

Interactive EXAFS Analysis Using IFEFFIT

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IFEFFIT is an interactive program for XAFS analysis. It combines the high-quality analysis algorithms of AUTOBK and FEFFIT with graphical display of XAFS data and general data manipulation. *TKATOMS* is a crystallography program for the absorption spectroscopist and uses elements of IFEFFIT. *ATHENA* and *ARTEMIS* are programs built on top of IFEFFIT which bring interactive, graphical EXAFS data analysis to the desktop. *ATHENA* is a program for data processing and with *ARTEMIS* you can use theoretical standards computed by FEFF to analyze your EXAFS data. Written in Perl and using the Tk graphics toolkit, *TKATOMS*, *ATHENA*, and *ARTEMIS* run on Unix, Windows, and Mac OSX.

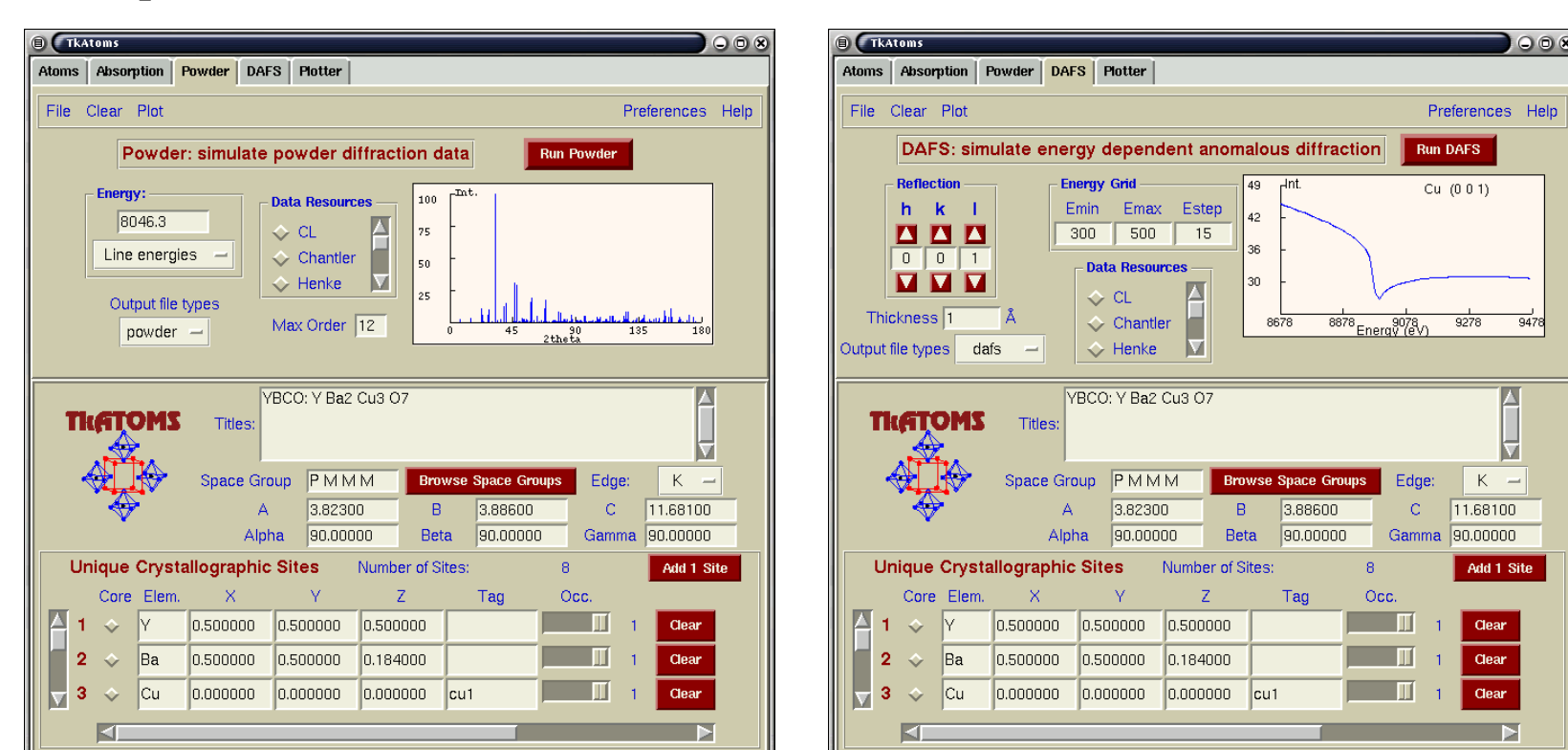
TKATOMS

TKATOMS is a user application providing crystallographic functionality useful to x-ray absorption spectroscopists. The main use of *TKATOMS* is to generate input data for the *ab initio*, multiple scattering, x-ray absorption spectroscopy code FEFF⁸ or earlier versions². This version of *ATOMS* uses the same input files as older version, but offers many significant improvements, including highly configurable output, robust handling of monoclinic space groups, a clever space group symbol parser, unlimited size atom lists, and command line, graphical, or web-based interfaces.

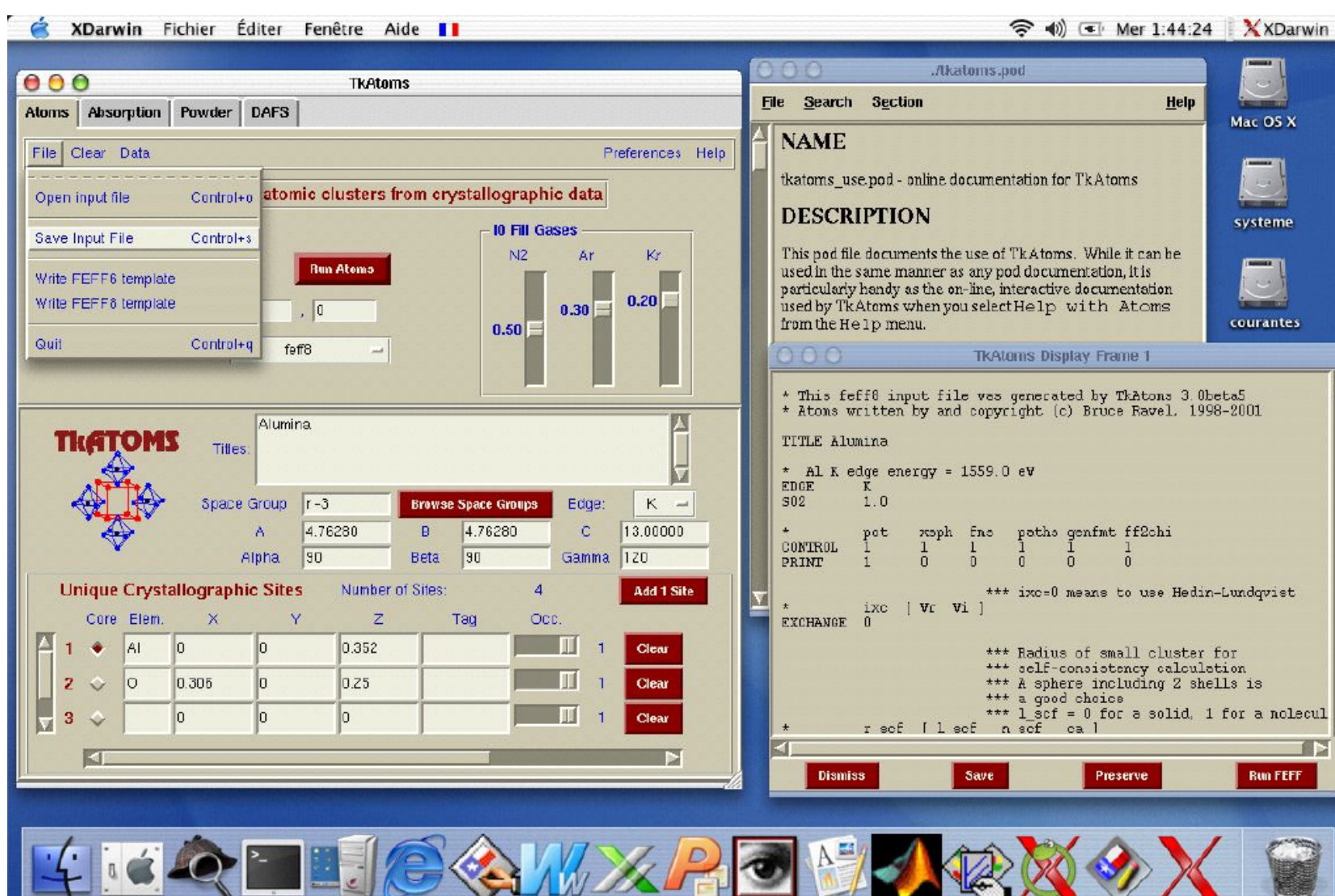
The input data to *TKATOMS* is the structural data commonly reported in the crystallography literature. Here is an example:

```
title YBCO: Y Ba2 Cu3 O7
space P M M M
rmax=5.2 a=3.823 b=3.886 c=11.681
core=cu2
atoms
! sym x y z tag
Y 0.5 0.5 0.5
Ba 0.5 0.5 0.184 cu1
Cu 0 0 0.356 cu2
O 0 0 0.5 o1
O 0 0 0.158 o2
O 0 0 0.5 o3
O 0.5 0 0.377 o4
```

From these input crystallographic data, *TKATOMS* generates FEFF input files or atom lists. It can also make several useful calculations involving tables of absorption coefficients and simulate powder diffraction and Diffraction Anomalous Fine-Structure (DAFS) spectra.



This is a shot of *TKATOMS* running natively in Mac OSX with X-Windows for Darwin. It shows the main window along with the on-line help and a FEFF8 input file.



The ATOMS Periodic Table

ATOMS comes with a periodic table of X-ray edge and line energies for all the elements which also computes absorption lengths and transmitted fractions for the pure elements and convert all energy values to wavelength. *Very handy at the beam line!*

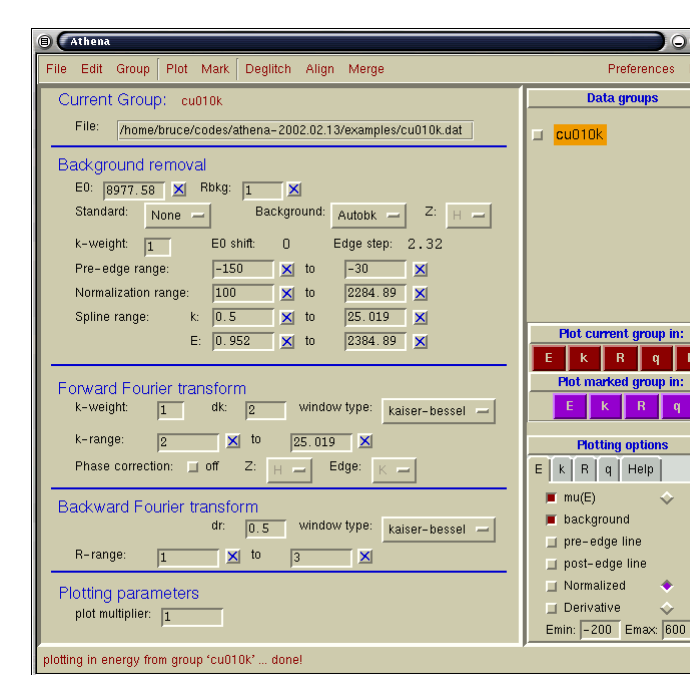
Free Software

IFEFFIT, *TKATOMS*, *ATHENA*, and *ARTEMIS* are all free software and are built using tools which themselves are free software. This means that you may download and use them without cost. In that sense, they are like *free beer*. But it also means that you are guaranteed certain liberties with respect to their use, including the freedoms to redistribute the programs to others, to modify the programs for your own benefit or for the benefit of others, and to examine the algorithms for reasons of security or suitability of purpose. In that sense, they are like *free speech*. Like all forms of free speech, free software comes with some costs in the form of additional responsibilities. We ask that, if you modify the codes, you contribute the modifications to the authors so that others may benefit by your inspiration. We require that, if you redistribute the programs, you also distribute the source code. And we ask that you cite our work in your published articles.

ATHENA

ATHENA is a program for generic EXAFS data processing, including:

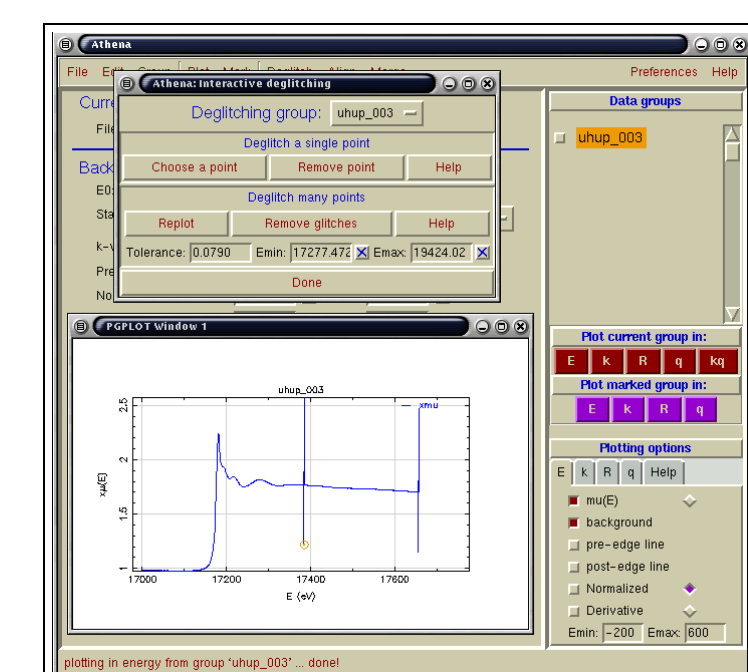
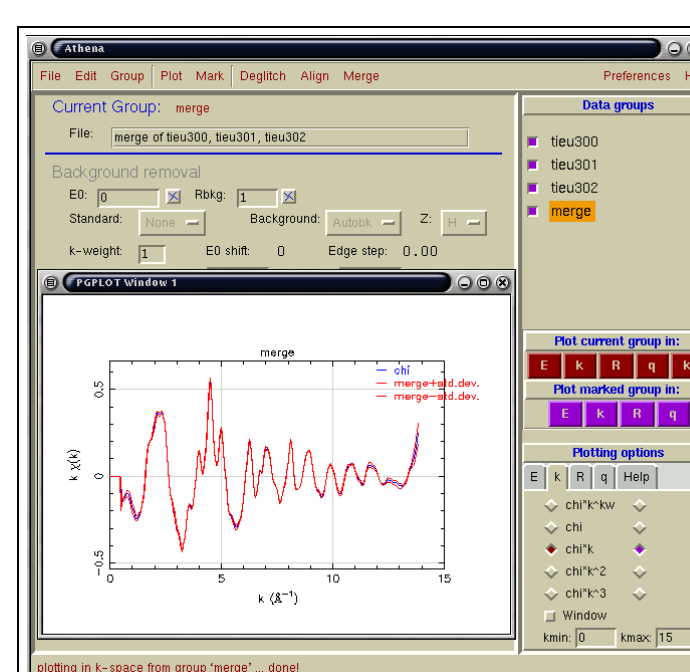
- converting raw transmission or fluorescence data into $\mu(E)$ spectra
- deglitching
- merging spectra
- data alignment
- difference spectra
- background removal using the AUTOBK³ algorithm
- normalization to Cromer-Liberman calculations⁴
- forward and backward Fourier transforms with optional central atom phase corrections



A generic dialog allows for conversion of raw column data into $\mu(E)$ spectra by selecting columns and options. *ATHENA* allows various input data types besides raw column data, including $\mu(E)$, $\chi(k)$, and output files from FEFF. Additionally, many data preprocessing chores may be automated by comparison to a previously defined data standard, including setting data analysis parameters, interpolation, alignment, deglitching, and truncation.

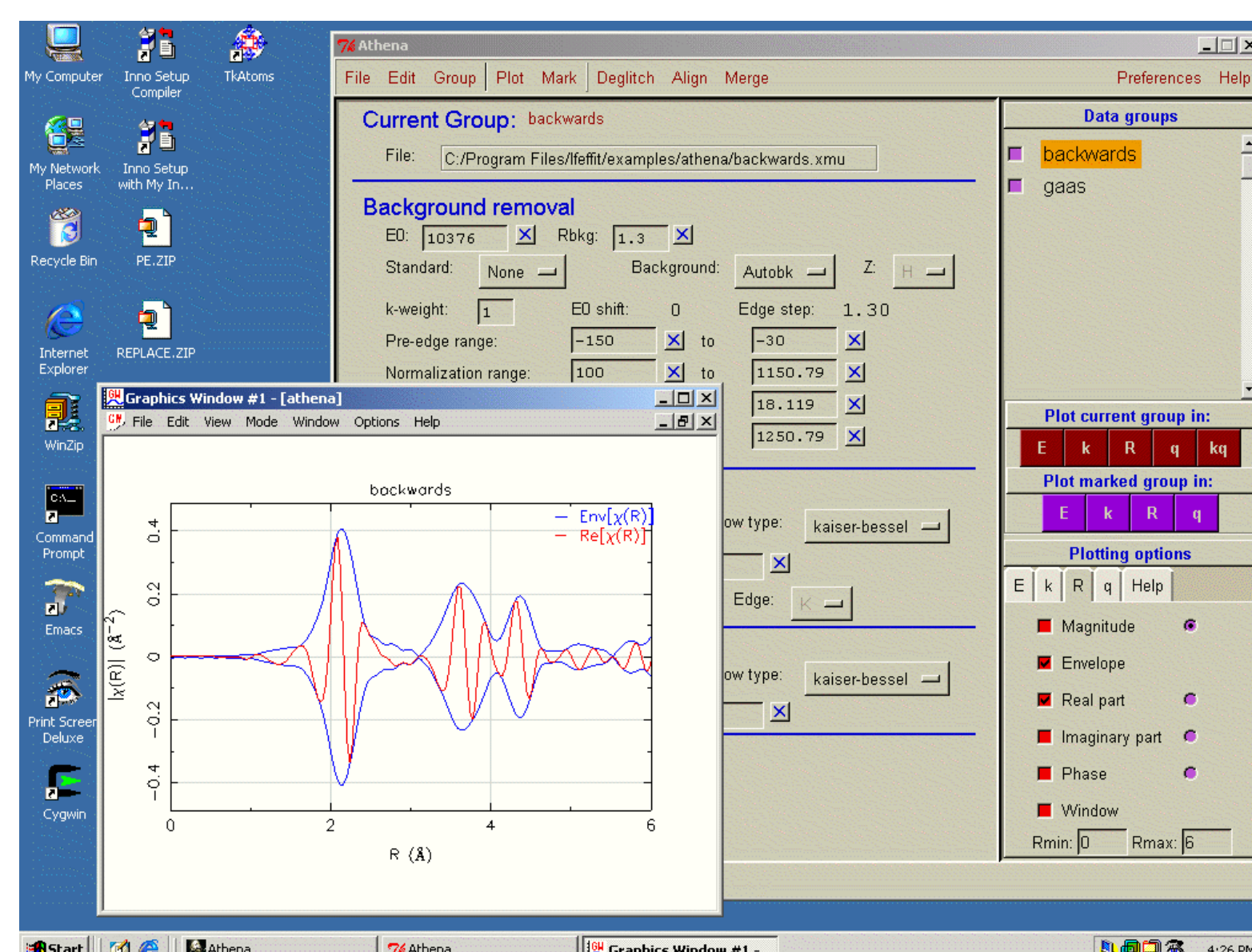
There are two noteworthy features of *ATHENA*. First, **the only active buttons are for plotting** in energy, *k*-space, *R*-space, or back-transformed *k*-space (which is called *q*-space in *ATHENA* and *ARTEMIS*). Whenever one of these buttons is selected, *ATHENA* will perform background removals, Fourier transforms, and other operations as needed to display data in the requested space. Second, **performing analysis or plotting operations is just as simple on single groups as on sets of marked data groups**. A group is marked by pressing the small purple button next to its name. Pressing a red plotting button will plot the *selected* group. Pressing a purple button will overplot *all marked* groups, as shown in the figure. Merging and other operations work on the set of marked groups.

ATHENA allows you to merge data. Each data group that you want to include in the merge is marked by pressing the small purple button next to its name. The Merge menu in the menubar has options for merging $\mu(E)$, normalized $\mu(E)$, $\chi(k)$, $\tilde{\chi}(R)$, or $\tilde{\chi}(q)$. Shown in the picture is the merge of three data groups in *k*-space. The plot is of the averaged data along with the average data plus and minus the standard deviation.



With *ATHENA*, you can deglitch data point by point, as shown, or use an algorithm which attempts to identify and remove groups of glitchy points.

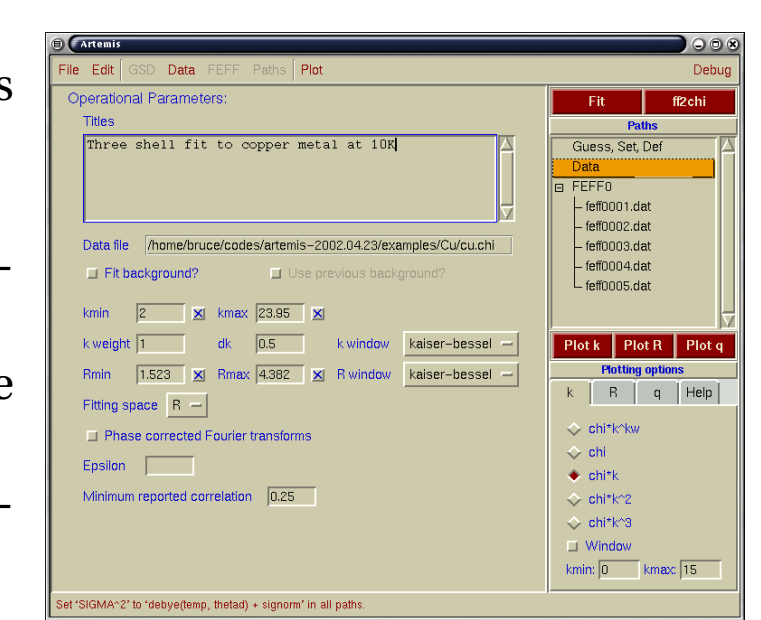
Here is a shot of *ATHENA* running on Windows 2000. This shows how interesting plots are made using the Plotting Options.



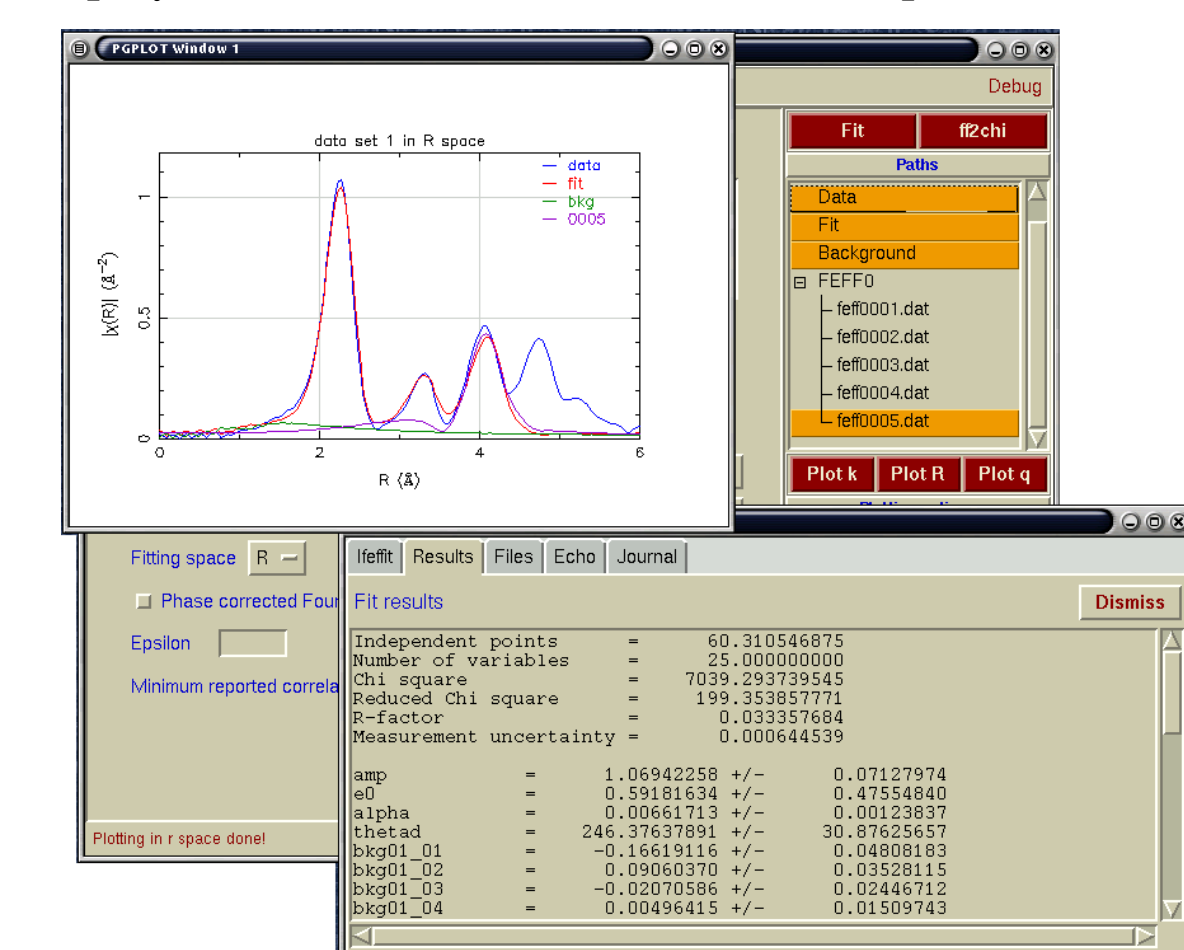
ARTEMIS

ARTEMIS is a program for quantitative and statistical analysis of EXAFS data.

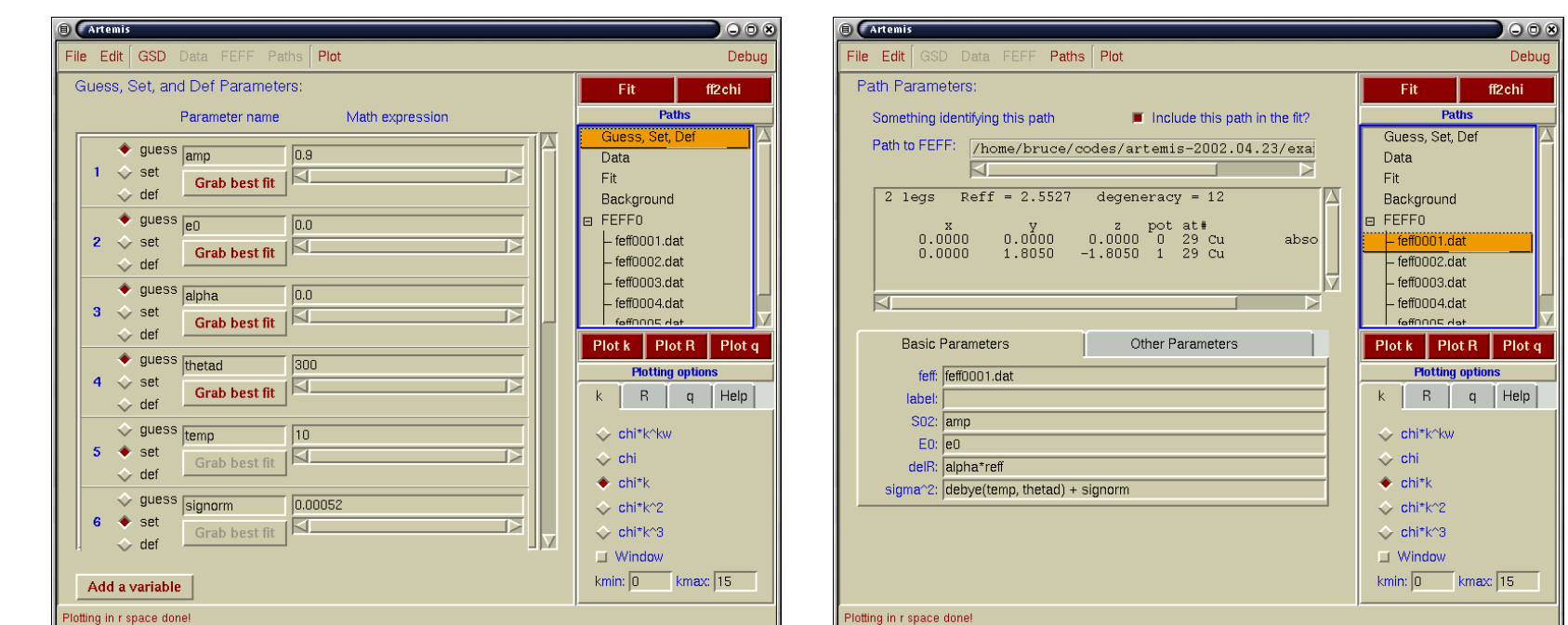
- A forms-based interface to setting fitting parameters
- A forms-based interface to setting constraints and restraints between parameters
- Co-refinement of a background spline
- Plotting in *k*-, *R*-, or back-transformed *k*-space
- Plotting of data, the best-fit function, the background spline, and individual paths
- Display of error bars on and correlations between variables
- Import input files from the old FEFFIT program



Here is the result of a fit to an EXAFS spectrum of a copper foil. The plot shows the Fourier transforms of the data and the best fit along with the co-refined background and the third-shell, single-scattering path. The best-fit parameters and their error bars are displayed in the pop-up palette. The χ^2 , *R*-factor, and other statistical parameters are displayed, as are the correlations between parameters.



These two pictures demonstrate how constraints are set in *ARTEMIS*. Variables are defined in the *Guess*, *Set*, *Def* form. Guess parameters are varied in the fit. Set and def parameters are fixed and may be expressed in terms of other parameters by math expressions. In the *Path* Parameters form, parameters from the EXAFS equation are set for each path included in the fit.



In this example, the correlated Debye model is used to compute σ^2 for each path using a single variable parameter, the Debye temperature θ_D . The ΔR for each path is computed from a thermal expansion coefficient, α .

URLs

The IFEFFIT homepage:

<http://cars.uchicago.edu/ifeffit>

Bruce's EXAFS software homepage:

<http://feff.phys.washington.edu/~ravel/software/exafs/>

The IFEFFIT mailing list:

<http://cars9.uchicago.edu/mailman/listinfo/ifeffit/>

Citing this software

IFEFFIT

M. Newville, J. Synchrotron Rad. (2001) **8**, pp. 322–324

ATOMS

B. Ravel, J. Synchrotron Rad. (2001) **8**, pp. 314–316

ATHENA and ARTEMIS are currently unpublished.

Bibliography

1. Ankudinov, *et al.*, Phys. Rev. **B58**, #12, (1998) pp. 7565–7576
2. Zabinsky, *et al.*, Phys. Rev. **B52**, #4, (1995), pp. 2995–3009
3. Newville, *et al.*, Phys. Rev. **B47**, #21, (1993), pp. 14126–14131
4. Cromer and Liberman, J. Chem. Phys. **53**, (1970), pp. 1891–1898

This poster was prepared on May 13, 2002. On that date, the current versions were IFEFFIT 1.0071, ATOMS 3.0beta5, and ATHENA 2002.05.13 and ARTEMIS 2002.05.13, although the pictures in this poster may differ from current versions.

Platforms

IFEFFIT, *TKATOMS*, *ATHENA*, and *ARTEMIS* have been extensively tested on a variety of platforms, including

- Linux and SGI. Other unices should require minimal porting effort.
- Windows 2000 and NT. The installer package and the programs will all work on XP, 95, 98, and ME as well.
- Macintosh OSX. Earlier Mac systems are unsupported.