XAID:
Software tools for visualization and analysis of XAFS spectra

XAID is a user-friendly package to perform XAFS data analysis. It is intended for visualization, averaging, extraction, filtering, etc. of single or multiple sets of raw data. For a more sophisticated analysis, including fitting to a model or *ab-initio* calculations, other codes should be used. See the XAFS Software Catalog and chose your preferred code.

Modules for standard XAFS analysis:

- XAID_MU2CHI EXAFS signal Extraction
- XAID_FF Fourier Filtering
- XAID_CALIB Calibration of dispersive XAFS spectra

Modules for multiple spectra analysis

- EXODUS Visualization, interpolation, reesampling, averaging, linear combination and fit from multiple spectra contained in SPEC data files. This module has been especially written for ID26.
- DELIA Simultaneous visualization, interpolation, calibration, extraction and Fourier filtering on a bunch of spectra (typically dispersive XAFS experiments). This module has been especially written for ID24.

DABAX tools

- Tables of atomic scattering factors f1 and f2
- McKale phases
- EXAFS spectra database
- XANES spectra database

Starting the program

If you are at ESRF (www.esrf.fr), the programs are installed in the NICE cluster and may be accessed by any workstation. For that enter (this command is also good for any Unix installation):

```
xop xaid
```

or (in case this fails):

```
/sware/exp/xop-2.0/xop xaid
```

If XAID starts correctly, a window like this one should appear:

From this window you should start the different XAID modules using the `Start...` menu.

Installation

XAID can be freely installed in virtually any kind of machine. It is distributed as a part of the XOP software package. Two steps must be followes (see XOP website /www.esrf.fr/computing/scientific/xop)

1. Download and install XOP
2. Download and install XAID as an "XOP extension"

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Module XAID_Mu2Chi

Module characteristics

- **Goal:** to obtaing the XAFS signam *Chi(k)* starting from the absorption signal *Mu(Energy)*
- **Input:** A 2 column file with *Mu(Energy)* data. It may also receive data from other XAID modules.
- **Output:** To a 2-column ASCII file, or passed to the XAID_FF module, or passed to XPLOT module for better visualization and further processing, or a combination of them.
- **Tricks:**
  - Zoom at any time by selecting a box in the window.
  - You may use `View->XPlot` at any time to get more details on your data.
  - It is recommended to display *Mu* in *k* scale before starting the post-edge fitting, although this is not stricktly necessary.

Follow the steps

1. **Load** a 2-colums ASCII file with input data (Energy in eV in the first column and Mu(Energy) in the secondone) by using the `File->LoadFile` menu. Use for example the file: Ge_calib.dat.
2. **Preparation of the data:** you may use the `Operation1->Cut` item to select the good interval for the analysis, or may be `Operation1->Interpolation` to change the number of points.
3. **Selecting of Eo:** using `Operation1->Get Eo`
4. **Pre-edge fitting** Usually done by fitting the pre-edge with a straight line. Use `Operation1->Fit Polynomial->Least Squares` option for that. If the results of the fir is satisfactory, then substract the Fit from the Mu(Energy) signal using `Operation2->Substraction`
5. **Jump calculation** using `Operation1->Jump`
6. **Display Mu(k)** using the buttons in the lower part of the window
7. **Post edge spline** This is the more delicate part and the quality of your *Chi(k)* signal depens on your ability to perform this fit. It is more an art than a science. Use `Operation1->Fit Multispline` option. The default option may work, but, select the minimum of the fit interval around 2 or 3 Angstroms. By default, it presents the full interval. A technical trick: negative values are presented (although they do not exist physically). This is to obtain smoother fits in the case of selecting the full interval). You may use the zoom option (just by selecting the box to be zoomed). Zoom back is done using `View->Refresh` or just clicking on the window. If you do not like this spline, you can perform another one by reselecting `Operation1->Fit Multispline`. If you want to carefully study your data and the spline, it is recommended to use `View->XPlot`

option. See an example window.

8. **Extraction** Once you have a satisfactory post-edge spline on the screen, go to `Operation2->Extraction` to obtain the *Chi(k)* signal. Three options are available, that apply different extraction algorithms:
    - Experimental: `{chi(E)=(mu(E)-mu_at(E))/(mu_at(E)-mu_bck(E)) }`
    - Constant: `{chi(E)=(mu(E)-mu_at(E))/jump}`
    - Lengeler-Eisenberg: `{chi(E)=(mu(E)-mu_at(E))/jump*LE(E)}` with `LE(E) = 1- (8/3) [(E-Eo)/Eo]`

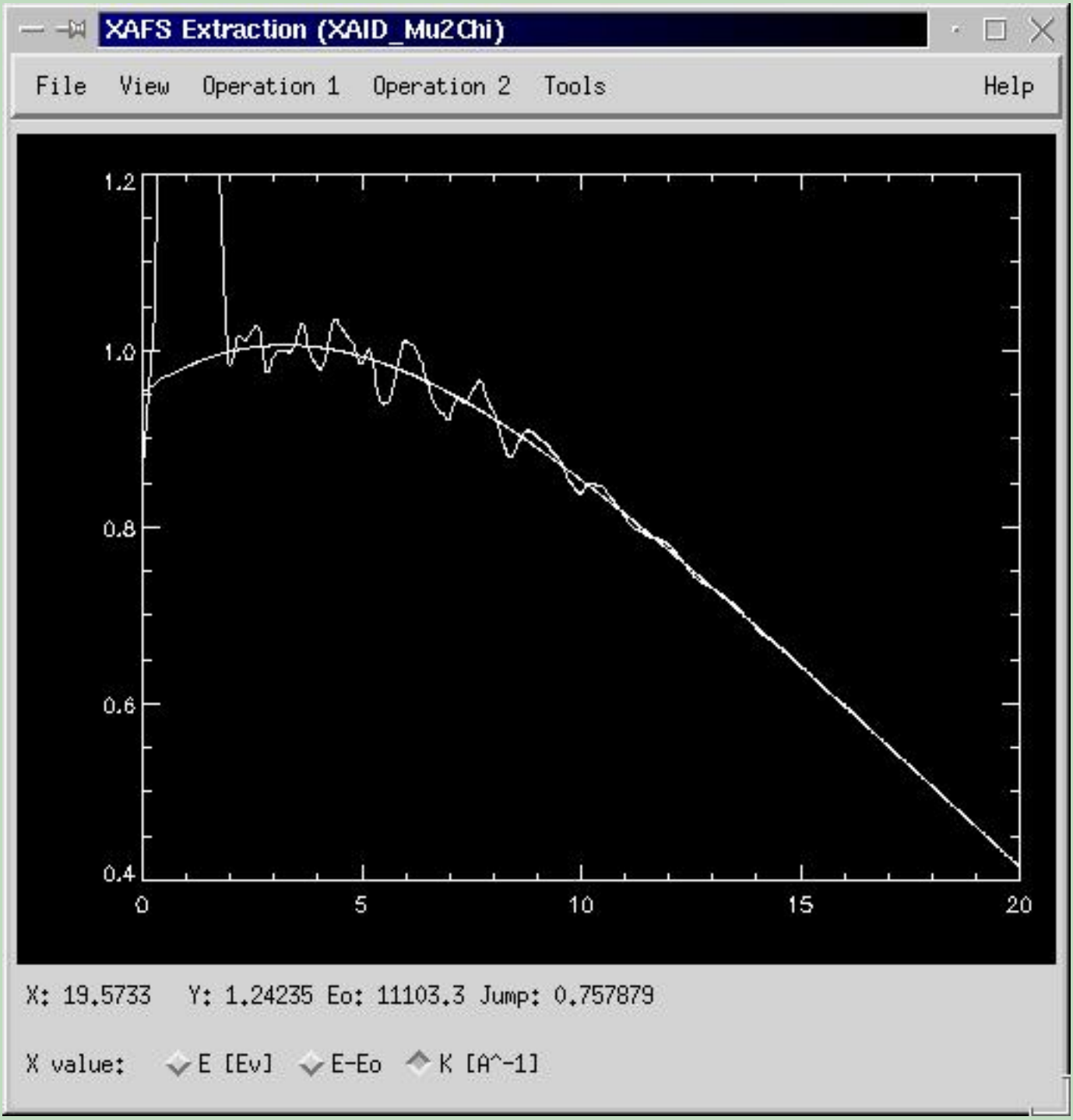
    After the extraction you are asked to either substitute or go to XPlot for a better look. Click `substitute` if you are sure you do not want to go back to post-edge spline.
9. **End** After the extraction you can save the result to a file using `File->Save File` or inject the result in the Fourier filter application XAID_FF using `Operation1->Fourier Filter`. In most cases, specially when you have negative *k* values, it is recommended to cut your spectrum to a useful interval before saving.

FAQs

- **Can I load a scan from a SPEC file in XAID_MU2CHI?**
  Not directly. You can however open XPlot (e.g., `Tools->XPlot`, load your SPEC data file in XPlot, and start XAID_MU2CHI with your selected scan from the XPlot `Calculations->XAFS->Xafs Extraction (xaid_mu2chi)`
- **Do I need to follow literally the given steps?**
  No. But you need some logic in your analysis: in a widget application you risk to get any bad result or even crash the program because the combination of different possible actions is close to infinity and the author does not have the time to check all of them.
- **What do the strange labels "Operation 1" and "Operation 2" in the menu bar mean?**
  "Operation 1" refers to operations with a single data set (i.e., when you see only a line in the graphical window). "Operation 2" refers to operations between two data sets (two lines displayed).

Window example

This is the window (zoomed) at the step 7 using the example data file and performing the post-edge spline starting at 3 A.


XAFS Extraction (XAID_Mu2Chi)
File
View
Operation 1
Operation 2
Tools
Help
1.2
1.0
0.8
0.6
0.4
0
5
10
15
20
X: 19.5733 Y: 1.24235 Eo: 11103.3 Jump: 0.757879
X value:
E [Ev]
E-Eo
K [A^-1]

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Module XAID_FF

Module characteristics

- **Goal:** to calculate the Fourier Transform (FT) of a XAFS spectrum *Chi(k)* and the Back Fourier Transform (BFT) of a selected region of the FT. *Chi(k)* can be weighted with powers of *k* (from 0 to 4) and many weighting windows are available.
- **Input:** A 2 column file with *Chi(k)* data. It may also receive data from other XAID modules.
- **Output:** A SPEC-formatted data file with signal, FT and BFT (Use `File->Save File`).
- **Tricks:**
  - After changing any parameter, press "Enter" to refresh calculations.
  - The syntax of the intervals is: [min,max]. The square brackets and the separating coma are must always be entered.

Follow the steps

1. **Load** a 2-colums ASCII file with input data (*k* in A in the first column and *Chi(k)* in the secondone) by using the `File->Load File` menu. Use for example the file: Ge_calib.chi.
2. **Input:**
   - The *k* limits for the FT (in left window)
   - The *R* interval in central window (limits for the FT plot).
   - The *R* limits for the Back Fourier (in central window). The BFT is calculated from the FT within these limits in *R*. The selected limits appear as vertical lines in the FT window (central window). This helps to select more accurately the wanted limits, normally including one or several peaks in the FT.
   - The *k* limits for the congugated variable (BFT in the right window). Note that this interval must be smaller than the "k limits for the Fourier Transform" interval in the left window, otherwise some numerical inconsistences appear.
   - The "Shell radius *r*for the back phase". This affects only the BFT phase. The BFT is written as *A(k)*sin(2kr+Phi(k)*). The phase is *Phi(k)*.
3. **Press `Enter` for calculating and updating the windows after entering any new parameter.** See an example window.

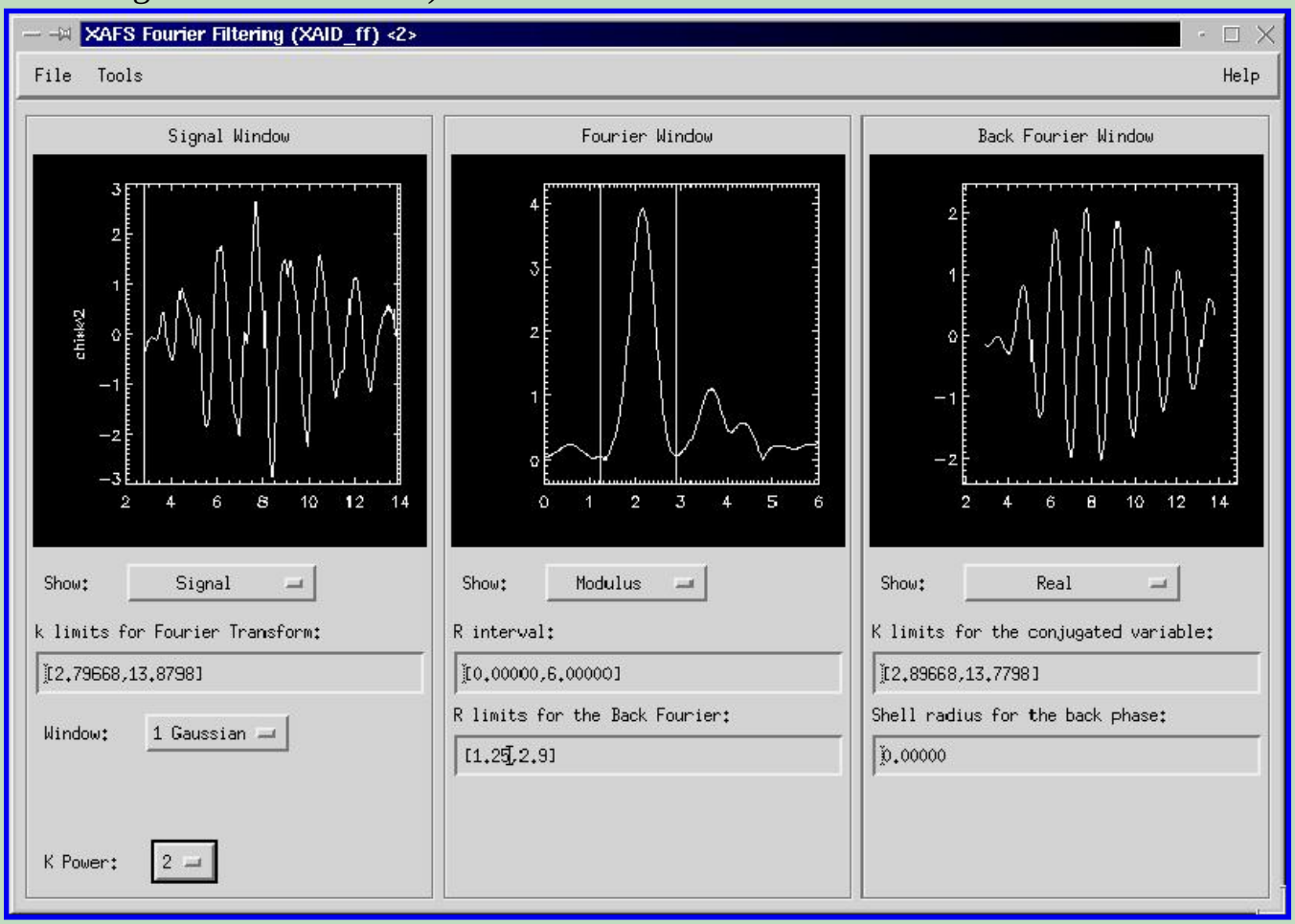
FAQs

- **Can I load a scan from a SPEC file in XAID_FF?**
  Not directly. You can however open Xplot (e.g., `Tools->Xplot`, load your SPEC data

file in Xplot, and start XAID_FF with your selected scan from the Xplot `Calculations->XAFS->Xafs Extraction (xaid_ff)`

Window example

(click on the image for full resolution)



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XPLOT

XPLOT is the common visualization tool for most XOP applications. A manual for an older version is available at: http://www.esrf.fr/computing/scientific/xop/xplot/

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Module XAID_CALIB

Module characteristics

- **Goal:** to calibrate a XAFS spectrum *Mu(x)*. Calibration is done by calculating *Mu(Energy)*, where the energy is calculated as a second degree polynomial in *x*. In other words, this module helps in finding the *a,b,c* coefficients in:
  Energy_eV[i] = a+b(x[i]-x[0])+c*(x[i]-x[0])^2*
  being *i* the index of the *i*-th point. (The substraction of x[0] is essential for TurboXAS experiments performed in ESRF/ID24 beamline).
- **Input:** Two files:
  1. A 2 column file with calibrated spectrum (reference file) *Mu(Energy_in_eV)*.
  2. A 2 column file with spectrum to calibrate *Mu(x)*.
- **Output:** The *a,b,c* coefficients (displayed in main window).
- **Tricks:**
  - Remember you always move the dashed (calibrated) plot, and the continous (reference) remains fixed.

Follow the steps

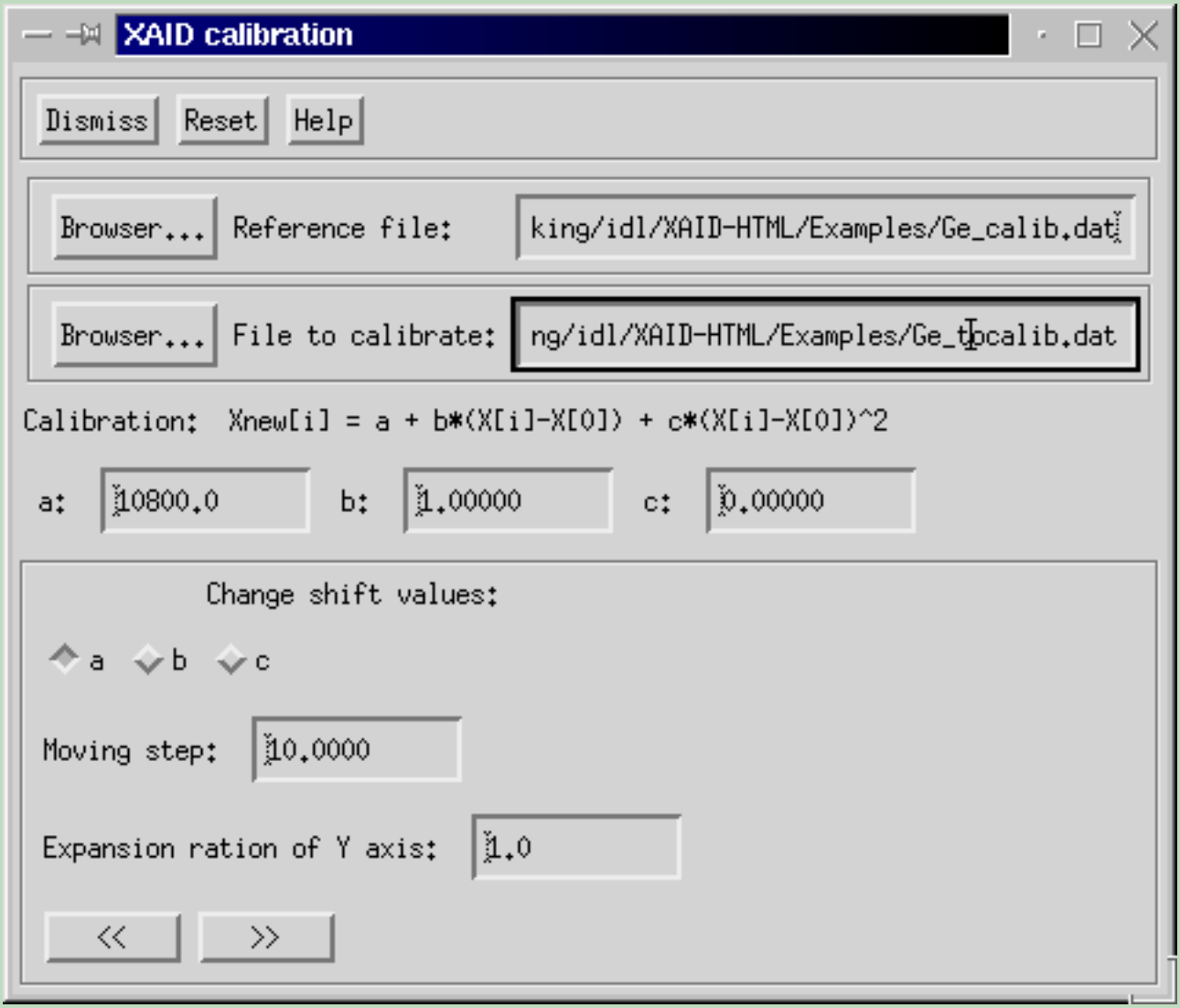
1. From the main window (see Example window 1), **Load** two files, the first one with the reference spectrum and the second other with the spectrum to calibrate. As examples, use the files Ge_calib.chi and Ge_calib.chi, respectively. Once both spectra are loaded, an auxiliar XPLOT window (see Example window 2) appears. An estimated *a* value appears automatically.
2. Change *b* manually with the expansion compression value. In the example, I estimate that the dashed spectrum must compress at least 20 times to fit the solid one, so I put .05 in b and **then I do not forget to press ENTER for refreshig the plot**.
3. Change *a* manually to a better estimation. You can estimate the value that the edge of the dashed (calibrated) spectrum must move to align to the continuous (reference) spectrum by using the (x,y) cursor position in the XPLOT window. In the example, I estimate that it should be moved 200 units (11100-10900) to the right, so I changed *a* from 10800 (initial guess) to 11000. **And then I do not forget to press ENTER for refreshig the plot**.
4. Then I click on the *a* button, and fine tunning the *a* value using the "<<" and ">>" buttons. You may change the step of the movement.
5. Then I click on the *b* button, and do the fine tunning. I may neede iterating *a* and *b* tunning. It may also be necessary to use the non-linear term *c*.
6. Occasionaly, the heigth of the twe spectra is different avoiding a good overlapping. For that you can expand the Y axis using the value "Expansion ratio of Y axis". This helps in

the fine tunning but does not affect the resulting coefficients.

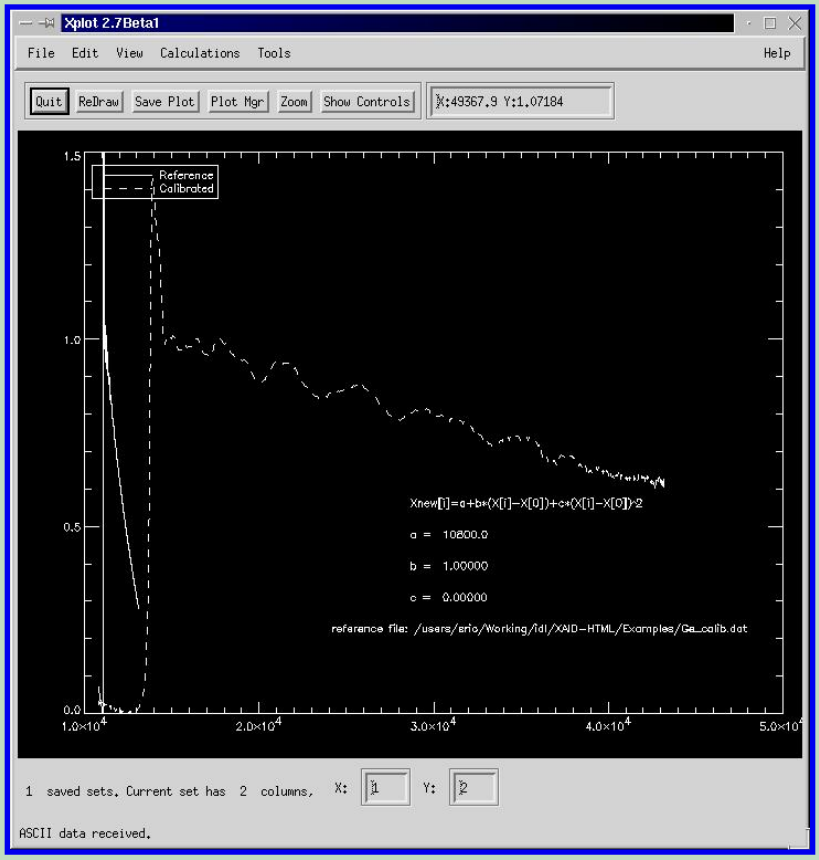
7. A calibration (not exceptional) is shown in example window 3.

Window example

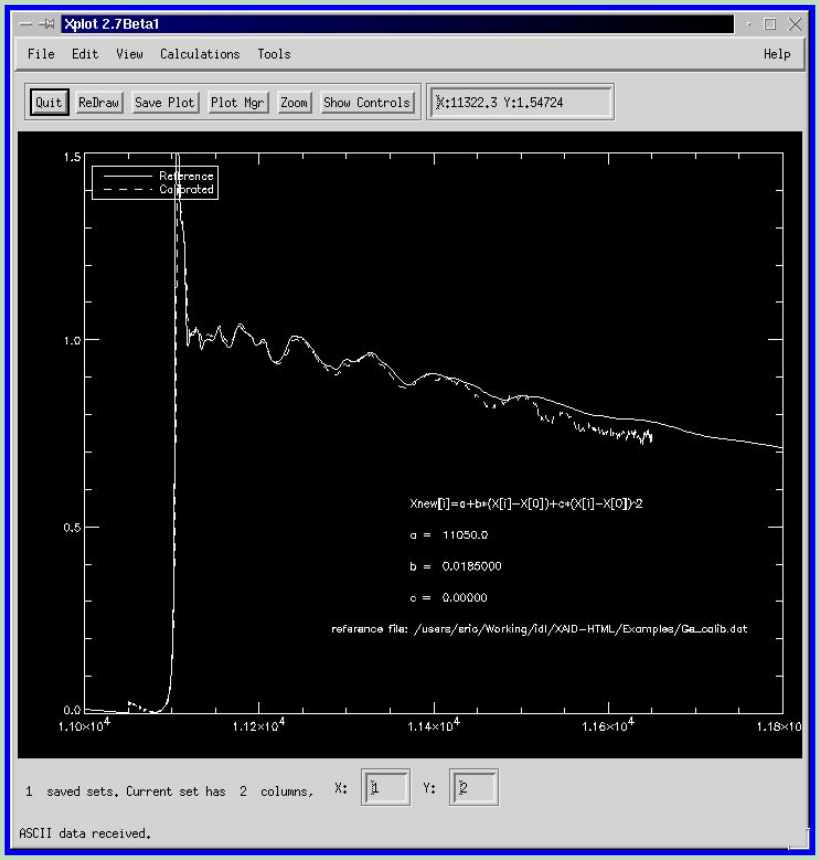
Window 1: Main window after loading the two example files.



Window 2: XPlot auxiliar window after loading the two example files.
(click on the images for full resolution)



Window 3: XPlot auxiliar window with a result of calibration process.



FAQs

- **May I zoom the image and fix the limits to the zoomed area?**
  Yes. Just select the wanted area to zoom, click the `Zoom` button and go to `Edit->Limits->Set Limits as Selection Area`. The next plots will be displayed in the selected area. To go back to the defaults, go to

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Module EXODUS (EXafs Of DilUte Samples)

Module characteristics

- **Goal:** to load a SPEC file and selecting, viewing, averaging, and perform operations with data from multiple scans. This applications has been designed for the particular needs of the ESRF/ID26 beamline. However, it can be useful for any data analysis involving manipulation with data from **several** scans from a single or multiple SPEC data files.
- **Input:** A SPEC file (use `Import->SPEC file`)
- **Output:** The results of the operations performed with EXODUS can be injected into other XAID applications, into XPlot, and they can also be written to a file (ASCII, SPEC or DELIA format).
- **Tricks:**
  - **Multiple selection:** for exploiting all the possibilities of EXODUS, it is essential to know how to select multiple lines in the lists. Click on a line for a single line selection. Then press `Shift` and click on another line on the same window (while `Shift` is pressed) for selecting a block of lines. For selecting multiple individual lines use `Control` instead of `Shift`.

Follow the steps

1. **Import a SPEC file** The list of scans appears in the left window.
2. **Copy from left (import) window to right (process) window the data to be processed**
   - Several controls in the left panel allows you to identify the scans you want to use and their scan columns.
     - `View Scan` button allows to display the header and/or data of a single scan. You can visualize other scans by either using the `View Scan` button in the left panel of the main EXODUS window or by using the `Scan Sel...` button in the created window containing the scan.
     - `Plot Scan` button allows to plot a single selected scan. The XPlot window helps in identifying the wanted columns. Double-clicking in a scan line has the same effect as selecting it and the pressing `Plot Scan`.
   - When you identify a single or multiple scans containing the data you want to use (process), then fill the wanted columns in the `Cols X` and `Cols X` boxes, select the multiplication factor of the X column to obtain X in eV (e.g., use X*1000 if the scan energy is in keV) and press the `=>` button in the central panel. With this, your selected data is copied to the right panel (processing area)
     Use `*=>` button if you want to copy all the scans (independently of the selection). If you want to process data included in several SPEC files, then `Import->SPEC file` the next file and repeat the process. The data copied to the right window is not deleted when other files are imported.
     The example window 1 shows the look of the window after the two first steps.
3. The right (process) window allows different operations:
   - **Visualization of a single data set:** select a single line and press `Plot` button (the same effect os obtained by double-click on the data line). The data is sent to an XPlot window for visualization. You may use all the features of XPlot for analysis.
   - **Visualization of multiple data set:** select several lines (using `Shift`+click or/and `Control`+click) and then press the `Plot` button. An "EXODUS multiple plot" window appears

containing an overplot of all data sets. You can zoom a selected region just selecting the wanted region with the mouse (use `Zoom Out` button or just click on the graph to zoom back). This window also allows to display the different spectra shifted vertically one respect to the other. For that press `Edit Parameters` button, select a "Shift spectrum factor" different from zero (zero means no shift, one means shift a distance equal to the height of the first displayed spectrum). Then press `Accept` and a shifted plot appears.
    - **Delete** the data sets: use the `Delete` button to delete the currently selected data sets, or use the `*Delete` button to delete everything.
    - **Edit labels** use the `Edit:->Title` option to change the labels of the data sets for a more meaningful text.
4. **Operations** with data sets in the right (process) panel. This is the most important part in processing your data with EXODUS. It allows you to perform a selected operation (interpolate, average, sum, perform a customized operation and fit a linear combination) on the selected data sets:
    - `Operations:->Interpolation` This option builds interpolated or resampled data sets from the selected ones. The interpolated/resampled data sets will have the same abscissas array. The abscissas array can be selected between different options: i) like the first data set, ii) customized with constant step in *Energy* scale, and iii) customized with constant step in *k* scale. The results can be added to the list of data sets (right panel) or be injected in XPlot for visualizing in 2D (multiple column format) or in 3D. You may want to save the results in XPlot to a file using `XPLot->File->Write ASCII file with current set...` option.
      Two algorithms are available:
        - **Interpolation:** linear interpolation. The y value for the new x value is calculated by linear interpolation between the two closer neighbours. This option is recommended when the number of points of the interpolated array is of the order or bigger than the number of points of the original array.
        - **Resample:** Some kind of smooth interpolation. For each resampled point *x[i]* of *xNew* it calculates yNew consisting in the average y values of all points *(x,y)* sitting in the interval *[x[i]-0.5*step1,x[i]+0.5*step2]*, with *step1=x[i]-x[i-1]* and *step2=x[i+1]-x[i]*. In the case that step1 or step2 are undefined (first and last points) we used *step=[x[1]-x[0]]* instead *step1* or *step2*.
    - `Operations:->Interpolation` This option averages the selected data sets. For that, if the abscissas are different, it makes an interpolation (see before). The result is added to the list in the right panel.
    - `Operations:->Sum` This option sums the selected data sets. For that, if the abscissas are different, it makes an interpolation (see before). The result is added to the list in the right panel.
    - `Operations:->Customized` This option allows you to program a customized operation. The result is added to the list in the right panel.
    - `Operations:->Fit LinCom` This option allows you to perform fit a given data set in the list (target) as a linear combination of other data sets (components) in the list. This option is useful whilst analyzing XANES spectra of compounds or mixtures, and wanted to know the percent of its components. The data sets to be used as target and components are identified by their indices in the right panel list, starting from zero. If the list is long, you may want to use the `View:->Info` option to help in identifying the indices of the wanted data sets. The fit is performed using the Levenberg-Marquardt [MINPACK-1] method as implemented in the MPFit IDL routine. The result of the fit is added to the right panel list.
5. **Export** options: the data sets in the right panel list can be exported to other applications (like XAID_MU2CHI or XAID_FF) or to a file in the following formats:
    - **ASCII file** a file containing two columns and an optional commant line. **Only a single data set (not multiple sets) can be stored in an ASCII file.**

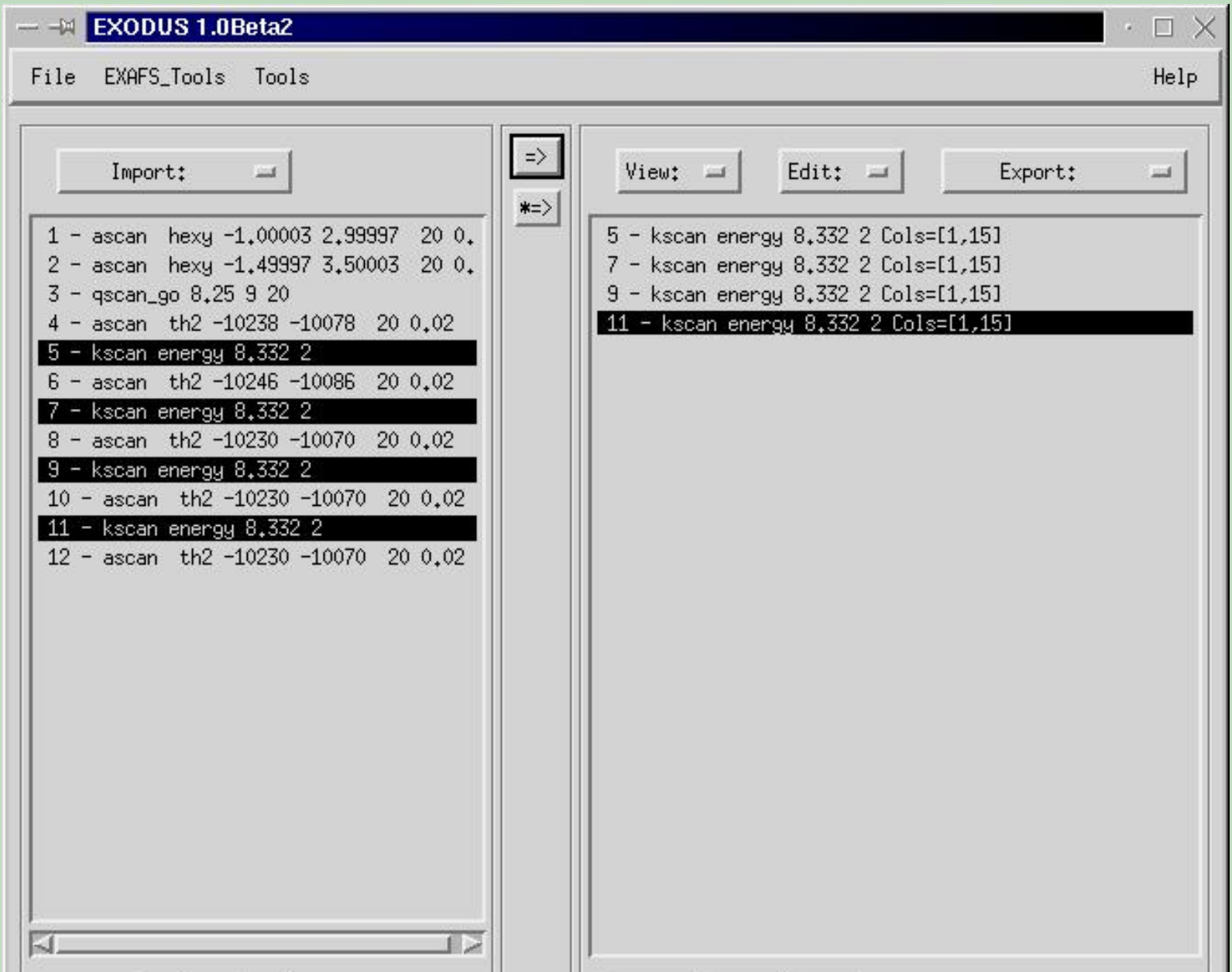
- **SPEC file** The selected data sets are written to a new SPEC file or added to an existing SPEC file. This option is particulary useful to save some kind of workspace of the current work: just select all data sets in the right panel and save to a new SPEC file. The resulting file can then be imported in a new EXODUS session.
- **DELIA file** The selected data sets are written to binary file in DELIA format. Note that this option does not save the labels. The data sets will be indexed in the DELIA file as they appear in the right panel.

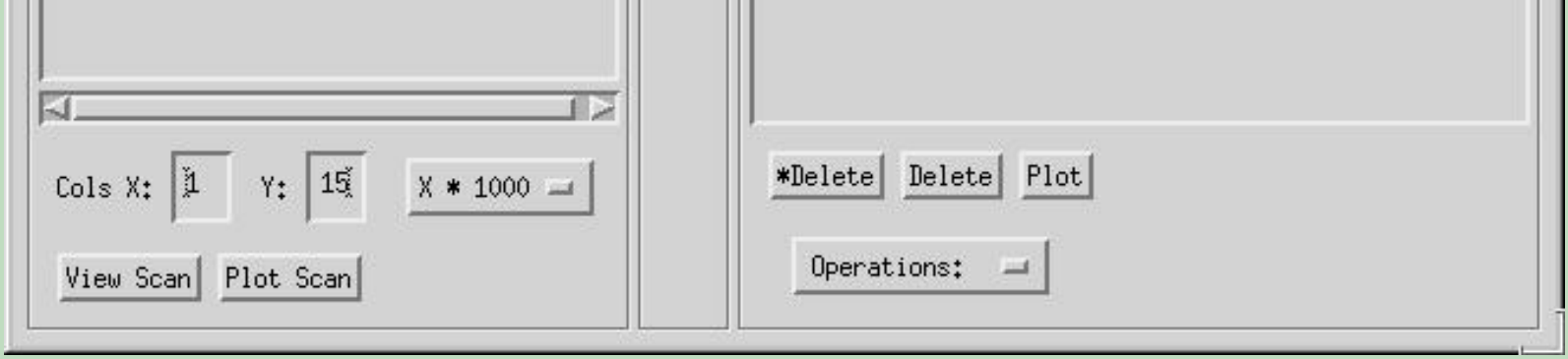
FAQs

- **Can I do other operations like spline, convolution etc. on the spectra?**
  Yes, but on a single spectrum. Just double click on the data set line in the right panel, and use the `Caluclations` menu in the XPlot winwdow.

Window examples

Window 1. Status of the EXODUS window after steps 1 and 2.




Cols X: 1
Y: 15
X * 1000
View Scan
Plot Scan
*Delete
Delete
Plot
Operations:

[Back]

Module DELIA (Dispersive Exafs caLIbration and Analysis)

Module characteristics

- **Goal:** To perform operations over a bunch of spectra. Operations: calibration the spectra, extraction of the XAFS signal and Fourier (and back-Fourier) filtering. This applications has been designed for the particular needs of the ESRF/ID24 beamline. The Dispersive XAFS and Turbo-XAS techniques generate a huge amount of XAFS spectra in few seconds or minutes. This module allows the user to visualize the spectra, calibrate them, extract the XAFS signal and perform Fourier and back-Fourier transforms simultaneously over all the spectra by simply point-and-click.
- **Input:** a file with raw data. The standard input file contains three columns with X,Mu and Index, all floats, written in binary format by a big endian system. The file size is then number_of_points*3*8 bits. Note that you can run DELIA in both little or big endian systems, but the file must be written by a big endian system (or also by a little endian system but swapping the byte ordering). To load a standard raw data file use the `Browser...` buttin in the "Raw" control panel.
  DELIA also accepts other ASCII input files (using the `File` menu:
  - **ASCII RAW data:** a multicolumn file containing at least three columns (more columns also accepted) with X,Mu and index. The index can be any value that identify the spectrum. Usually indices are 0,1,2..., but can be, for example, a temperature value, etc.
  - **Mu(E):** a multicolumn file containing in the first column the Energy values in eV, and then one additional column for each spectrum (Mu(Energy)) value. When this kind of file is used, the interpolation and calibration analyses are skipped.
  - **Mu(E):** a multicolumn file containing in the first column the Chi values in A, and then one additional column for each spectrum (Chi(k)) value. When this kind of file is used, the interpolation, calibration, and extraction analyses are skipped.
- **Output:** The results of the operations performed with DELIA can be saved in either multicolumn ASCII data files or in sequential ASCII data files. They are usually saved from an XPlot window using the menu `File->Write ASCII file with current set...`.
- **Tricks:**
  - Better use binary raw input files: they are smaller and load quicker.

Follow the steps

The DELIA analysis is done in four main steps, Each step is implemented in a different panel in

the main window: **Raw, mu(E), chi(k) and Fourier**. You should pass from one panel to the next one after completing the operations in the current one. The names are self explanatory:

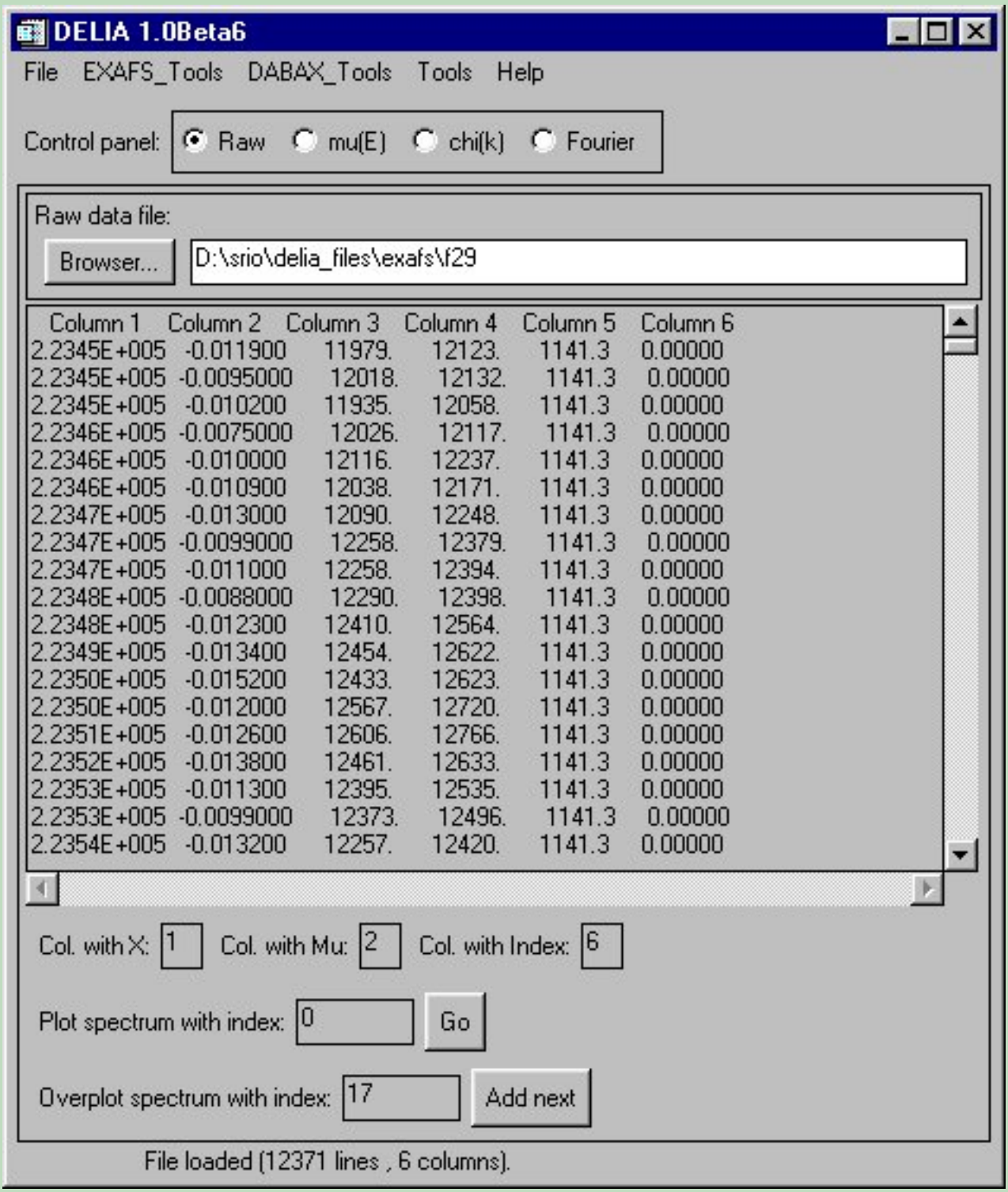
1. **Phase I [Raw]:** allows to read raw data, visualize the individual spectra, overplot them. The user must identify the columns with X, Mu and indices. Using the ASCII raw sample file f29 I obtained the sample window 1.
2. **Phase II [mu(E)]:** Interpolation and Calibration. It allows the user to input the parameters. Default parameters for the interpolation limits are presented. The minimum correspond to maximum value between all the abscissas spectra minima, and the maximum corresponds to the minimum between all abscissas maxima. They may be changed by the user. The user should also supply the calibrating coefficients *a,b,c*. By using the `Get...` button, the XAID_CALIB application is started to help in finding the coefficients. The coefficients found in this way are automatically transferred to the DELIA window. Once all parameters are filled, predd the `RUN interpolate & calibrate` button to make calculations over all spectra. The results appear in the "Result:" text window and also in a newly created XPlot window. The results can be visualized using the `2D` and `3D` buttons.
   If you want to create a file for further use with DELIA, press the `2D` button, and from the XPLot window, select `File->Write ASCII file with current set...`, select then `Data to save: All columns` and `Include header (SPEC type): No`. The resulting file can then be loaded using the DELIA `File->Load file with Mu(E)...` menu. Some example windows are in windows 2 and 3.
3. **Phase III [chi(k)]:** extraction of the XAFS signal, i.e., calculate *Chi(k)* from *Mu(Energy)* over all the spectra. For selecting the appropriate parameters for the extraction, the user must perform interactively the extraction on a single spectrum (select its index and then press the `Go` button to start XAID_MU2CHI module (remember to perform the extraction in *k* space). The parameters of the extraction are copied automatically to their respective boxes. The results can be visualized in 2D or 3D and saved to a file for further use in DELIA as shown in Phase II. See examples in windows 4 and 5.
4. **Phase IV [Fourier]:** Fourier transform and filtering. As in the previous phase, the user must first perform the Fourier Filtering on a single *Chi(k)* spectrum, by using the XAID_FF module. The parameters are copied automatically. A sample can be found in window 6 and

FAQs

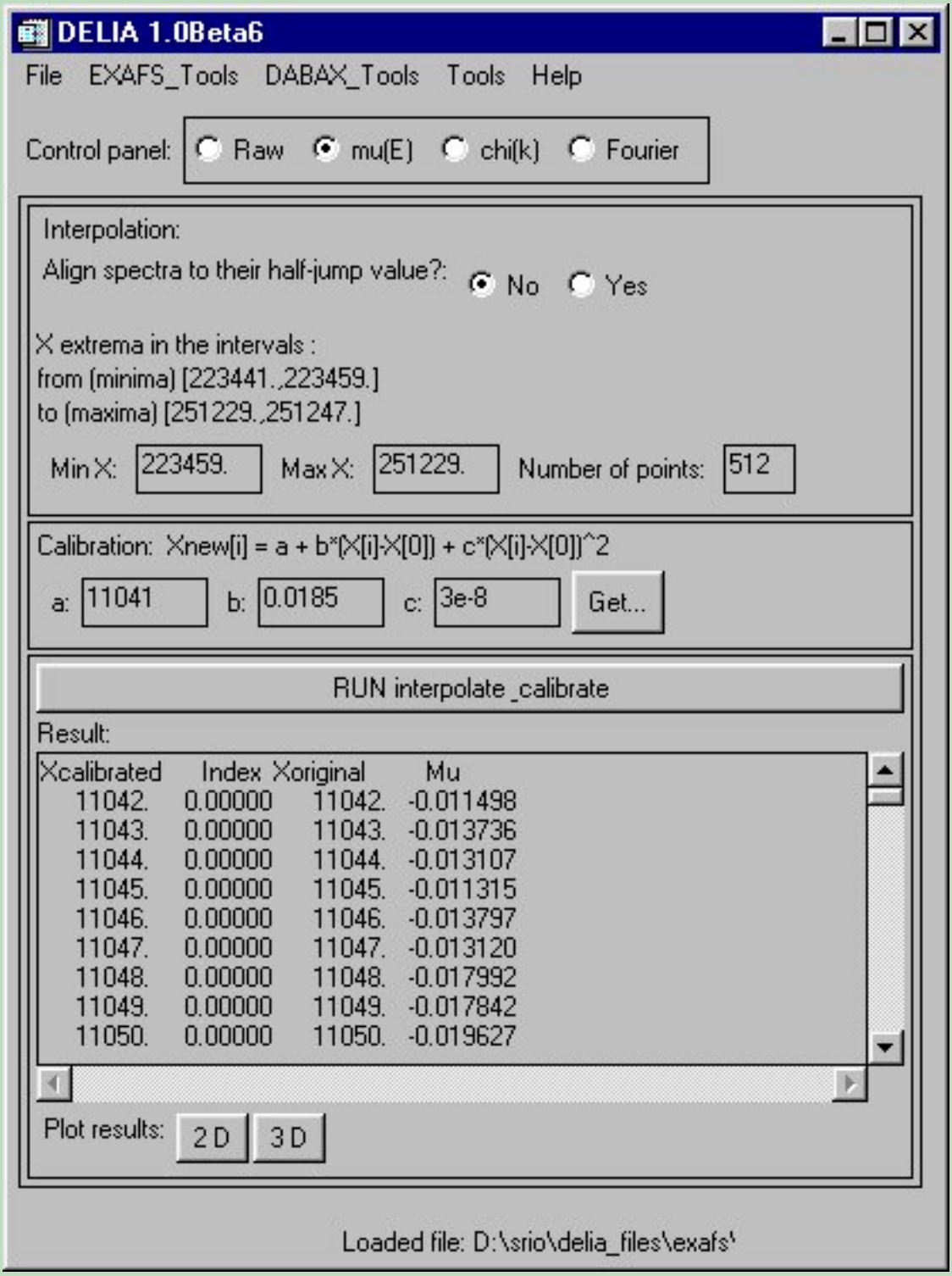
- **What to do if the programs crashes?**
  Restart from scratch.

Window examples

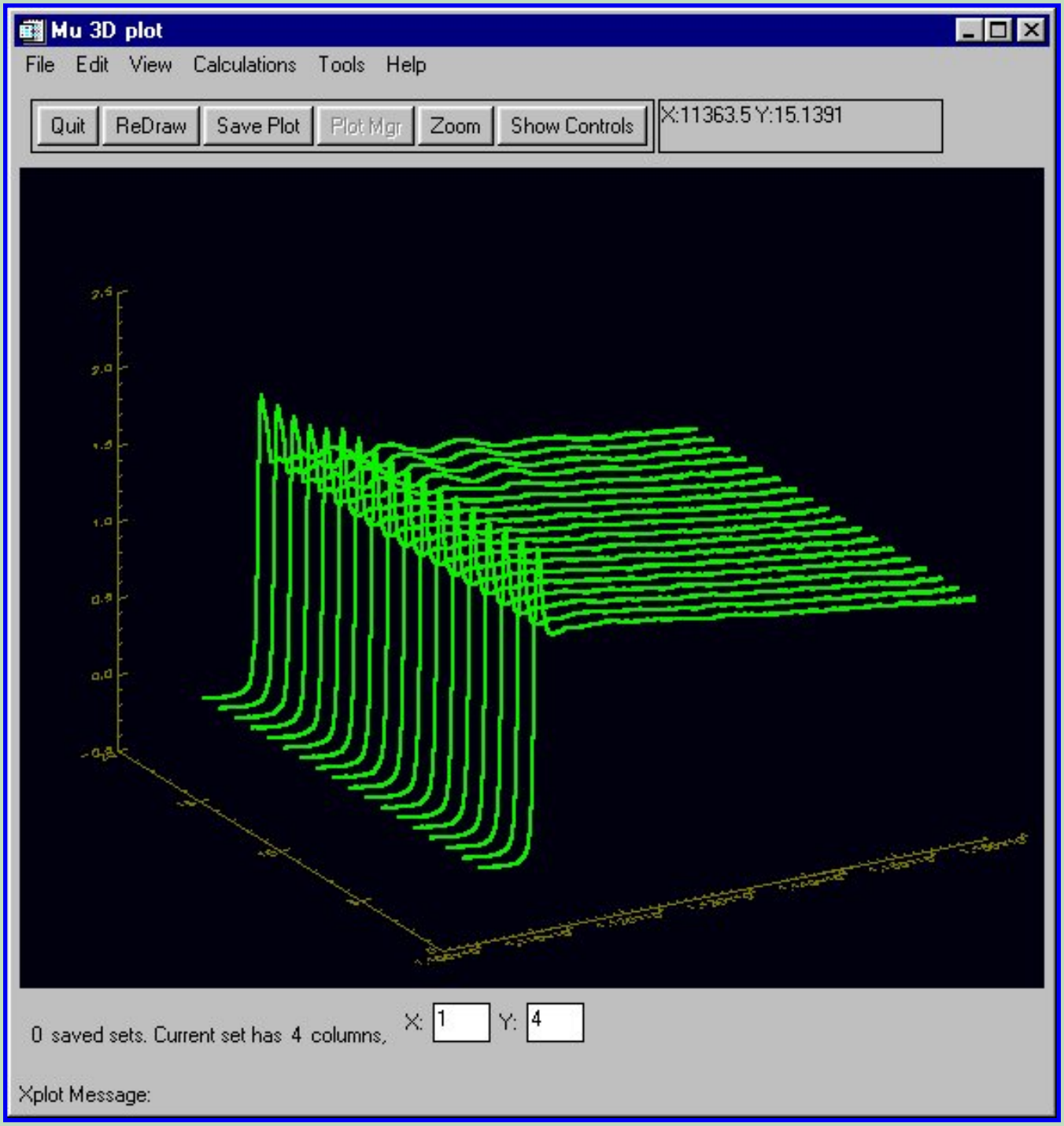
Window 1. Main panel after loading the ASCII raw data file f29.



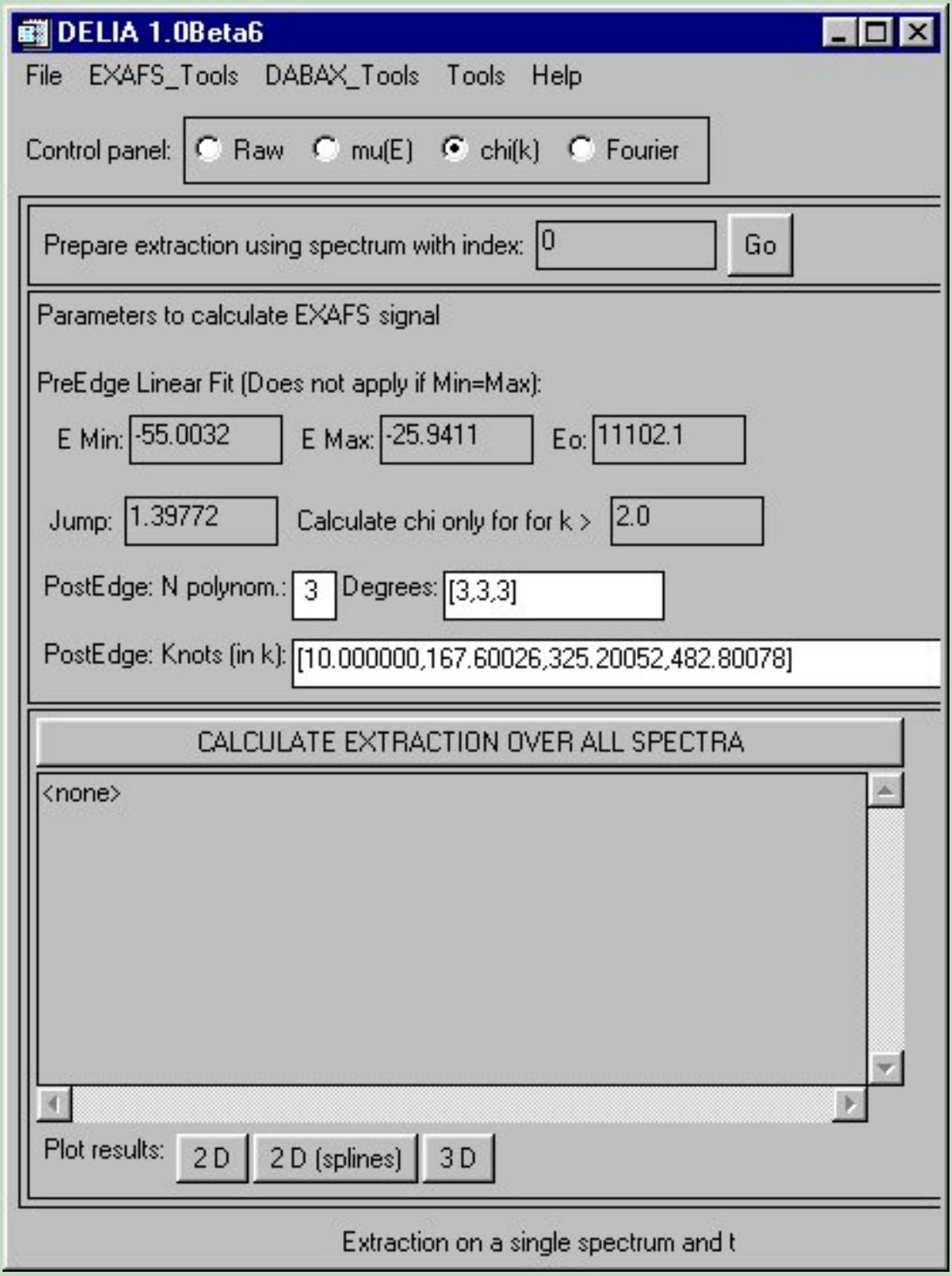
Window 2. Main panel after interpolation and calibration (Phase II).



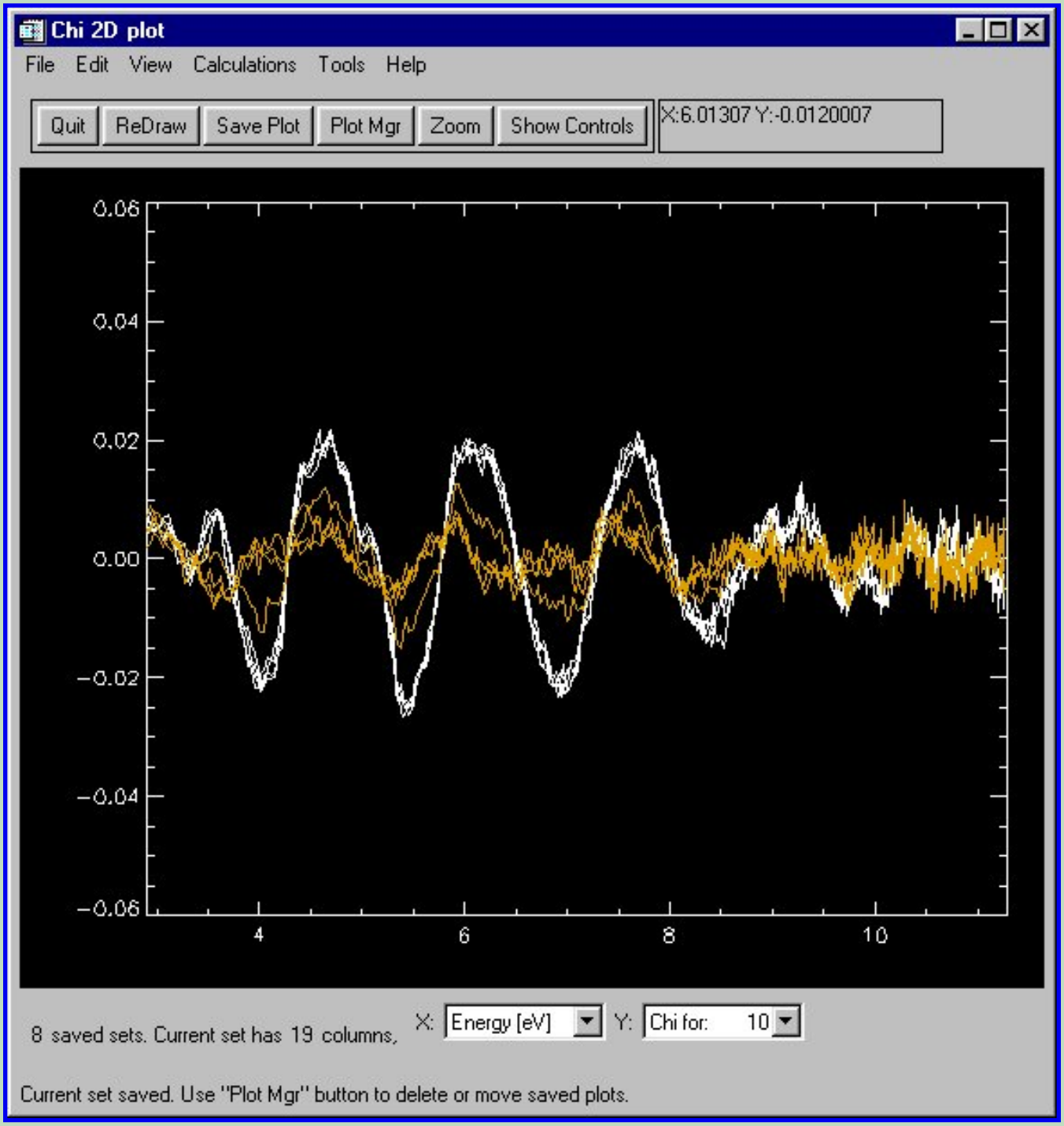
Window 3. XPlot window after interpolation and calibration (Phase II).
(Click on the image for full resolution.)



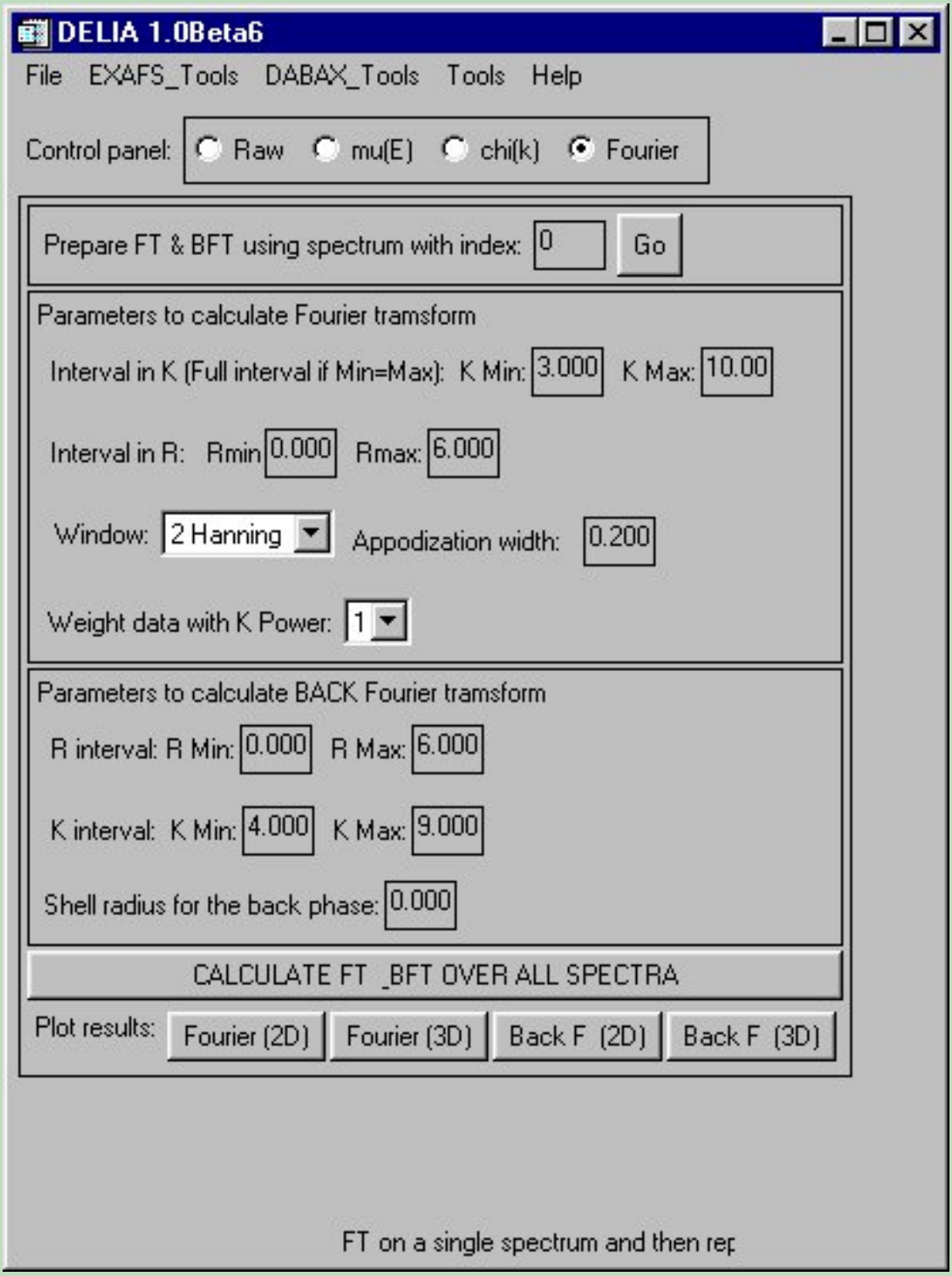
Window 4. Main DELIA window during XAFS extraction (Phase III).



Window 5. XPlot window after XAFS extraction (Phase III).
(Click on the image for full resolution.)



Window 5. Main DELIA window during Fourier Filtering (Phase IV).



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