

XAID: a package for XAFS data analysis based on IDL.

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Abstract. A set of IDL functions and procedures to perform basic XAFS data analysis has been developed. XAID provides the necessary tools to perform background subtraction, Fourier transforms, Fourier filtering, etc. The library routines can be used as modules to be included in the users's customized programs or for creating widget applications. Stand-alone main programs and Graphical User Interfaces to perform standard data analysis are also presented.

1. INTRODUCTION

The purpose of this set of routines is to provide a high level tool to perform basic XAFS data analysis. IDL [1] has been chosen because of its simplicity, power, modularity, build-in tools, programming facilities and portability. The XAID library has been developed in a Unix (HP) environment, but it should run without problems in any other platform supported by IDL (IDL is available for PC, MacIntosh and almost all Unix platforms). IDL is a commercial package which runs only on licensed platforms. It has a high degree of flexibility and modularity which allows the user to write his own user code in a short time. Routines do not need special compilation, and almost all the data are created and can be accessed interactively, and they allow splitting, cutting, pasting and redirecting intermediate data.

2. IDL LIBRARY ROUTINES OF THE XAID PACKAGE

2.1 Terminology

Data analysis, and in particular XAFS data analysis, is based on different operations done on data arranged in spectra. A spectrum is in its simplest way a couple of arrays of the same length, one for the abscissas and the second for ordinates. A more complicated spectrum can contain additional arrays or columns with errors or any other associated value. We define a *set* as one matrix of data containing a spectrum. It has at least two columns (in the IDL language is `fltarr(2,npoints)`) but occasionally it can also hold multiple columns (`fltarr(ncolumns,npoints)`). The set is the basic unit of communication between the XAID functions and procedures. A typical user code reads a set, makes specific operations and saves the results as a new set. The possibility of defining a more complex structure for spectra (with data headers, for instance) has been neglected deliberately to simplify the creation of the data sets by the user.

2.2 Routines for set management and Input-Output

This set of routines are intended to facilitate the work with the sets of data. They are used for reading a set from a file (routine `read_ascii`), writing a set to a disk file (`writeset`), visualization (`plotset`), zooming (`zoomset`), and making general mathematical calculations like derivation (`derivset`), integration (`integset`) and polynomial fitting (`fitset`). Other routines have been written with the aim of helping to input data (routines `gettwoabscissas`, `getvalue`, `getyesornot`, `pause` and `terminal`).

2.3 XAFS routines

This group of XAID routines are intended to provide specific parameters of the XAFS extraction (`gete0` calculates the edge value or E_0 of a set of data and `getjump` calculates the jump of a set of data). The change of spectrum abscissas scale between E (Energy in eV) and k (wavenumber in \AA^{-1}) is performed by the routines `e2k` and `k2e`. The routine `postedge` calculates the post-edge fit of a XAFS spectrum to the atomic absorption coefficient by using polynomial spline least squares fit (in routine `polspl`).

2.4 Fourier and Fast Fourier filtering

Inside the XAID packages there are routines to perform the Fourier transform (FT) and back Fourier transform (BFT) of XAFS data. The user can select between either the standard method to calculate the FT and BFT (using integrals) or the Fast Fourier Transform method. The latter is faster in computer time, but requires an interpolation of the data in order to have a regular grid and to allow control on the resolution in the conjugate variable. The standard method allows a non-uniform gridding of the data and does not require previous interpolation. The procedures `ftrset` and `bftrset` are drivers for all the routines referred here.

Data are usually windowed with a given window function before performing the FT. When calculating the BFT of the same data, the result has to be divided by the same window. In XAID, the data can be weighted automatically with any window contained in the `window_fft` procedure. Presently the windows available in this procedure are: Gaussian, Hanning, Hamming, Parzen, Welch, Tukey and Kaiser (or Bessel).

3. A MAIN PROGRAM FOR A MENU-DRIVEN XAFS DATA EXTRACTION

By using the IDL functions and procedures described above and a few other mathematical and graphical facilities provided by IDL, the user can load and analyse the XAFS data. This requires a limited amount of work. For instance, a procedure called `CNPICK` was created to perform XAFS data reduction. The program data flow is similar to the one used in the package `NPI` [2]. It analyses a spectrum passing sequentially through different phases, which are presented to the user as menus. Therefore, the user only has to select the options, and it is always possible to redo any operation. The phases are the following: 1- *Setup* of the terminal and load file with the experimental data. 2- *Preparation* of the data. 3- *Selecting the E_0* . 4- *Pre-edge* fitting. 5- *Post-edge* background removal. 6- *Normalization*, where the user can select between the three possibilities (the so-called experimental, constant and Lengeler-Eisenberg methods). 7- *End*. After the extraction the user can display the signal weighted with a power of k , calculate the integral and CDF (cumulative distribution function), calculate the Fourier transform and write the extracted signal in a file. After the interactive analysis, a file called `cnpick.log` is created. It contains an IDL program with all the active operations performed. This allows to repeat the analysis and can be applied to other files with slight modification. It can be used to make a loop for analysing automatically a set of several files with the same values of the one analysed interactively.

4. GRAPHICAL USER INTERFACES

The XAID functions and procedures can be used to create sophisticated Graphical User Interfaces (GUI) for XAFS data analysis using the IDL widget toolbox. The GUI called `XAID_mu2chi` is a point-and-click application which provides the same functionality of `CNPICK`. Here the user can perform the operations without being constrained to follow a given sequence. The application `XAID_ff` (see Fig. 1) is designed for interactive Fourier filtering of XAFS spectra. All the XAID GUI are also integrated naturally with our `XPLOT` application which visualize and analyse files with ASCII and SPEC[3] format. Reference spectra and electronic tables from *ab-initio* calculations can be accessed from the XAID GUIs and from the WWW by using our DABAX data base [4].

The XAID package is available from `ftp://ftp.esrf.fr/pub/expg/xop` directory. WWW information is in `http://www.esrf.fr/computing/scientific/xop/`

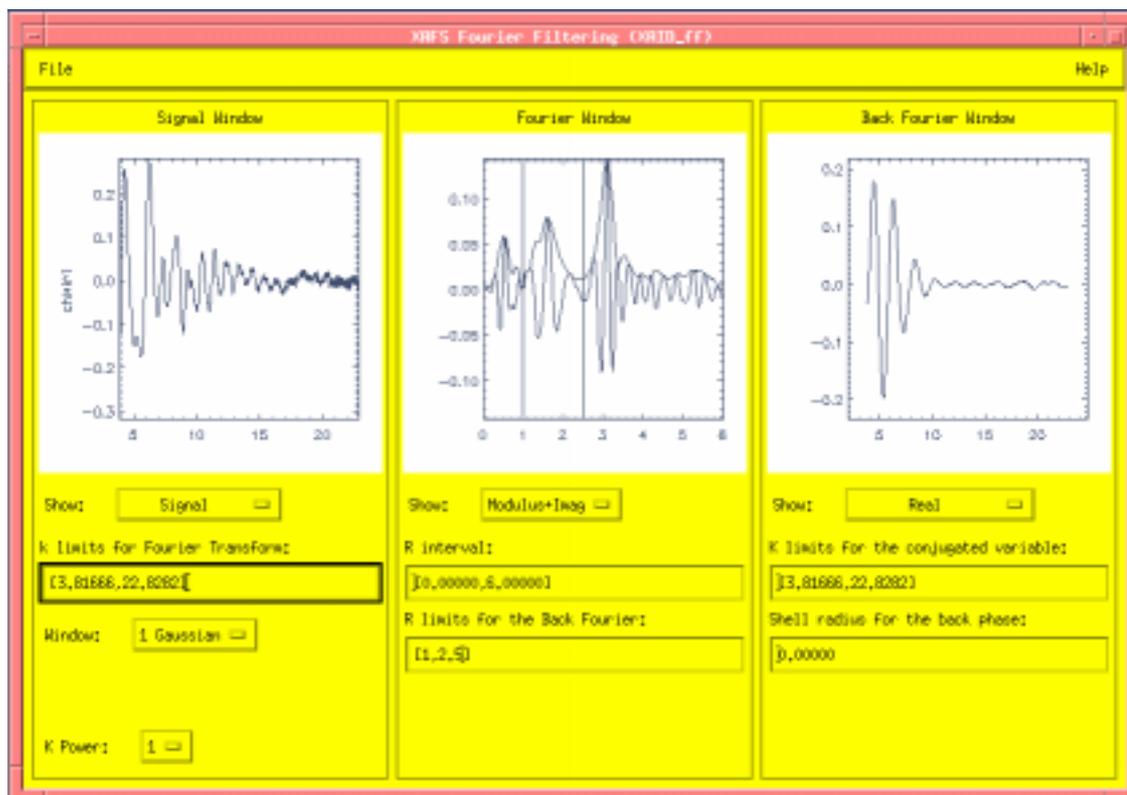


Figure 1: Main window of XAID_ff application for Fourier filtering.

References

- [1] IDL, Interactive Data Language. Trademark of Research Systems, Inc. <http://www.rsinc.com>
- [2] M. Sánchez del Río, J. Chaboy and R. Djerbi, *Computers Chem.* 19(1) (1995) 59. Retrievable from <ftp://ftp.esrf.fr/dist/expg/HP700>
- [3] SPEC is the main program used for instrument control at the ESRF. Trademark of Certified Scientific Software, <http://www.certif.com>.
- [4] DABAX, Data Base for X-ray applications. B. Roux and M. Sánchez del Río. In preparation.