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APEX version 2.0: latest version of the cross-platform analysis program for EXAFS

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This report describes recent progress on APEX, a free, open source, cross platform set of EXAFS data analysis software. In a previous report we described APEX 1.0 (Dimakis, N. and Bunker, G., 1999), a free and open source code suite of basic X-Ray Absorption Fine Structure (XAFS) data analysis programs for classical data reduction and single scattering analysis. The first version of APEX was the only cross platform (linux/irix/windows/MacOS) EXAFS analysis program to our knowledge, but it lacked important features like multiple scattering fitting, generic format conversion from ASCII to University of Washington (UW) binary-type files, and user friendly interactive graphics. In the enhanced version described here we have added cross-platform interactive graphics based on the BLT package, which is an extension to TCL/TK. Some of the utilities have been rewritten in native TCL/TK, allowing for faster and more integrated functionality with the main package. The package also has been ported to SunOS. APEX 2.0 in its current form is suitable for routine data analysis and training. Addition of more advanced methods of data analysis are planned.

Keywords: EXAFS; software.

1. Introduction

APEX ("Analysis Program for EXAFS") version 1.0 (Dimakis, N. and Bunker, G., 1999) provided a cross platform open-source interface to the UW/NRL EXAFS analysis programs. These implement standard methods of data reduction and analysis: background subtraction, fourier transform/filtering, nonlinear least squares fitting in single scattering approximation using empirical or theoretical standards, and include various utilities. The APEX package presently consists of the UW/NRL Fortran 77 code base supplemented with a graphical front end written in TCL/TK (Ousterhout, J., 1994, Welch B., 1997), which runs on a wide variety of the operating systems: Linux, Silicon Graphics IRIX Version 6.5, Apple MacOS 8.0/8.1+, and PC compatibles under Windows 98 and NT) for EXAFS data reduction. With the exception of MacOS, APEX 1.0 was executed as a shell script i.e. text file. The open source SpecTcl 1.1 was used as a GUI (Graphical User Interface) builder and also as a TCL/TK compiler for the Macintosh case.

At its inception APEX was the only cross platform program that run under no emulation, was easy for novices but also useful for experts. The development strategy was to start with a proven code base, incrementally remove its limitations, and add more advanced features. More recently our primary goals have been to develop better interactive graphics; include multiple scattering fitting; rewrite some of the utilities in native TCL thus improving integration with the main package; adding a generic data ASCII to UW conversion capability; and at the same time to keep the cross platform character of APEX. Secondary but also important goals included adding

more utilities, using TCLPro to create binaries for the non MacOS platforms, and having interactive help in addition to the local and on-line help already available.

The first task was to improve the interactive GUI. New interactive graphics should be also open source, have at least the same functionality of the old Interactive Data Plotting program (IDP) used by APEX 1.0, but also be more flexible, support high quality output, and be easy to use for beginners and also be useful to experts. We elected to use the BLT package for two dimensional graphics and OpenGL for three dimensional graphics, since OpenGL or public domain work-alikes such as MESA are standard on the target platforms. One drawback to this approach is that the BLT extension has not yet been ported to MacOS 8.0-9.0, although it is in progress, and but it should readily be ported to MacOS X because of its BSD unix API layer. For MacOS 8.0-9.0 a version of APEX 1.5 that includes all new features except the BLT-type graphics has been implemented. APEX1.5 incorporates the original Interactive Data Plotting program (IDP) as the primary graphical user interface.

Our next priority was to add a generic data conversion format card so a user could create and save its own format. Also there was a necessity for multiple scattering analysis within APEX. To do this we have added a FEFFIT card (Newville, M., *et al*, 1995). Other improvements are the addition of two utilities, for example Mucal, which, among other things, calculates the absorption and scattering cross sections of a given compound as a function of energy, and a utility to export a UW file to a column data ASCII for further plotting or analysis using other software.

A limitation of APEX 2.0 is that the Random Data File format (RDF) UW file format upon which it is based are platform dependent e.g. a MacOS UW file will not be directly usable in an SGI environments. It is clear that a different cross-platform binary standard file format (e.g. HDF) is required for future use in APEX, and this is planned. Official versions of APEX 2.0 will be made available at the APEX, BioCAT home pages and mirror sites.

2. Discussion

APEX 1.0 used IDP as main interactive graphics for XAFS data analysis. This program is quite capable, offering interactive graphics using text-based commands. but it has a sufficiently steep learning curve that it is intimidating for new users. IDP is based on the XFP plotting package which as fortran source code is cross-platform except for a device dependent graphics driver. The graphics uses very basic primitives which enhances portability but does not produce presentation quality graphics. For MacOS, IDP used two windows, one for the graphics and one for the command line. Under UNIX it used only one window for both purposes thus sometimes causing confusion to the user. The BLT extension has many advantages: it is simple, open source, cross-platform, directly produces postscript output (which is convertible to pdf), and it can be integrated easily with the existing TCL/TK code.

Using the same approach as in the main APEX program, the new interactive graphics allows the user to customize the foreground and background colors simply by a mouse and modifier key combination. Also pen and point size for graphics elements are fully customizable. Once the user opens a UW file, the number of total records is shown and the first record, by default, is plotted. Depending on the type of the file e.g. XMU, various entries appear at the top of the graph. For example, in case of an XMU graph edge jump (E_0), Step, and the two pre-edge values appear as entries (E_{f1} , E_{f2}). When the user sets the edge energy then this value will be automatically shown in the corresponding entry. If the user moved

to a another record then the energy of this record, if has been previously set, will be displayed. The user could also plot scans one over the other and by clicking the corresponding label on the legend can highlight the particular scan (Fig 1). In this case every new scan will be automatically colored with a different color and plotting symbol than the previous scans so to be easy for the user to identify the particular scan. BLT graphics offer zoom capabilities.

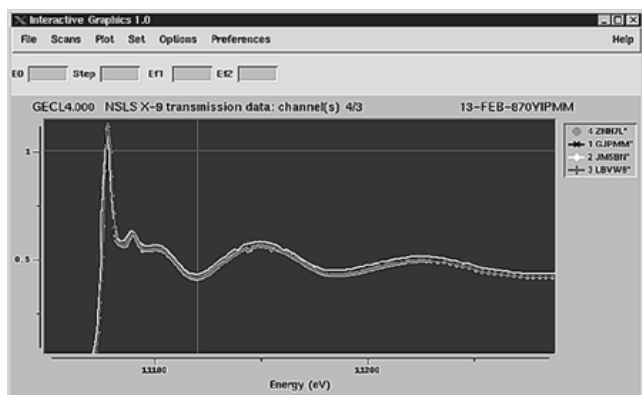


Figure 1
Linux version of the Interactive Graphics 1.0. Four records of Absorption vs Energy for $GeCl_4$ are plotted (zoom operation). Each record is represented by a different color and symbol.

As mentioned before, APEX 2.0 offers much more than just incremental improvements. A screenshot of the generic data conversion card is shown in Fig 2. The user selects title, documentation and data lines by clicking the appropriate color buttons (colors are user configurable). Then the user selects the type of conversion.



Figure 2
IRIX 6.5 version of the generic format card.

Buttons are automatically enabled or disabled depending on the procedure thus helping further the user. In Fig. 3, which represents a first attempt to a FEFFIT top level interface, the user could put all the corresponding information using the entries and then do a path by path selection, and may also edit the final feffit.inp file to add a more advanced keyword or for a 1st minute change. Also utilities that read the number of records of a UW file and display the documentation buffer of a record has been written in native TCL/TK.

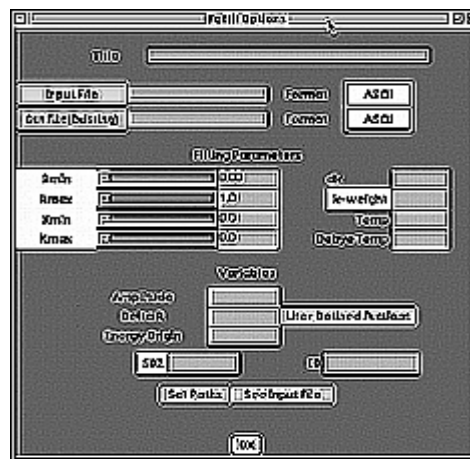


Figure 3
IRIX 6.5 version of the generic format card.

Many users rarely read help manuals. Whenever they encounter a difficulty they try to experiment before they think about reading the help manual. Therefore we have included an interactive help system in addition to the local and internet help APEX 1.0 offered. By clicking a label a dialog box provide brief description about an entry or a menu.

Future plans include designing a new type of RDF file that will replace the platform specific UW format files, writing more utilities in native TCL/TK code, adding a card for AUTOBAK, incorporating the new interactive feffit (called IFEFFIT), interactive path selection using 3D graphics, and extension to regularization. Some advanced programs such as AUTOBAK, FEFFIT, and FEFF must be obtained by contacting the authors of those programs; they are separately licensed and are not part of the APEX package.

3. Conclusion

The latest version of APEX is to our knowledge the only open source, cross-platform (no emulation) EXAFS data analysis package that offers a friendly user interface, fast data analysis, and is friendly to new users. Forthcoming versions will offer 3D path selections for multiple-scattering, more native TCL code for most of the utility routines, and advanced features not presently available in any analysis programs.

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