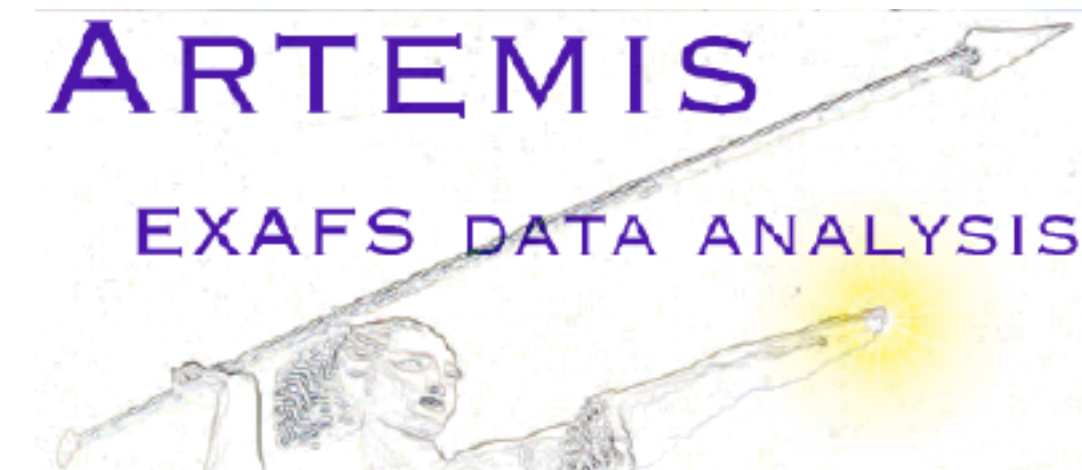


Athena and Artemis: Interactive graphical data analysis using Iffeffit

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We introduce a new software package for analysis of XAS data. This package is based on the Iffeffit library of analytical and numerical algorithms and uses the perl/TK graphics toolkit. The two main components are Athena, a program for XAS data processing, and Artemis, a program for EXAFS data analysis using theoretical standards from Feff. These programs provide high quality analytical capabilities in a manner that is accessible to novices yet powerful enough to meet the demands of an expert. The programs run on all major platforms and are freely available under the terms of a free software license.



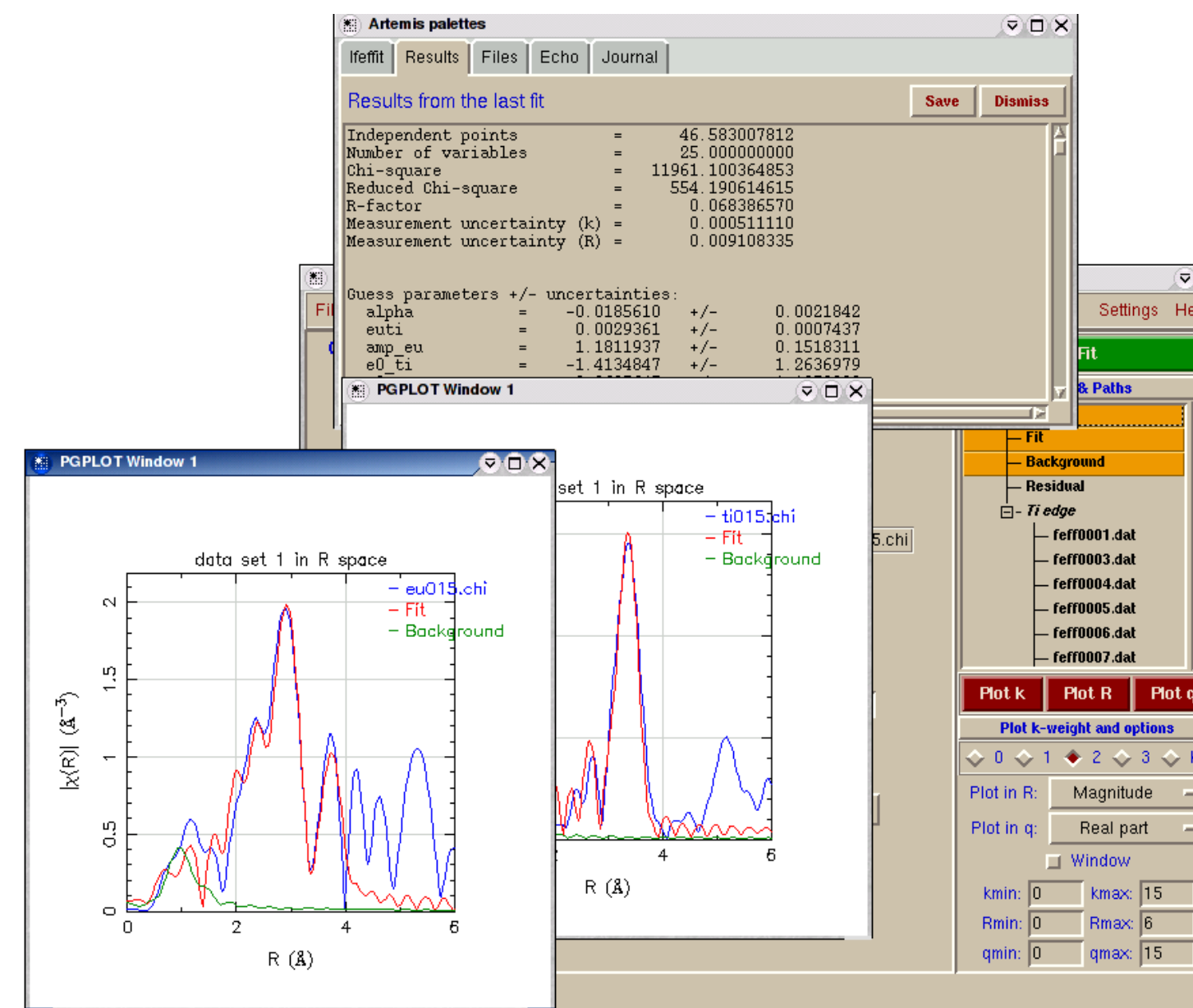
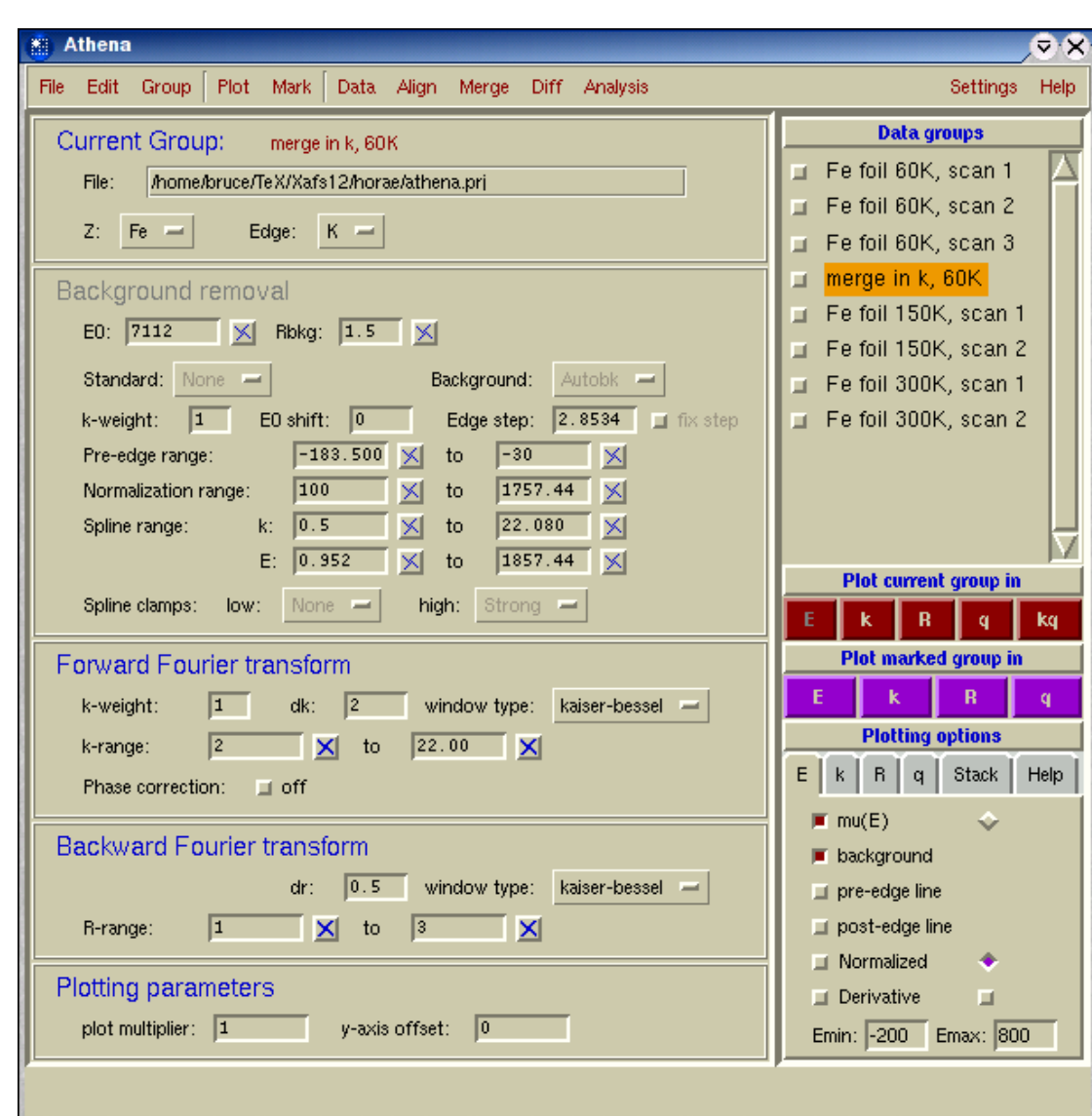
Features

- Convert raw transmission or fluorescence data into $\mu(E)$ spectra
- Degitch by point selection or by an algorithm
- Merge spectra and compute the standard deviation spectrum
- Align and calibrate data
- Compute difference spectra for XANES, dichroism, and EXAFS
- Remove background using the Autobk algorithm
- Normalize to Cromer-Liberman calculations
- Perform forward and backward Fourier transforms with optional central atom phase corrections
- Do log-ratio/phase-difference analysis
- Fit XANES data
- Do data truncation and data smoothing
- Plot individual or many data sets in k -, R -, or back-transform k -space
- Constrain background removal and Fourier transform parameters between data sets in a flexible way
 - Do Principle Component Analysis (coming soon)
 - Fit XANES by linear combination of standard spectra (coming soon)
 - Do self-absorption and dead-time corrections (coming soon)
- Process and visualize large quantities of data easily

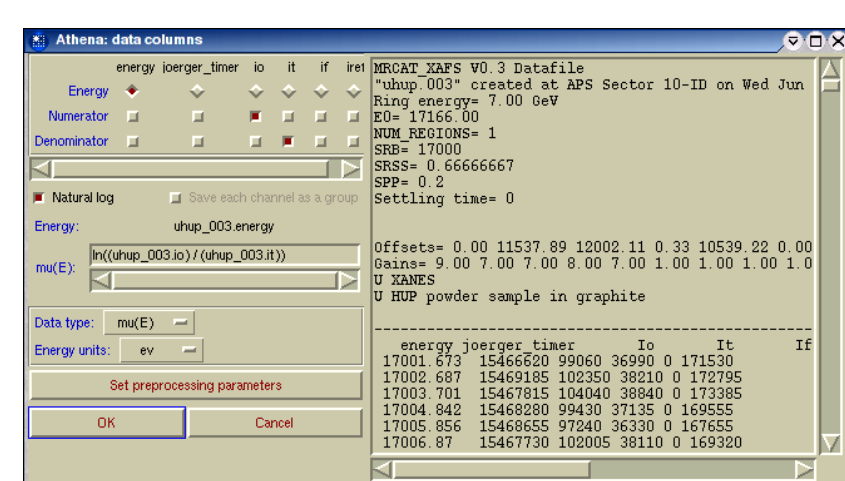
Features

- Use of theoretical fitting standards from Feff
- Fit using single or multiple data sets
- Fit using single or multiple Feff calculations
- Co-refinement of a background spline to uncover correlations between the background and the fitting parameters
- Fit using one or more values for the k -weight
- Set arbitrary constraints between and restraints on fitting parameters
- Plot in k -, R -, or back-transformed k -space
- Plot the data, the best-fit function and the background spline as well as the individual paths
- Report on fitting statistics, including error bars and correlations between variables

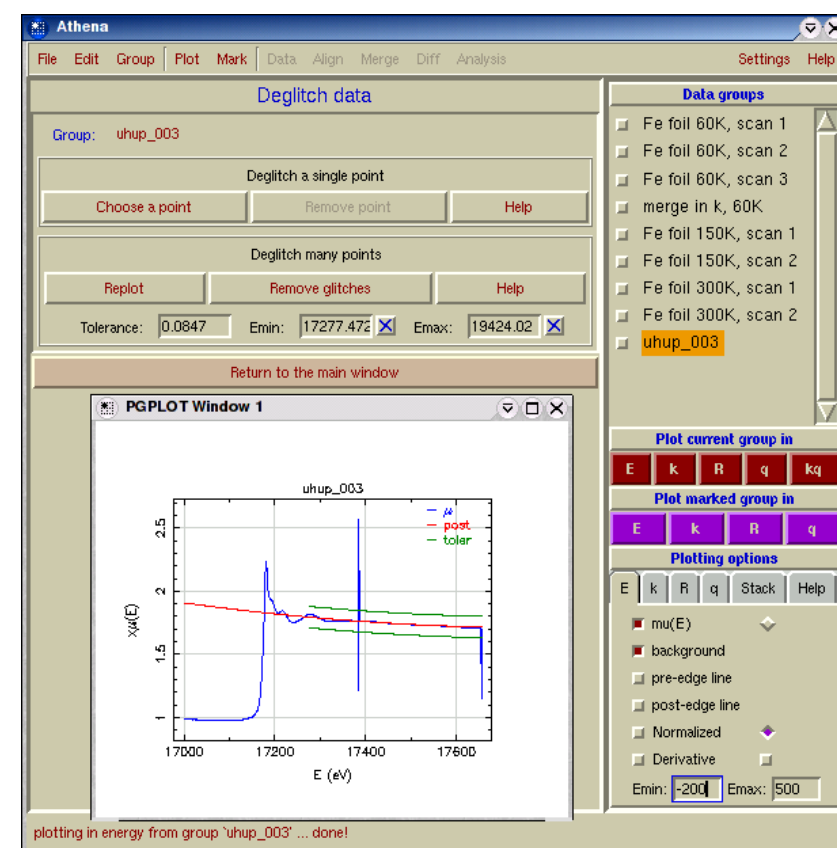
This composite image shows the results of a multiple-data-set fit to the $Ti K$ and $Eu L_{III}$ edges of $EuTiO_3$. Upon completing a fit, Artemis plots the data and best-fit function and displays the statistical results, including best-fit values, error bars, and correlations.



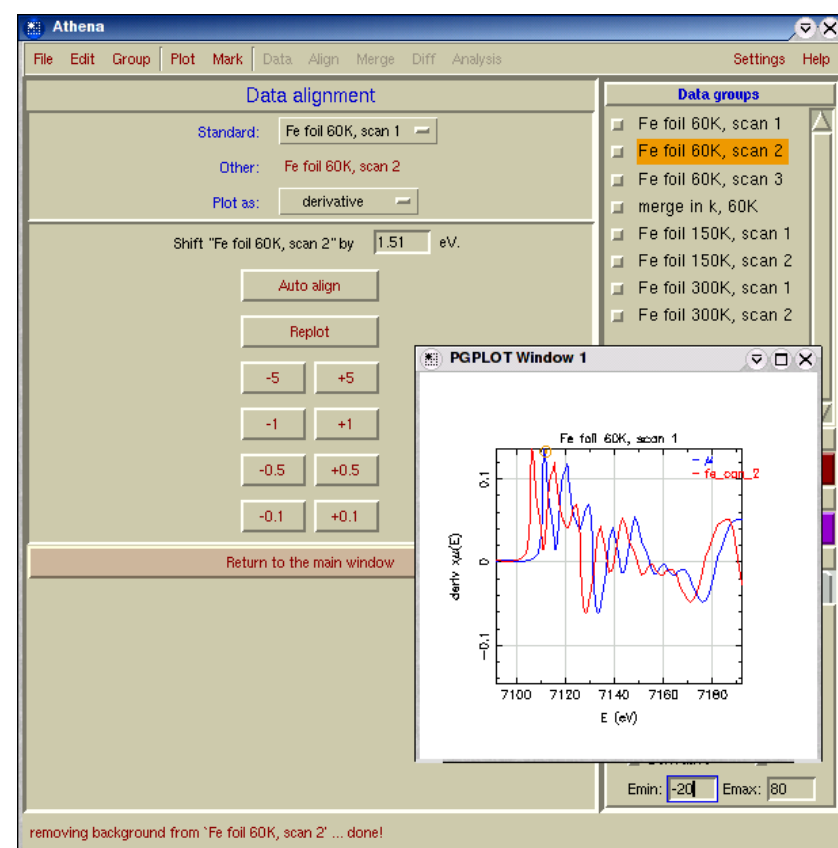
Data processing with Athena



Data import in Athena is very flexible. Column data can be combined to form $\mu(E)$ data for transmission, fluorescence, or electron yield. Multi-element detector data can be summed on the fly or each channel can be read as individual data groups. Data can also be degitched, truncated, and/or aligned on the fly as it is imported. Feff's 'xmu.dat' and 'chi.dat' files can also be imported.

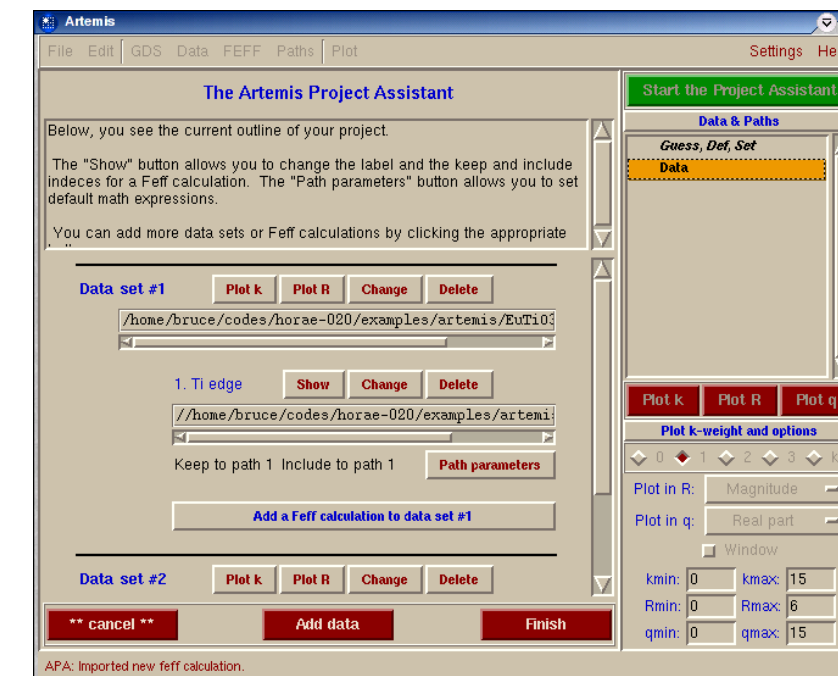


Degitching is handled interactively, either by selecting and removing individual points or, as shown, by defining margins outside of which points are flagged as spurious.

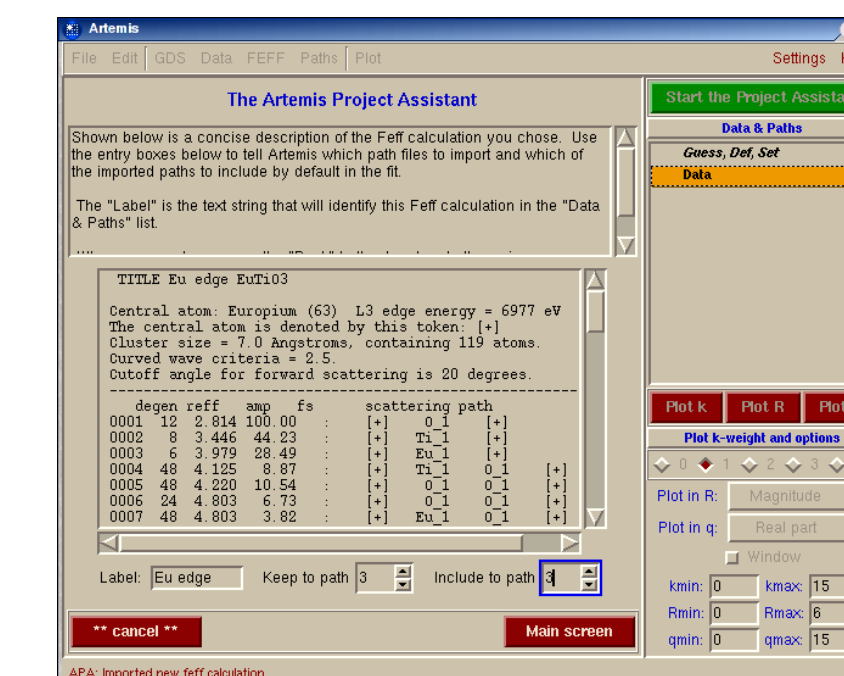


A simple, automated alignment scheme based upon a comparison of derivative spectra is available. If that is not adequate, data can be aligned by hand.

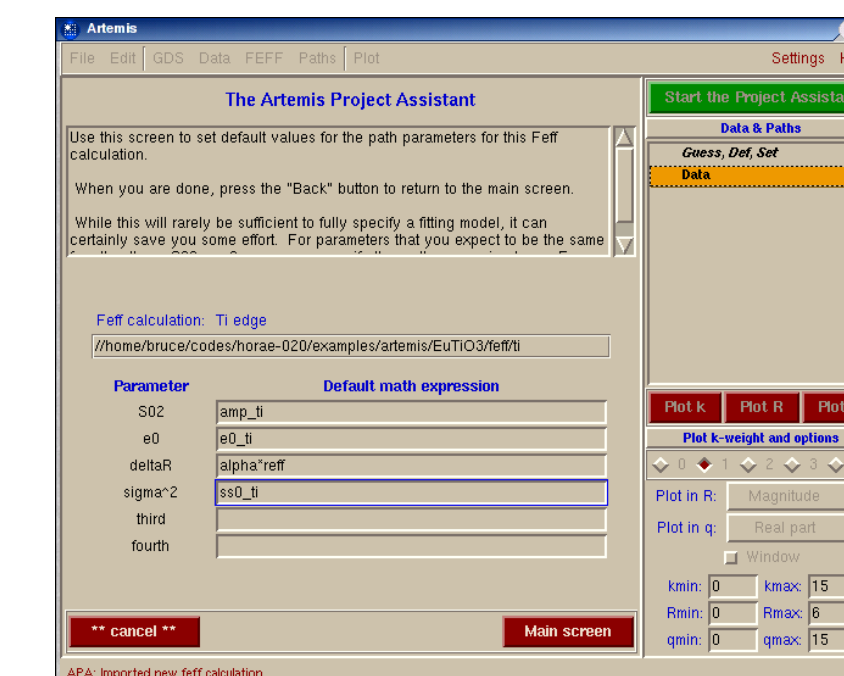
The Artemis Project Assistant



The Project Assistant is a wizard to help you through the initial steps of setting up your fitting project. Here we begin to set up a multiple-data-set fit on $EuTiO_3$. The Project Assistant has guided us through importing data from the two edges.

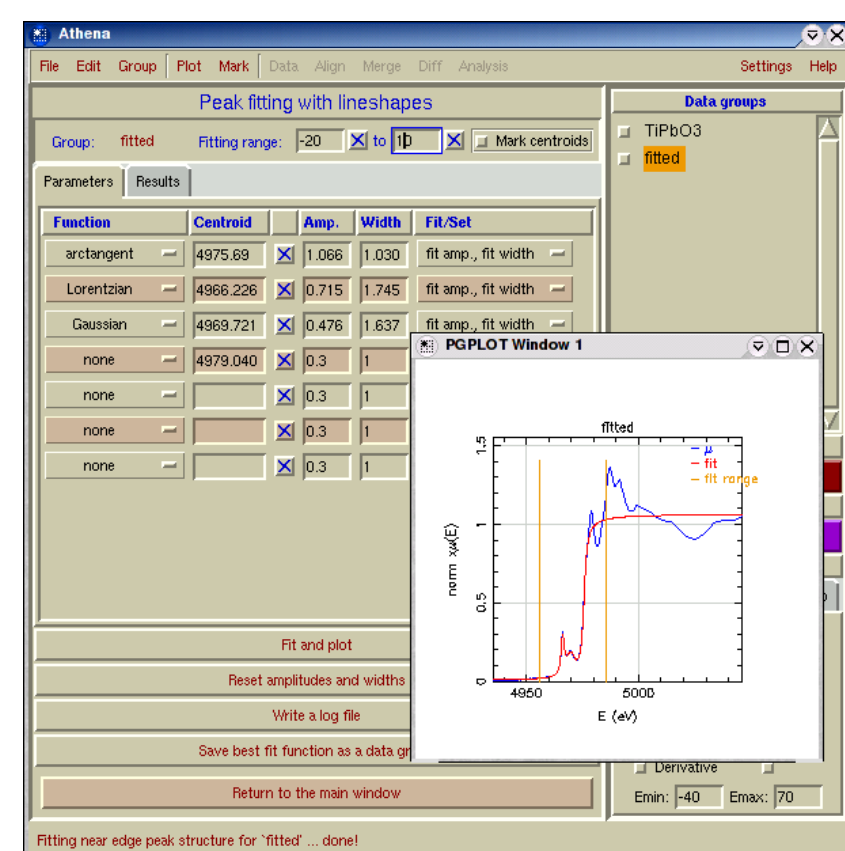


After importing a Feff calculation, the Project Assistant displays a summary of the imports and allows us to limit the number of paths we import and the number we will initially use to fit the data.

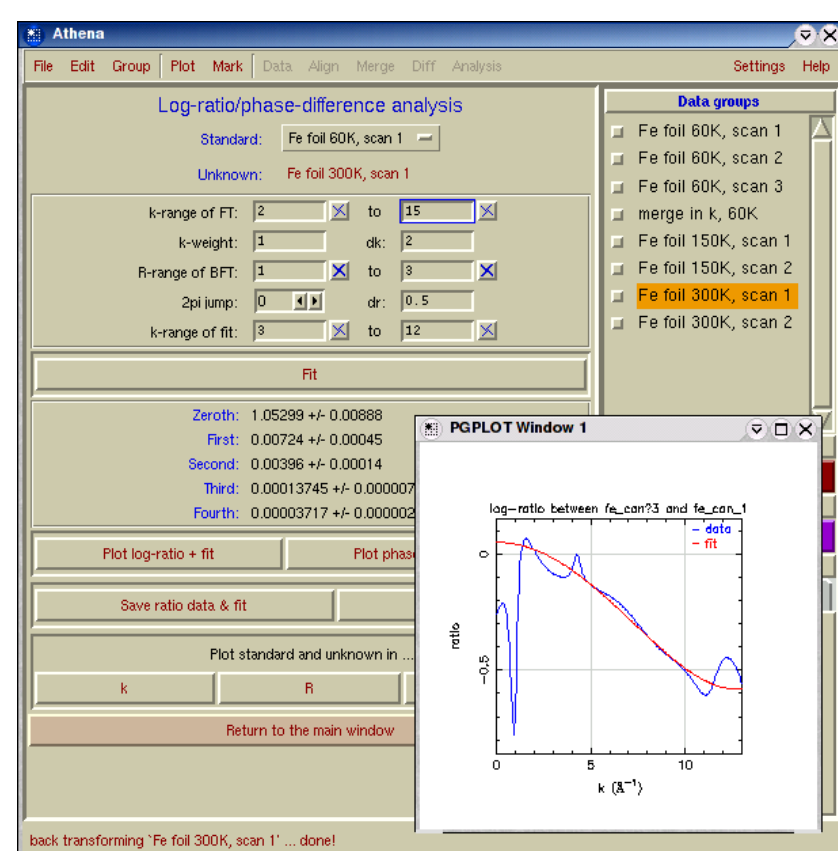


Finally the Project Assistant allows you to specify a template for the path parameters associated with each data set. Variables will be harvested from these math expressions and used when the project is imported.

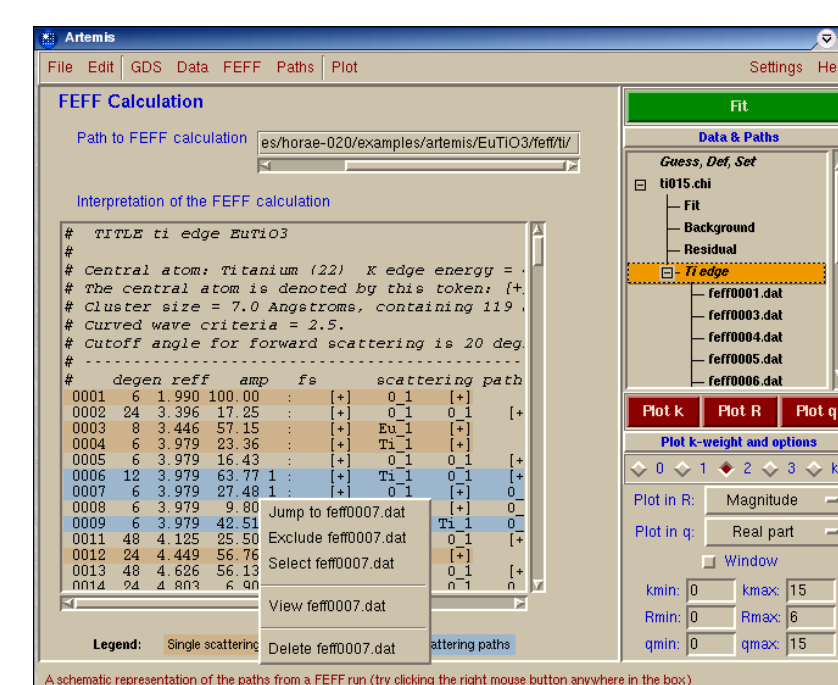
Data analysis with Athena



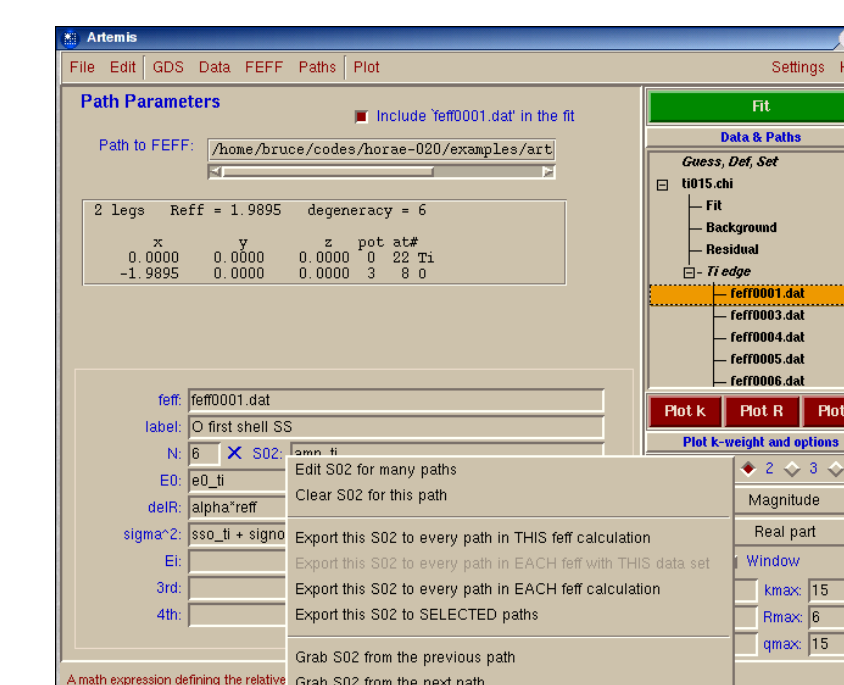
Athena supports simple data analysis for your XANES and EXAFS data. To the left is an example of Athena's peak fitting interface. Here XANES data is modeled as a sum of line shapes. To the right is Athena's log-ratio/phase-difference interface. Changes in EXAFS data can be measured by comparing the Fourier filtered spectrum of a standard to an unknown. PCA and fitting XANES as a linear combination of standard spectra are among the features under development.



Managing Feff calculations and paths

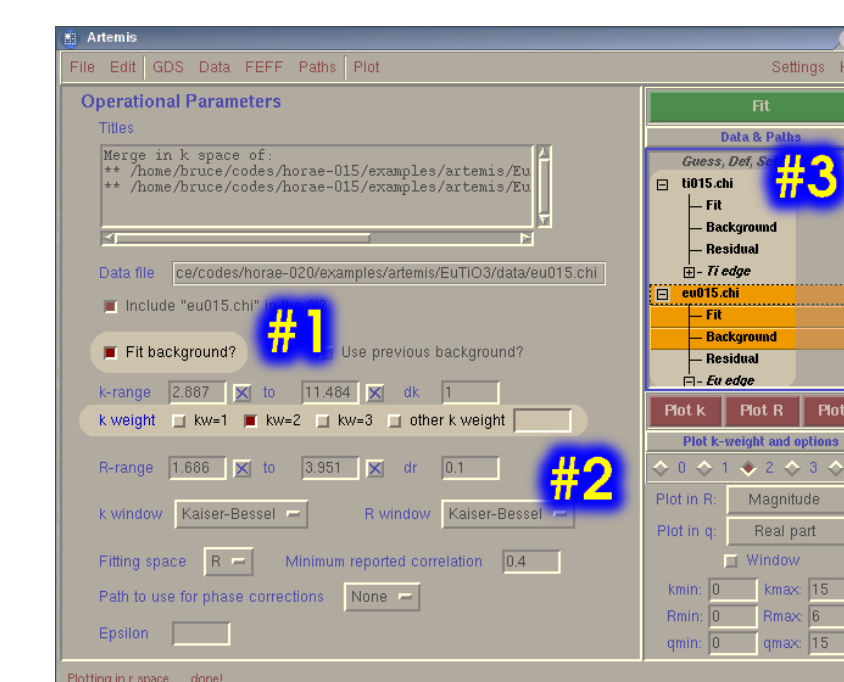


To the left is the concise summary of the Feff calculation. The pop-up menu shown is seen by right-clicking on a line in the summary and allows you to manage paths for viewing, plotting, or including in the fit. To the right is an example of the view of an individual path and the interface for setting the path parameters. A right-click menu offers a variety of editing shortcuts to help you create your fitting model.



Advanced features in Artemis

- #1: Co-refinement of a background spline is useful to reveal correlations between the background and the fitting parameters. Enabling this co-refinement is as simple as clicking this button.
 - #2: Multiple- k -weight fits can help reduce correlations between parameters with different k -dependencies, such as S_0^2 and σ^2 or E_0 and ΔR . Simply toggle as many k -weight buttons as you would like to use in the fit.
 - #3: Multiple data sets and multiple Feff calculations are easily introduced into the fit. Simply import as many you wish to include and they will all be displayed in this list. Fitting parameters can be constrained between data sets and between Feff calculations.
- Constraints between and restraints on parameters can be arbitrarily defined to reflect your prior knowledge of your fitting problem.



Free source code and the scientific method

Full disclosure of experimental procedures and results is one of the cardinal rules of the scientific method. We, as scientists, cannot and should not accept results which cannot be reproduced by independent investigators. Consequently, we are obligated to explain enough detail of sample preparation, experimental procedure, theoretical background, and interpretation of the data that any reader with adequate background and inclination can fully reproduce a result. Most journals would refuse to consider publication of an article that hides details behind a veil of secrecy.

We believe that full disclosure is essential to science and to the dialogue between scientists, and that full disclosure applies to the software that is used in data analysis. In this day, most scientific disciplines depend on computer technology for many aspects of data collection and analysis. In particular, XAS is heavily dependent on computerized control for its data collection and on computer algorithms such as the Fast Fourier Transform and general non-linear modeling algorithms for its analysis.

It is essential that any reader of a scientific publication who has the necessary background and inclination be able to scrutinize the details of the codes used for the analysis. This requires that source code be freely available.

Freely available source code allows independent scrutiny of the procedures used and also allows scientists to modify and improve these procedures for their own needs. By using an Open Source Software license, such modifications can be disseminated to the community either by the original authors or those making the modifications. In this way, new ideas and algorithms can build on and improve earlier work in an open and peer-reviewed manner to enrich the entire scientific community.

Acknowledgments

Particular thanks to Shelly Kelly, the first and best beta tester of both of these codes and a font of good suggestions. Thanks also to everyone on the Iffeffit mailing list for their support, enthusiasm, and suggestions — and especially for lots of bug reports. Paul Fons contributed the nice OSX screenshot. This poster was made using free software tools including *Blat*, *XEMacs*, *AUCfig*, *The Gimp*, *XSnapshot*, and *XGhoseView*. *Athena* and *Artemis* are written in Perl using Perl/TK. Data visualization uses the *PGPLOT* graphics library.

Iffeffit homepage: <http://cars.uchicago.edu/iffffit>

Athena and Artemis homepage: <http://teff.phys.washington.edu/~ravel/software/exafs/>

This poster shows Athena version 0.8.020 and Artemis version 0.6.005 (June 19, 2003). This poster and all images on it are copyright © Bruce Ravel, 2003. This poster is licensed under the Creative Commons Attribution-NonCommercial License. To view a copy of this license, visit <http://creativecommons.org/licenses/by-nc/1.0/> or send a letter to Creative Commons, 559 Nathan Abbott Way, Stanford, California 94305, USA.