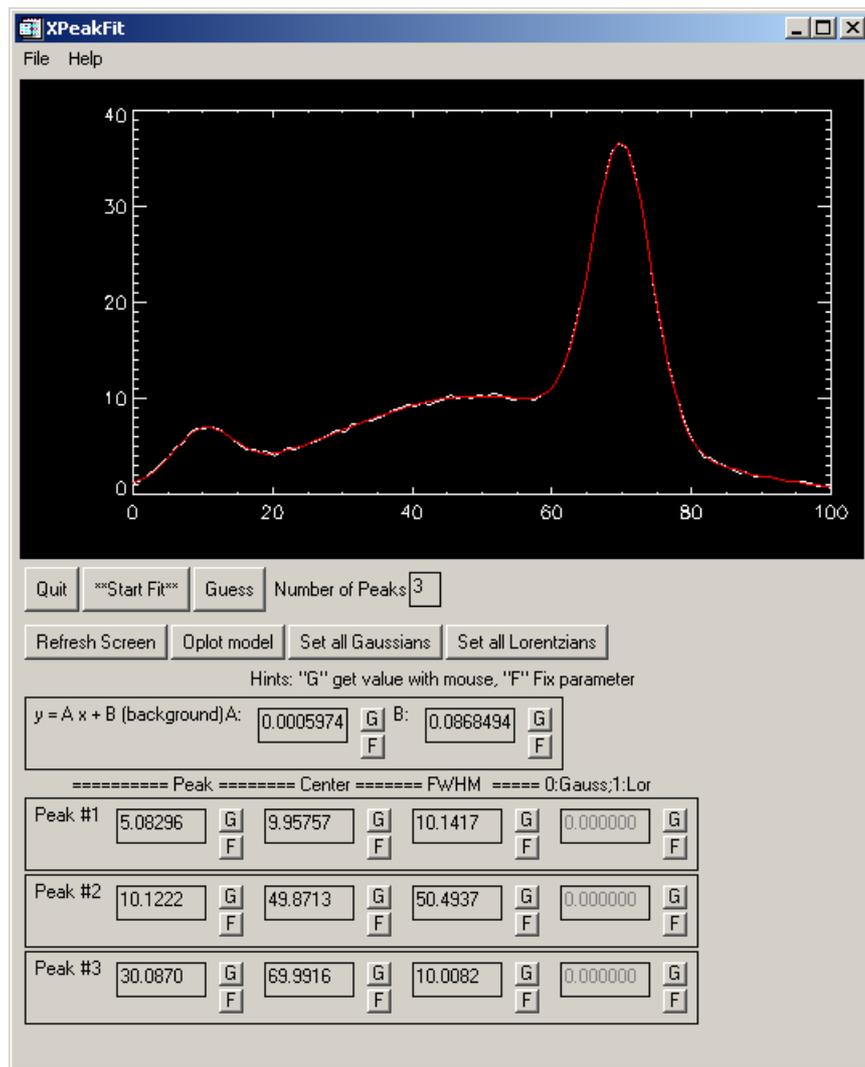
The proposed peak and background are not satisfactory for me, so I decided to improve them by hand. For that I will select the initial parameters with the mouse. Let us start with the Peak #1. Click the "G" (meaning GET) button close to the "Peak" or "Center" value. A info window will appear. Read it and click "no". Click on the plot on the top pf the first peak. A red asterisk will appear and the corresponding "Peak" and "Center" numerical values are updated. Click now "G" close to the FWHM value of the first peak. Select then two points in the plot that define the width of the first peak. I got:

Repeat the process for the second and third peak and click "Oplot model". You will see something like (if you clicked more or less where I clicked):

Note that the "guess" (in red) is higher than the data, because we selected single peaks and values what we got is the overall of all three peaks. It does not matter, it can make his work. Try then "**Start Fit**" and have a look at the look window. Click "Yes" to the question "Update parameters with fit results?". This is the result of the fit:

Non linear fitting (free function)

This option permits to fit the current set of data to a user-defined function, by using a non-linear fit. For the non-linear fit algorithm it is possible to choose between three models: MPFit (Craig B. Markwardt), CURVEFIT (IDL) and POWELL (IDL). The MPFit routine is highly recommended.

When this option is selected in Xplot, a new application window (XNLFit) is poped-up.

Warning: If you load a new data set (or change columns) in Xplot, you must restart the XNLFit to update the data.

The user must define the model function in IDL syntax as an expression of the independent variable x and a parameter array p. It should be placed in the `Model Equation` entry. For example a straight line is : p[0]*x+p[1], a gaussian is p[0]*exp((x-p[1])^2/p[2]) etc etc. Several

buttons are available to help the user to type the most standard functions (polynomials, gaussians and lorentzians).

The initial parameter guess must be provided in array notation in the `Model Parameters` entry: `[p(0),p(1),p(2),etc]`.

It is also possible to define the x range for the points to be used in the fit. By setting `xmin=xmax`, the program uses all the x interval for the fit.

The sigma (error) values for the data can be the unit for all points, or can be read from an external file, or can be set to statistical noise: sigma = sqrt(ordinate value).

In addition, the user may select the option to calculate covariance and error estimation on the model parameters.

When one of the fitting buttons is pressed, the resulting curve of the fit is overplotted in the main Xplot window with triangular symbols. Then the user is asked if he wants to update the model parameters to the fitting result. The overplotted triangular points (fit's results) disappear when the screen is refresh. If one wants to conserve the fitting data, them he should save them as a new data column, by using the `Put Model in a new column` button.

For example, let us fit the data in tmp1.dat with a sinus function `p[0]*sin(x/ p[1])`, with initial guessed parameters `p=[50,5]`. When clicking the `Start Fit` button, one gets:

The fit result is not excellent. Perhaps we should try another model…

Working with SPEC data files

A SPEC file is an ASCII file containing one or several blocks of data (called scans, the same as what we called sets) preceded by a header. Any header line is preceded by a # symbol #. After the # it contains a letter (or set of letters) to define keywords. Many standard and user-defined keywords can be present in a SPEC file. However, xplot needs only three keywords: #S to indicate the scan number and its title, #N with the number of columns, and #L with the labels for the columns **separated by double blank.**
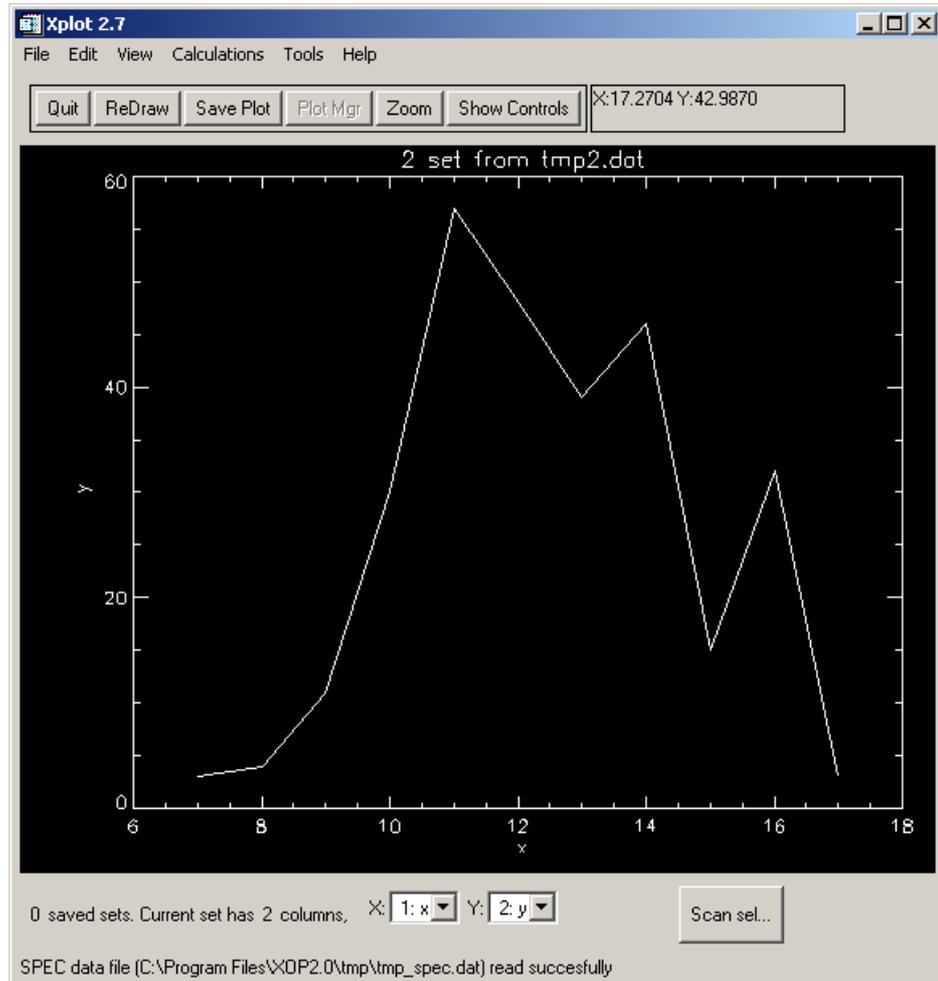
Generalities

Xplot has the availability of visualizing and analyzing SPEC formatted data. It includes tools to navigate between the different data sets stored in a SPEC file, and therefore to apply all the Xplot options to these data. In order to store a SPEC data file in Xplot, use the `File/Load data File...` option and select a SPEC file. Once you have done that, the first scan in the file is displayed in the Xplot window, and the bottom part of the Xplot window changes a bit its aspect, allowing to change columns with a pull-down menu and to change scan number with the "Sel Scan…" button.

Warninig: A SPEC file for Xplot must be ASCII, with the corresponding end-of-line character correctly set. This means that if you transfer to your windows-PC a SPEC file created in a Unix workstation using ftp in binary mode, or simply dragging it to your PC, you will not be able to open it with Xplot. You need to create the correct end-of-line characters (for example by opening and saving it with WordPad, not with Notepad).
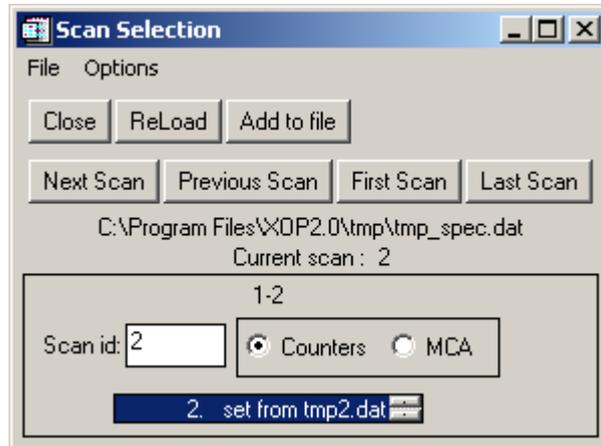
For example, let us build a SPEC file with the data we used from tmp1.dat and tmp2.dat. Let us call the new file tmp_spec.dat:

```
#S 1 set from tmp1.dat
#N 2
#L x  y
0 3
1 4
2 11
3 30
4 57
5 48
6 39
7 46
8 15
9 32
10 3
#S 2 set from tmp2.dat
#N 2
#L x  y
7 3.0
8 4.0
9 11.0
10 30.0
11 57.0
12 48.0
13 39.0
14 46.0
15 15.0
16 32.0
17 3.0
```

Load it in Xplot:

Now is possible to change the abscissas and ordinates of the current plot by using the drop-list widget with the titles of the SPEC columns in the current scan. In order to change scan number, just press the `Scan sel...` button, and a new window with this aspect will be created:

From this window is possible to change interactively the scan number by typing its identifyer in the `Scan id.` plus <enter>. Please read the documentation of the SpecAccess library in order to know the possible identifiyers of a scan in a SPEC file. By clicking the exclusif buttons Counters/MCA, you may select data from the scans with the two formats allowed in the SPEC files: the standard one and the MCA (Multi Channel Analyser) one. It is possible also to use the cursor up and down arrows to navigate in the scan list.

You can navigate and manipulate data in your display. Note, however, that possible modifications, etc, are not saved in the SPEC file, which remains intact.

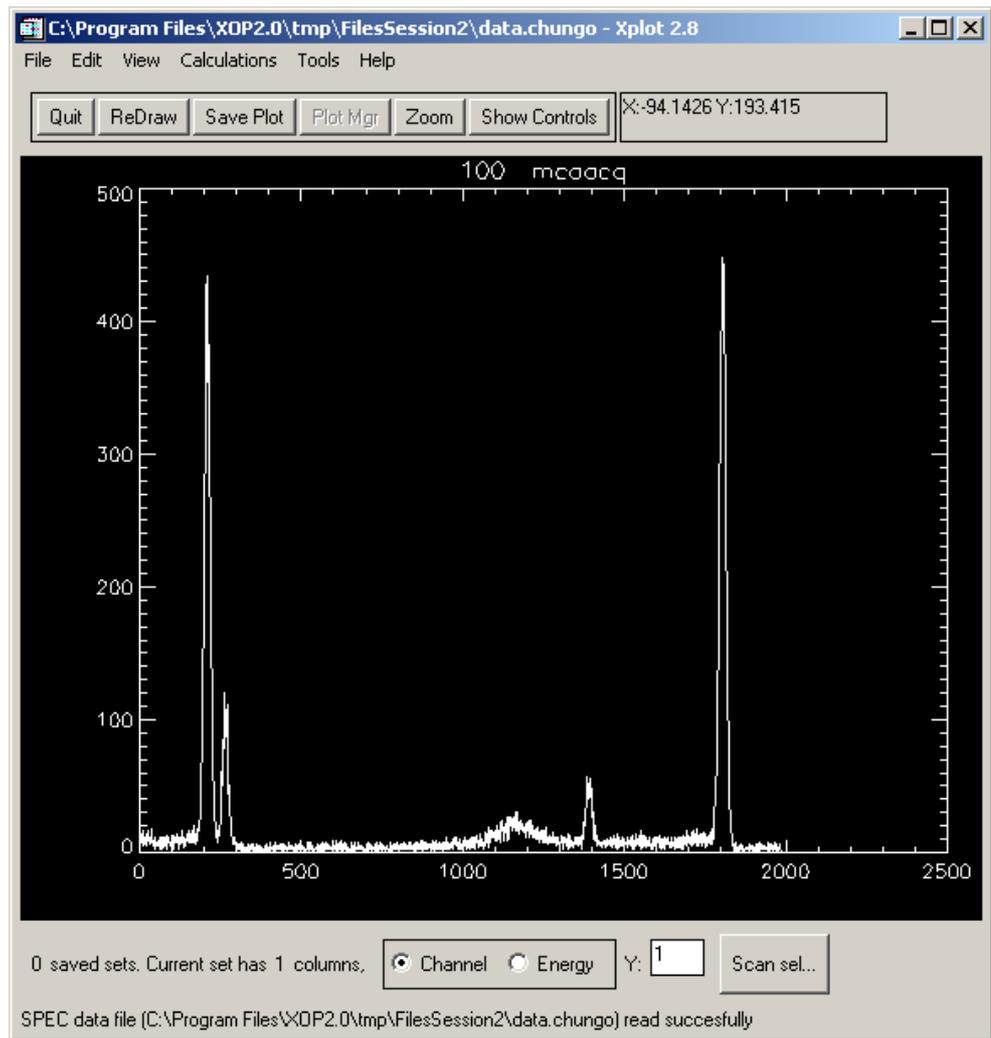## Change information in titles, scans, etc

You can see when you load a SPEC file that the SCAN number is displayed at the title of the plot and the column titles (motor and detector names, in the SPEC language) ate in the titles. For that some convention is needed. This is done in the Xplot|Edit|Titles… window. In order to get the column names in the X and Y titles, you must put "-1" in the corresponding title entry. In the main title, you can put a SPEC keywors (i.e., #S) and you will see in the graph window that the full line corresponding to that keyword appears. In the case that more than one keywords with the same value are found, Xplot displays the last one.

Cleaning files

A SPEC data file contains many scans, but only a subset of them are useful. The first step in our data manipulation can be to remove bad scans and perhaps to select the useful interval for the good ones. For that, Xplot proposed a mechanism consisting in creating a new file, and copying there only the good scans in the wanted interval. We call that "cleaninig". For doing that, open a SPEC file. In the Scan selection window (available by pressing the "Scan sel…" button, you must select the new file name in the File|Define file for storing cleaned scans… option. Then go to the first scan. If it is good, select the X interval containing the good data, and click "Add to file" button. If you want to write the whole interval, press first "ReDraw" in the main Xplot window, and then you will be asked if you want to copy the whole scan to the file. You can use the cursor arrows to change from one scan to the next or previous one.
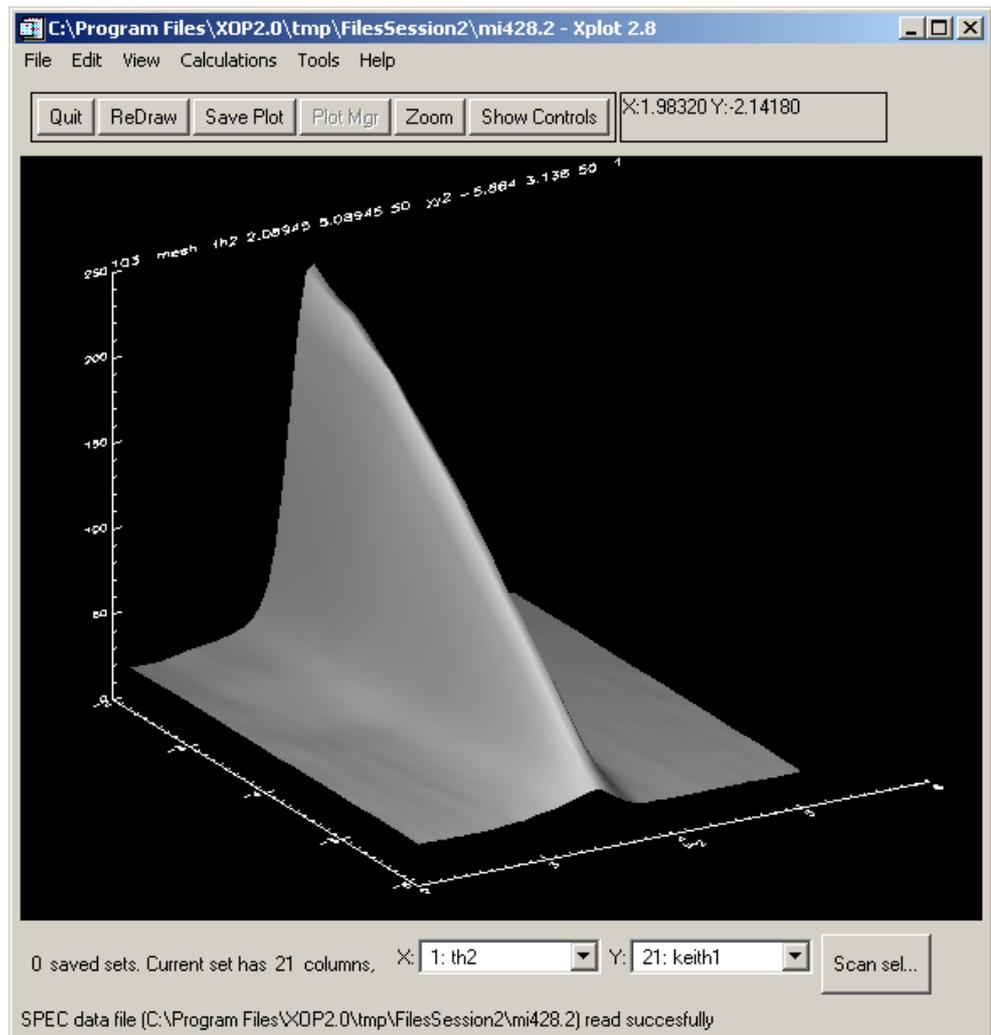
MCA

You can display MCA SPEC scans with Xplot. You can visualize then either in "channel" or "energy" scale. The energy (or "calibrated") scale is calculated using the A, B and C coefficients available in the MCA data header after the [#@CHANN](#) keyword. The energy values E are calculated as a function of the channel values X with: $E = A + Bx + Cx^2$

MESH/Surface plot...

Although Xplot has been designed to plot XY graphs, it can also display some graphs multiple data sets. A multiple data set is defined as a single data set with different plots one after the other. All individual plots must have the same number of points. The position where a plot ends and the next plot starts can be defined by the line position (or the number of points of the individual plots) of by an additional label column. The label column has a different value for each individual plot. Three kind of MESH view are possible: lines, surface and contour.

Operating with scans (Exodus)

Xplot can make operations with data from different scans only by exporting one scan to an auxiliary external file, and using Xplot|Calculations|Operations with sets… Sometimes, the user may need a quick access to data from several scans and average and operate with these data. For that, it is recommended to use the Exodus application (available in the Xop/Xaid extension) in combination with Xplot.

SpecAccess library and XOP macros

It is possible to write XOP macros to perform iterativeoperations with Spec files. For that one should call directly the routines in the SpecAccess library. An example to split a Spec file in many files, one for each scan, can be found in the file `splitspec.mac`.