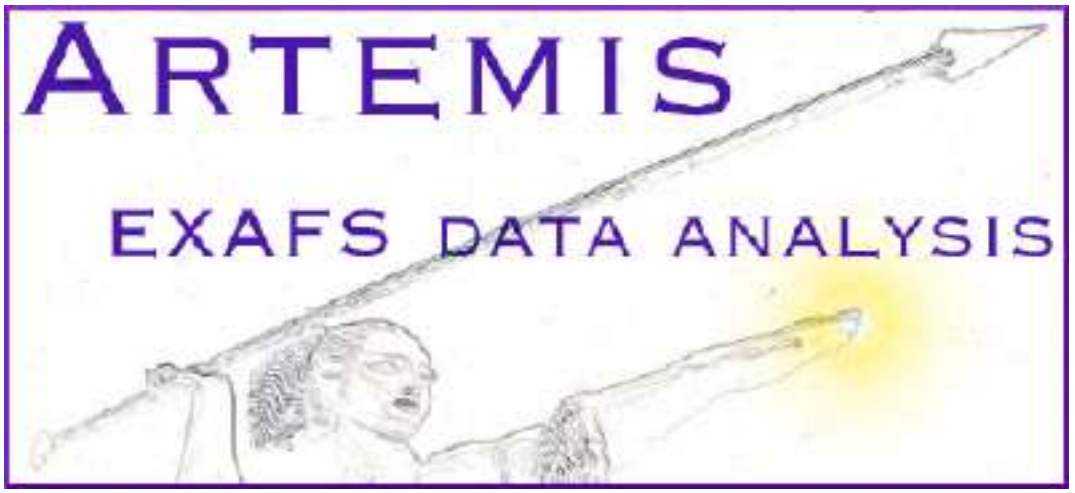

Preview of the 0.8 Branch of ARTEMIS

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What is This Document?

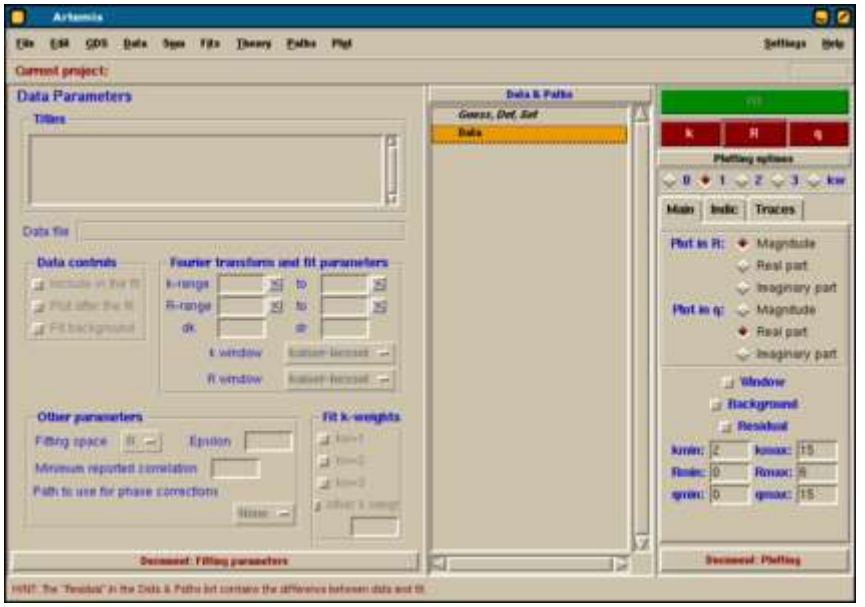
This document provides a brief overview of the changes between version 0.7 and 0.8 of ARTEMIS. Nothing here is explained in great depth, but if you keep this document by your side the first time you fire up the new version, it should help explore and understand all the new features.

<u>The central aims of version 0.8 include:</u>

1. Enhance the feature sets of the various parts of ARTEMIS to improve the user experience.
2. Expand the notion of the "project" by adding the fit history feature set.
3. Tighten the integration of ARTEMIS with ATHENA.

Startup screen

(1) The main screen is now divided into three sections
  (a) The main panel, which changes depending on what item is selected in the Data and Paths List
  (b) The central panel, which shows the list of data, fits, and paths
  (c) The right panel, which contains the plot buttons and the various plotting controls
(2) There is now a menu for doing summations of paths
(3) There is an indicator in the upper right hand corner which will tell you when your project has been modified



(4) There are several new plotting controls organized into three tabs.
(5) The controls for choosing how $\chi(R)$ and $\chi(q)$ are plotted are now radio buttons.
(6) Relevant document pages are accessible from all over the program.

Importing from ATHENA

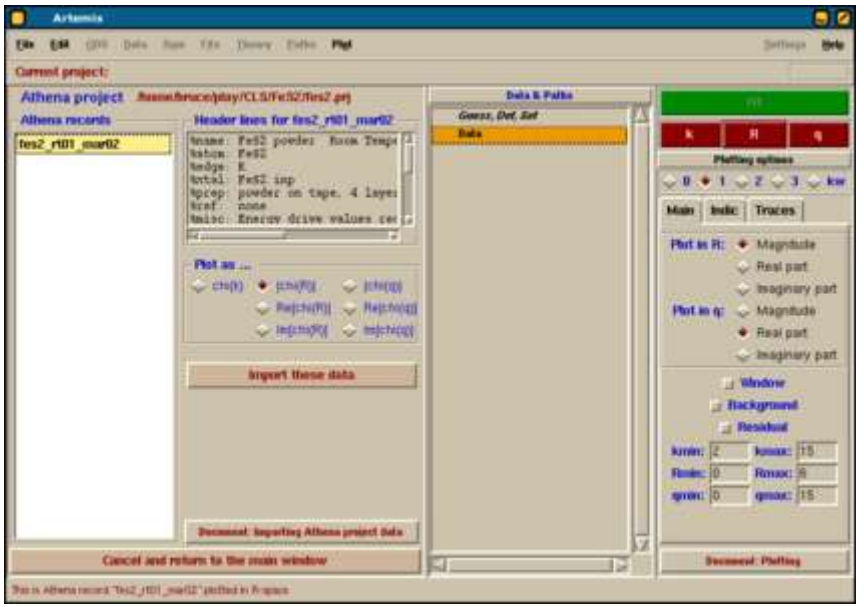
(1) Data can now be imported directly from ATHENA

(2) When an ATHENA project is imported, this screen is displayed.

(3) Every group in the project file is displayed in the list on the left.

(4) Groups from the project can be selected (highlighted in yellow) and plotted as χ(k), χ(R), or χ(q)

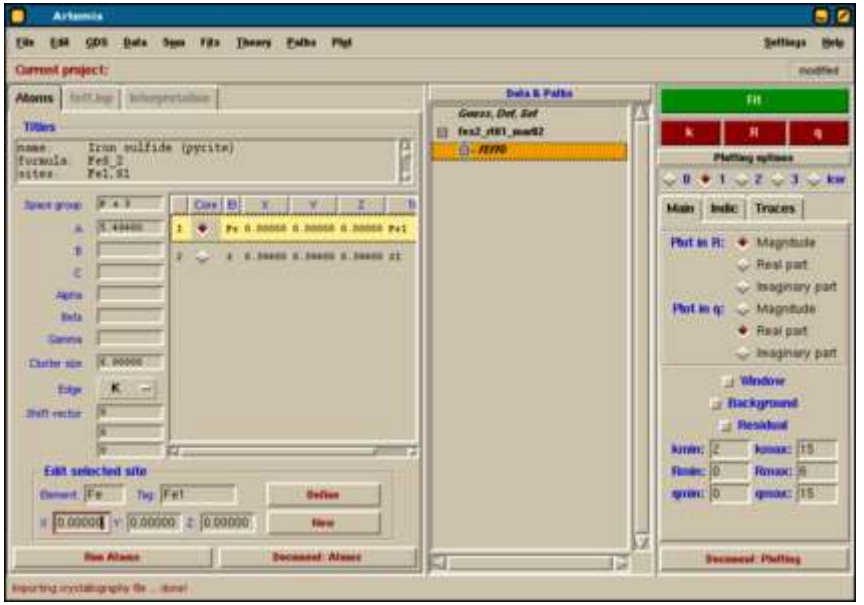
(5) When the import button is clicked, the chosen data is moved to the Data and Paths List and its Fourier transform, R-range parameters, and k-weight parameters are imported.



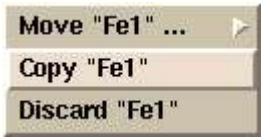
Note that the File menu now only has one option for importing all file types (`atoms.inp`, `feff.inp`, χ(k) data, ATHENA projects, ARTEMIS projects).

You can still import χ(k) files, just like before.

Improved ATOMS Interface



(1) The ATOMS page has been revamped and now works similarly to the Guess, Def, Set page.
(2) Selecting a site highlights it in yellow and inserts its coordinates in the editing area at the bottom.
(3) To define a new site, click the New button, enter its species, tag, and coordinates, then click the Define button.
(4) To alter a site, select it, edit it, then click the Define button to commit the change.
(5) The site list can be of unlimited length.
(6) There are items in the Theory menu which are relevant to the ATOMS page.



Right-clicking on a site will display this context menu with entries for manipulating the list of sites.

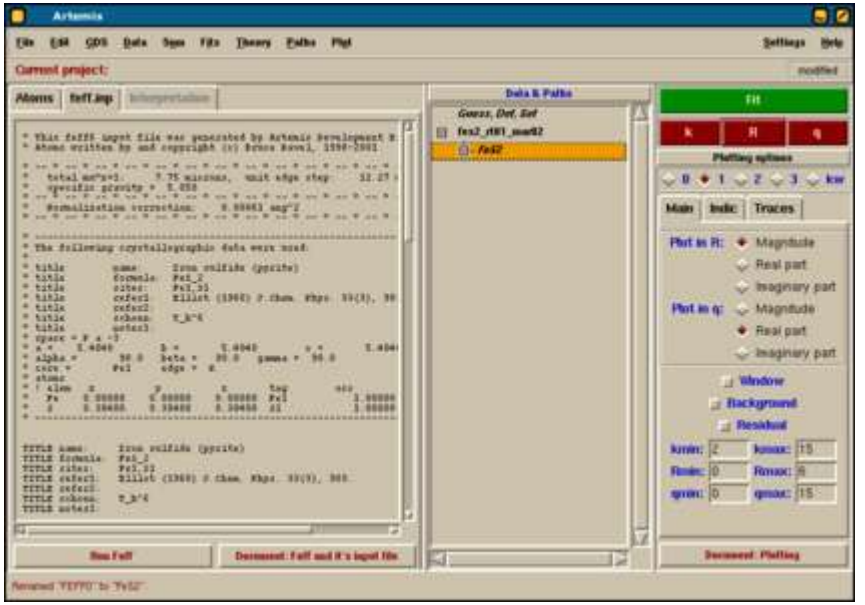
(7) You can import `atoms.inp` or CIF files.
(8) Configurable output for FEFF6 or FEFF8.

Changes in the FEFF Interface

(1) The FEFF interface is mostly the same as in previous version of ARTEMIS.

(2) In the Edit menu is an option labeled “Compact project.” Choosing this will make your project smaller by removing all unused files from your FEFF runs. Should you ever need to recover these files, simply rerun FEFF and, when asked how many paths to import, import none at that point.

(3) ARTEMIS now tries to parse FEFF's error messages and offer advice for how to fix the problem that triggered the error.



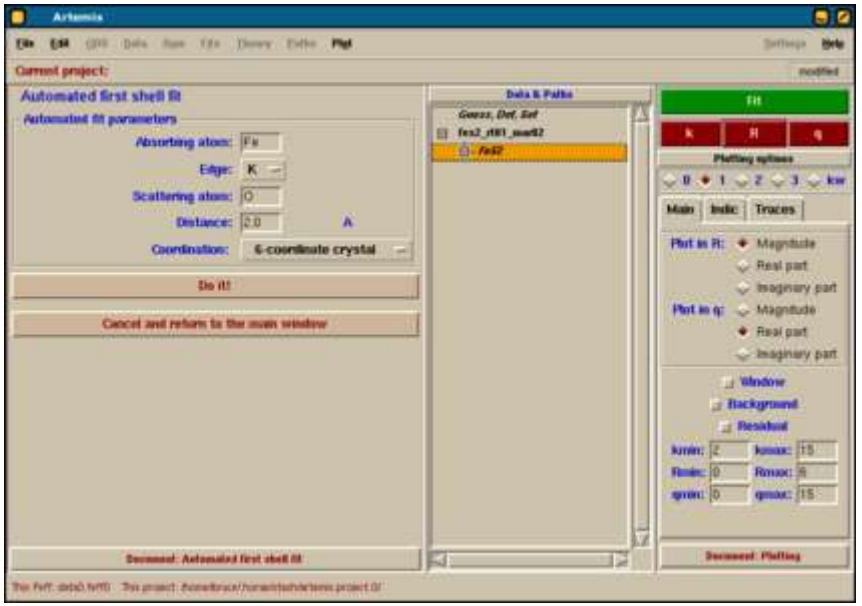
Quick 1st Shell Theory

(1) In the Theory menu is an option for “Quick first shell theory.” Selecting it shows this page.

(2) Here you can specify parameters for a simple first shell fitting problem, including the species of the absorber and scatterer, the bond length and the coordination geometry.

(3) Clicking the “Do it!” button will generate a suitable `feff.inp' file, run FEFF and import the first shell path.

(4) Fitting parameters for a cumulant fit will be auto-generated and inserted into the GDS list.



For many first shell problems, you can import some data, then run the quick first shell theory with sensible parameters, then hit the big green button, and expect a fit that is both good and reasonable!

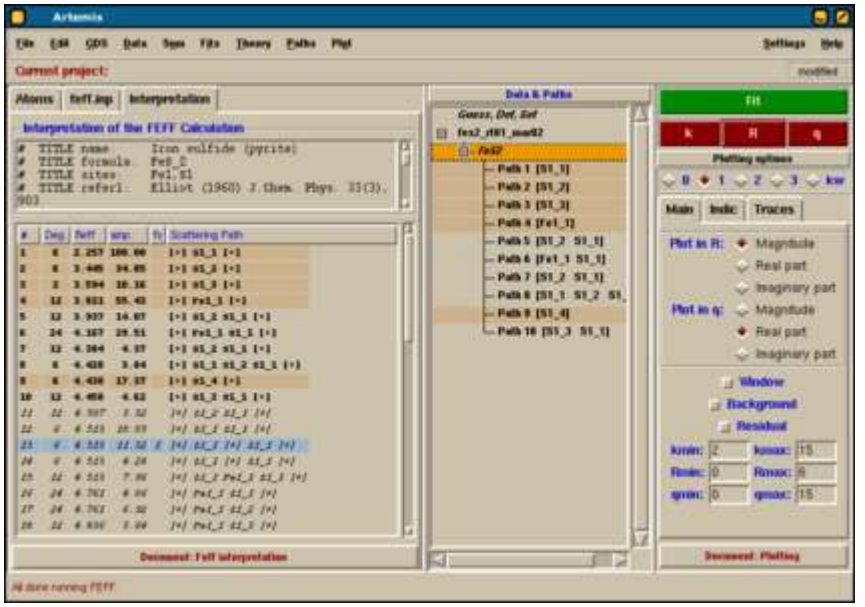
Changes on the FEFF Interpretation Page

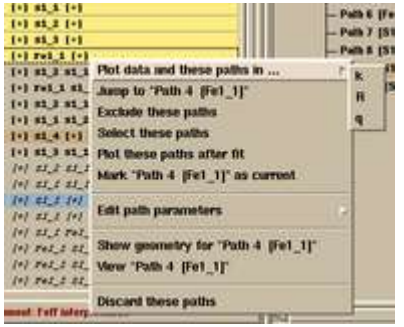
(1) The FEFF interpretation page has many new features based on a new method of displaying the information.

(2) Paths can be selected by clicking, click-dragging, control-clicking, and shift-clicking.

(3) Color and font indicates the state of each path in the project
   (a) **Black and bold**: included in fit
   (b) **Brown and bold**: excluded
   (c) *Italic*: available, not imported
   (d) *Italic and gray*: not in project
   (e) Tan background: SS path
   (f) Blue background: collinear path

(4) The background colors are also used in the Data and Paths List.





Right clicking on any path in the interpretation list displays this menu with many options for examining and manipulating paths. This menu is sensitive to the extended selection.

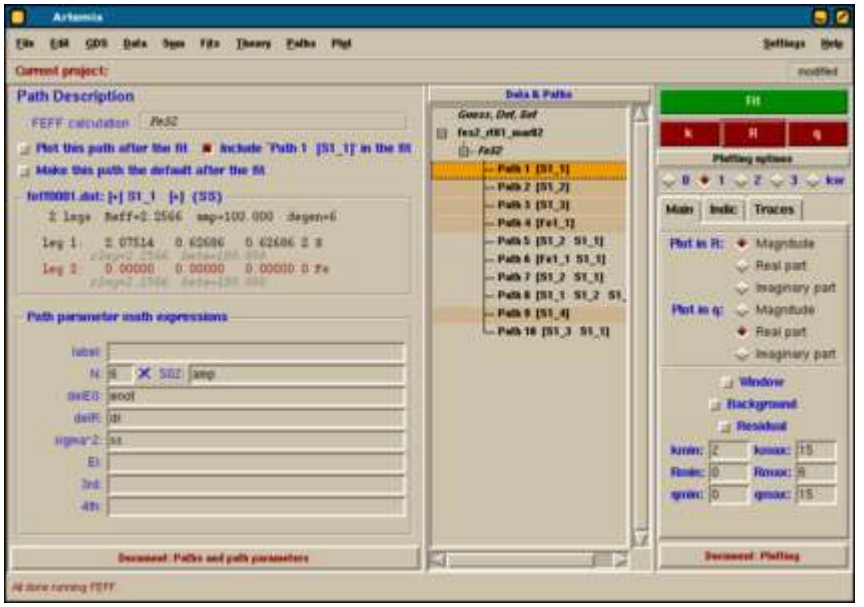
Changes on the Path Page

(1) The path description box has colored text.

(2) There is a toggle for telling ARTEMIS to plot the path after a fit is complete. That is, the paths selected for plotting will be added to the plot of the data and fit that is made upon completion of the fit. Any number of paths can be selected for plotting after the fit.

(3) The entry strings for the paths in the Data and Paths List no longer include the name of the FEFF path file.

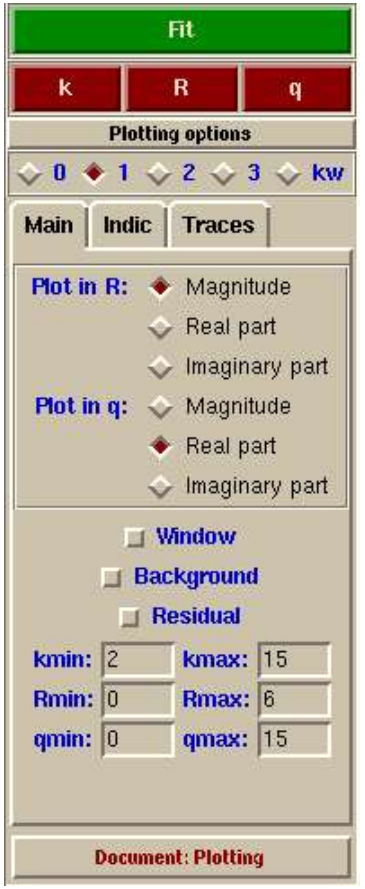
(4) The context menu for σ^2 includes options for inserting text appropriate to the Einstein and Debye models.

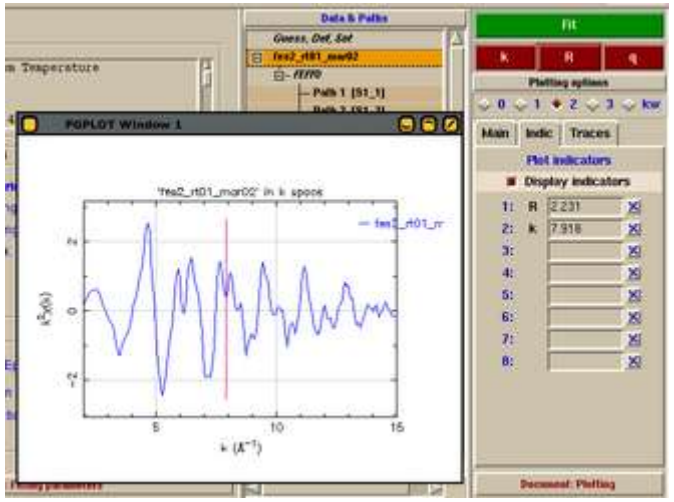


New Plotting Options

(1) The option menus for the parts of the χ(R) or χ(q) plots have been broken out into radio buttons.

(2) The background and residual spectra are no longer in the Data and Paths List. They are now plotted for each selected fit when selected with their check buttons.





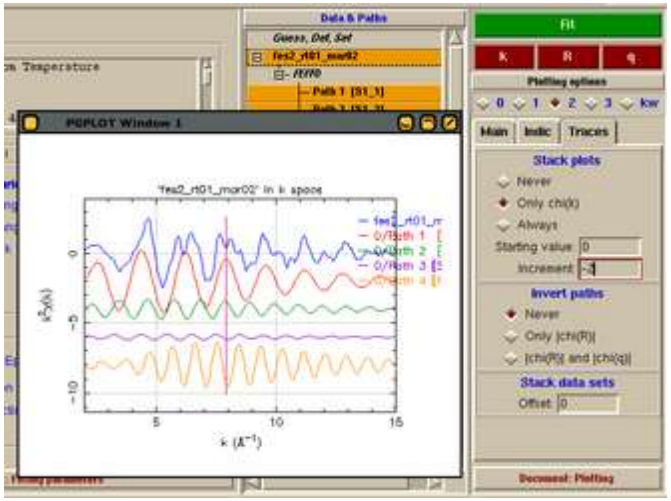
(1) Indicators have been implemented. These are markers that are repeated from plot to plot at a specified location.

(2) Indicators can be placed in k, R, or q.

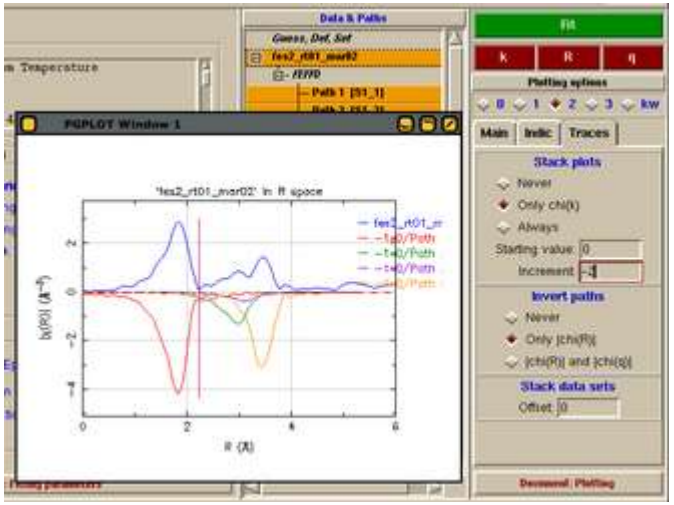
(3) Indicators in k will also be plotted in q and vice versa.

(4) The maximum number of indicators and their color and line type is configurable.

Stacked and Inverted Plots



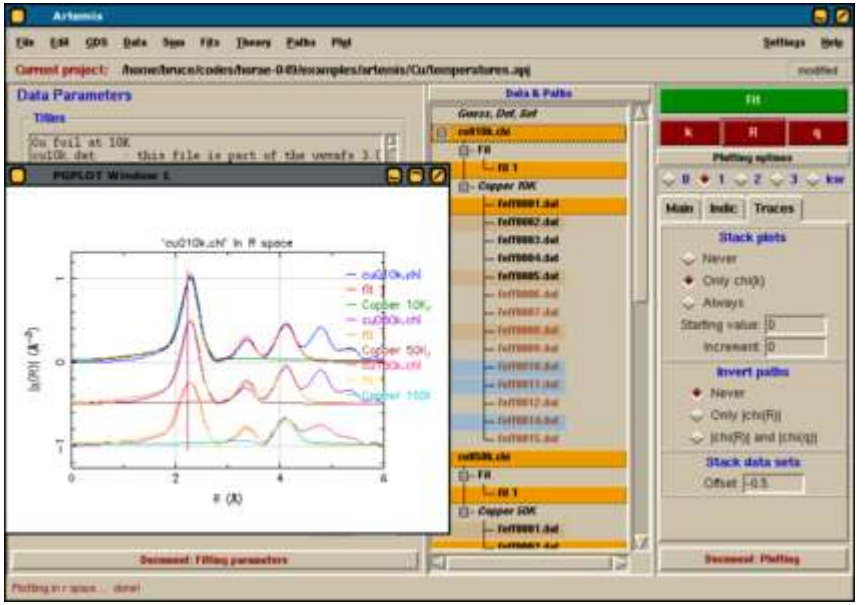
(1) Plots can be stacked, with a specified interval.
(2) This seems most useful for χ(k), but any plot can be stacked.
(3) Indicators and stacking play well together.
(4) Stacking over-rides inversion.



(1) Magnitude plots can have the paths inverted, providing another way of visualizing the contributions from the various paths.
(2) Only |χ(R)| or |χ(q)| plots can be inverted.
(3) Indicators and path inversion play well together.

Plotting Options for Multiple Data Set Fits

(1) Multiple data set fits can be stacked on a per data set basis. All traces associated with a data set are plotted at the same level.
(2) The increment between data sets is adjustable.
(3) Indicators and MDS stacking play well together.
(4) MDS stacking over-rides normal stacking.
(5) Any number of data sets in an MDS fit can be tagged for plotting after the fit.



Starting a Fit

(1) To accommodate the new fit history feature (see the next slide), ARTEMIS asks for some information each time a fit is run.

(2) There are default values and ARTEMIS can be configured to use them without asking.

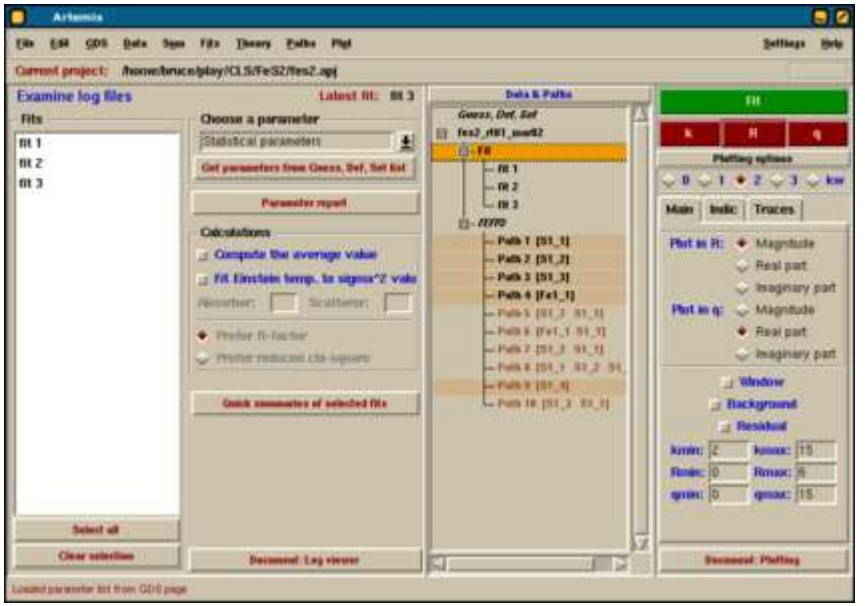
(3) The information in this dialog is written to the log file and used for several other purposes.
   (a) The label is used in the Data and Paths List
   (b) The comment is written to the Properties and to the top of the log file
   (c) The figure of merit is used in generating and plotting reports on fitting parameters

(4) Any fit can be selected from the Data and Paths List and plotted.

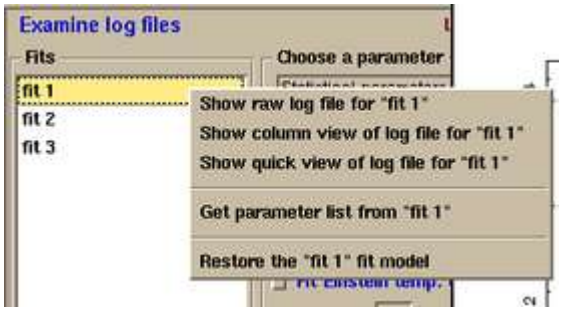
(5) If "Make a new fit entry" is selected, the fit will be added to the Data and Paths List.

(6) If "Reuse previous fit entry" is selected the most recent fit in the list will be overwritten. This is convenient for playing around with fitting models without needed to save each iteration.

Fit history



(1) Selecting a fit from the Data and Paths List displays the fit history page.
(2) ARTEMIS stores the data, best fit spectrum, log file, and description of the fitting model for every fit.
(3) Each fit is displayed in the list on the left of the fit history page.
(4) This list has a right click menu with options for viewing the log file. Double clicking will also display the log file.
(5) You can restore a fitting model, i.e. revert ARTEMIS to a previous state.



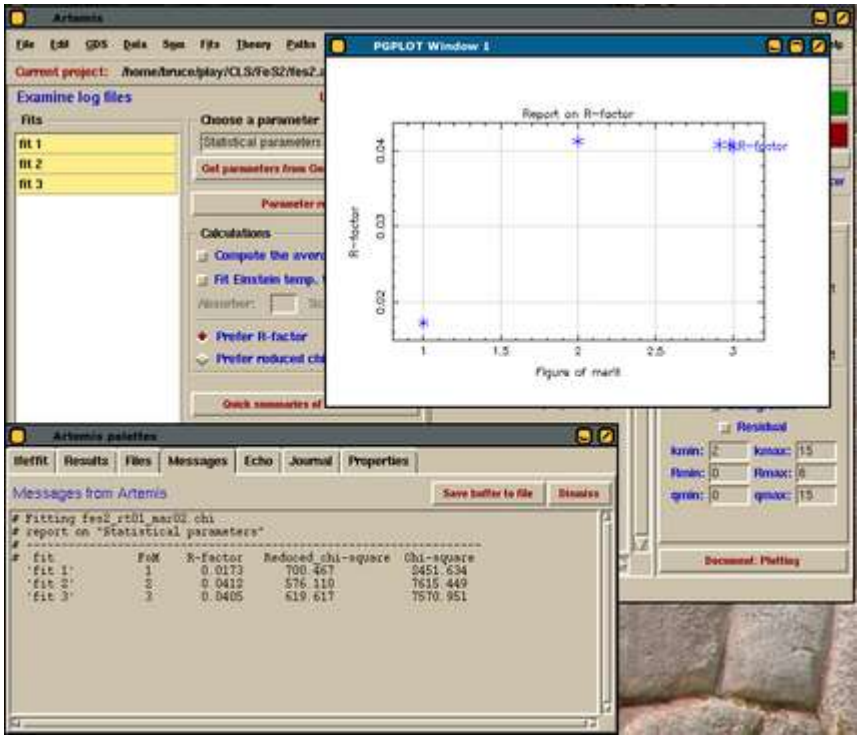
Writing and Plotting Reports

(1) The main use of this page is to generate and plot reports on fitting statistics or fitting parameters from the various fits.

(2) The list of fits works with extended selection and the selected fits are included in the report.

(3) Optionally, you can compute the average and standard deviation of a fitting parameter or fit an Einstein temperature to a sequence of σ^2 values.

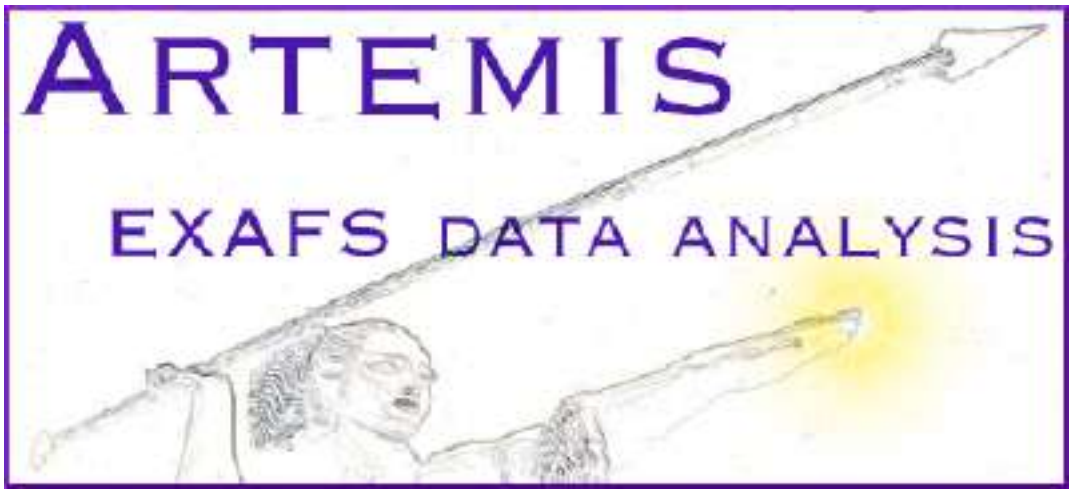
(4) The "figure of merit" from the fit dialog is used as the abscissa of the plot. For some data, e.g. temperature series, FOMs should be chosen appropriately.



(5) FOMs and labels can be changed at any time.

What's Next?

(1) Split the data page into two tabs. The additional tab would be like ATHENA's main page, allowing you to tweak the background removal before fitting.
(2) Improved space group browser (currently broken)
(3) Syntax highlighting in the path parameter entry boxes on the path page.
(4) Batch processing, i.e. run a fitting model on a series of input data files. This will be useful for temperature or other series.
(5) χ^2 or R-factor maps of parameter pairs to search for false minima of the fit.



(6) Import complete IFEFFIT scripts.
(7) Convert a data file into a `feffNNNN.dat'-style pseudo-path by Fourier filtering for situations involving hydrogen.
(8) Import/export of atomic coordinate lists in PDB format.

What else?