
Using AARTEMIS

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1 NAME

Artemis - interactive EXAFS data analysis

2 DESCRIPTION

Artemis is a program for analyzing EXAFS data using theoretical standards from **Feff**. **Artemis** includes interfaces to **Atoms** and **Feff** as well as forms for defining parameters and applying those parameters to the paths from the **Feff** calculation. **Artemis** uses $\chi(k)$ as its input. It does not handle any data processing chores, such as converting raw data to $\mu(E)$ or doing background removal. **Artemis**'s sister program **Athena** is the data processing program.

3 SYNOPSIS

Artemis is a graphical and interactive program written in the perl programming language, using the Tk display engine, the **Iffit** EXAFS library, and the PGPLOT plotting library. (See below for a list of relevant URLs.)

Artemis helps you organize all aspects of a fitting project, including running the **Feff** calculation, settings parameters for the Fourier transform and fitting of the data, parameterizing the paths from the **Feff** calculation, running the fit, and plotting the results. The **Artemis** window is divided into three panels. The largest panel is the space where most of the work happens. Its content is model and depends on the state of the Data and Paths List. This list is in the center, skinny panel. The other skinny panel contains the controls the are used to specify how plots are made.

At the top of the window are the menubar and the project bar. The project bar displays the name of the current project file. It also contains an indicator that tells you if the project has been modified since the last time it was saved. Clicking on the modified indicator will save the project (just like C-s or the "Save project" item in the File menu). At the bottom of the screen is the echo area, where **Artemis** writes all sorts of helpful messages as you use the program.

The Data and Paths list contains a tree-like list of all of the objects that can be manipulated as you use **Artemis**. When the program starts, two such items are displayed. As you run **Feff** calculations, import **Feff** paths and other data sets, and run fits, more items are added to this list. In total, there are five kinds of entries in this list, each of which controls a different aspect of **Artemis**. These five kinds of list entries are: (1) fitting parameters, (2) data, (3) fits, (4) **Feff** calculation, or (5) **Feff** path. When you click on an item in the Data and Paths List, that item will be "selected" and "anchored". A selected item is highlighted in orange. An anchored item is outlined with a dashed line. Only one item can be anchored. 0, 1, or more items can be selected.

The anchored item determines the mode of the large panel. For instance, when the "Guess, Def, Set" item is anchored, the main panel will display a page used for setting the fitting parameters. When a data item is anchored,

the main panel will display a page for setting Fourier transform parameters, the fitting range, and other parameters associated with the data. Many functions in **Artemis** depend upon the mode of the main panel. Some features are available only in certain modes. Each of the modes is described in its own document section. See **SECTIONS OF THE DOCUMENT**.

Plots in **Artemis** are always made using the selected items. To plot, for example, data, a fit, and several individual paths, it is necessary to select each of those items. Many other functions in **Artemis** also work on the set of selected items.

Anchoring and setting paths is usually done by using the mouse in the Data and Paths List, although there are several other ways of changing the anchor and selection using the mouse or the keyboard. Here is a list of mouse events useful in the Data and Paths List:

Left mouse button

Clicking the left mouse button will clear all selections then select and anchor the item clicked. The main panel will display the page appropriate to the anchored item.

Center mouse button

Clicking the center mouse button will anchor the item clicked without changing the selection. The main panel will display the page appropriate to the anchored item.

Right mouse button

Clicking the right mouse button will anchor the item clicked without changing the selection. It will also post a menu of functions appropriate to the item clicked. These menus are the same as the menus in the menubar at the top of the window. The main panel will display the page appropriate to the anchored item.

Control key + left mouse button

Clicking the left mouse button while holding down the control key will add the item clicked to the group of selected items. The anchor is not changed.

Shift key + left mouse button

Clicking the left mouse button while holding down the shift key will select all items between the anchor and the item clicked, inclusively. The anchor is not changed.

Left mouse button + mouse drag

Clicking the left mouse button then dragging the mouse while holding down the button will select all items that you drag the cursor over. The item initially clicked will be anchored and the main panel will display the page appropriate to the anchored item.

Control-k, Control-j

Hitting the k or j keys while holding the control key will move the anchor to the previous or next item in the list without changing the selection. The main panel will display the page appropriate to the anchored item. These two key sequences, behave differently when the Guess, Def, Set item is anchored. See [The Guess, Def, Set page|artemis.gds](#) for details

Control-l

Hitting the l key while holding down the control key will put focus on the Data and Path List. This allows you to navigate the list using the arrow keys.

The color and font of the text in the Data and Paths List indicates the status of each item. Any item written in black, upright text is an item that can be plotted. When a data set or **Feff** path is excluded from the fit, it will be written in brown text. The Guess, Def, Set item and the **Feff** calculation items are written in italic text. The italic text indicates items that cannot be plotted. Although these non-plottable items can be selected, they will be ignored when a plot is made.

4 ARTEMIS: The Data Page

ARTEMIS - The data page

The data page is displayed in **Artemis**'s main panel when a data item is anchored in the Data and Paths List. See the [main document section](#) for an explanation of anchoring and selecting items in the Data and Paths List.

The data page is divided into five sections. At the top is a box containing the title lines associated with these data. These are read from the input data file, but can be edited at any time by the user. When the data are written to output files, the contents of this box are written as headers. Below the titles box is the name of the data file that was imported. Below that are four boxes containing groups of related controls.

Data toggles

This box contains three toggles that control certain aspects of the fit. The first two are only relevant in a multiple data set fit. When setting up a project containing a multiple data set fit, it is sometimes useful to exclude an entire data set from the fit without deleting it from the project. This can be done with the first toggle. When a data set is excluded, it and all items beneath it are shown in brown text in the Data and Paths List to indicate that they have been excluded from the fit.

After the fit is complete, **Artemis** wants to show off her handiwork and display a plot of the data and the just-finished fit. In the case of a multiple data

set fit, you might have a preference about which data set gets plotting. Click this toggle on for your preferred data set.

The third toggle tells **Artemis** to do a corefinement of the background spline when it performs the fit. This corefinement is, effectively, the same operation that was performed by **Athena** to remove the background from the data. The **rmin** parameter serves the same purpose as **Athena**'s **rbkg** parameter. When the fit is performed with the background corefinement, a spline is used to fit the Fourier components of the data below **rmin** and the **Feff** paths are used to fit the Fourier components between **rmin** and **rmax**. The number of parameters used to determine the spline is the number of independent points in that portion of the data: $2 \cdot \text{delta_k} \cdot \text{delta_R} / \pi$, where **delta_k** is the range of the Fourier transform and **delta_R** is the range between 0 and **rmin**. The advantage of doing the background corefinement, other than the possibility of making the fit look nicer at low R, is that correlations between the background parameters and the fitting parameters can be measured.

Fourier transform and fitting parameters

This box contains the controls used to set the ranges of the forward Fourier transform and of the fit. The fit range is also used as the backward Fourier transform range when a plot in q space is made. See **Pluck buttons** for a discussion of the little square buttons marked with a blue x.

Other controls are used to set the functional forms of the Fourier transform window used in k and R. The widths of the sills of those functions are set using the entry boxes labeled **dk** and **dr**.

k-weight parameters

The controls in this box are used to set the values of k-weight to be used in the fits. There are toggles for turning on k-weight of 1, 2, or 3. There is also a toggle for specifying an arbitrary value of k-weight.

These are the k-weight values used in the fit but not the k-weight used to plot the data. These two purposes of k-weight are handled independently by **Artemis**. See **Plotting in Artemis|artemis_plot** for a discussion of the plotting k-weight controls.

People sometimes get confused by the concept of multiple k-weights for fitting. The purpose of choosing a low or high value for k-weight is to attempt to emphasize either the low- or high-k end of the data. Because different regions of the data are sensitive to different kinds of parameters, one might choose a low or high value to increase the precision of measurement of certain parameters. Doing multiple k-weight fits is a sort of compromise – a way of emphasizing both ends of the data in the fit.

The fit is determined by minimizing a quantity called chi-square. Chi-square is evaluated by summing the squares of the difference between the data and the theory. Since the FT is complex, there is a real part and an imaginary part. So chi-square is proportional to:

$$\sum_R \frac{\text{Re}[\text{data}(R) - \text{th}(R)]^2 + \text{Im}[\text{data}(R) - \text{th}(R)]^2}{\text{R}}$$

In a multiple k-weight fit, there are simply more terms in the sum. Let's take a kw=1&3 fit as an example. This summation is made for the kw=1 data and theory. **And** the summation is made for the kw=3 data and theory. The summations are added together and the full sum is used to evaluate chi-square.

At the end of the day, there is only one set of guess parameters that have been optimized by the fit. These guess parameters along with the set parameters are used to evaluate the def parameters and the path parameters. The path parameters are used to evaluate the exafs equation for each path. The exafs equations for the paths are summed up to make the best-fit theoretical **chi(k)**. You have a data **chi(k)** and a best-fit **chi(k)**. Those can then be plotted however you like – even using a k-weight that was not used in determining the fit.

Other parameters

The last box contains several controls that did not fit into the other boxes. There is a menu for selecting the fitting space. You can choose to fit the data in any of k, R, or q space. The default is to fit in R.

Epsilon is the uncertainty used to evaluate chi-square. Normally it is fine to let **Artemis** use the default value (which is determined from the RMS value of the data between 15 and 25 angstroms in R-space). In some situations, you may find it useful to explicitly set a value for epsilon.

After the fit, **Artemis** writes a log file documenting the fit. Among the information in that log file are the correlations between all the fitting parameters. You can set the level below which **Artemis** will exclude a correlation from this report.

Finally, there is a menu for selecting the path to use for phase corrected plots. This menu contains the first five paths from each **Feff** calculation used with the data set. When a path is selected for phase corrected plots, the full phase shift of that path – both the central atom and scattering atom portions – will be subtracted from anything that is Fourier transformed before it is plotted. If a path is selected for phase correction and you make a plot of, say, the data, the fit, and several paths, the selected phase shift will be subtracted from each item before it is plotted. Phase correction is for plotting only. Fits are always done on non-phase-corrected data.

Pluck buttons

Several of the controls on this page have a small button with a blue x next to them. These are called pluck buttons and are used for grabbing values from the plot window. When you click on one of these buttons, a prompt will be written to the echo area asking you to click on a point in the plot. When you do so,

the value that you clicked on will be inserted into the entry box adjacent to the pluck button. **Artemis** is careful not to let you pluck a k-value from a plot in R, or vice versa.

Context menus

As you pass the mouse over labels on the data page, the text under the mouse will change color. This color change is an indication that mouse clicks will do something. A left mouse click on one of these labels will cause a brief description of that parameter to be displayed in the echo area. Many of these descriptions also suggest reasonable values for the parameter.

Clicking the right mouse button on one of the labels will post a context menu of useful function. One such function is restore that parameter to its default value. If you have a multiple data set fit, the other menu options allow you to constrain the parameter between data sets.

The labels at the top of the boxes are all sensitive to the left mouse button. The labels atop the Fourier transform and fit range box and the k-weights box are also sensitive to the right mouse click.

5 ARTEMIS: Guess, Set, Def Parameters

ARTEMIS - Guess, set, def parameters

This page is used to define the parameters of the fitting model. In **Artemis** there are six kinds of parameters:

Guess

Guess parameters are the ones that are optimized during the course of the fit to best-fit the theory to the data.

Def

Def parameters are typically expressed as math expressions which may be functionally dependant upon other parameters. These math expressions are updated throughout the course of the fit. As the guess parameters are updated, so are the def parameters.

Set

Set parameters are evaluated at the beginning of the fit and not updated throughout the fit. This is the main difference between def and set parameters. Set parameters can be numbers or math expressions.

Restraint

Restraints are math expressions which, like def parameters, are updated throughout the course of the fit, but which take on a special role in the fit. A restraint is evaluated and added in quadrature to the evaluation of the chi-square parameter. A restraint, therefore, can be used to incorporate

a a bias in the fitting result towards a piece of prior knowledge about the physical system. See the **Iffit** for a complete discussion of restraints.

Skip

Skip parameters are maintained in the project but are not used in any capacity in the fit. The point of a skip parameter is to maintain but not use a complicated parameter with a complicated math expression.

After

An after is similar to a def parameter in that it may be a math expression dependent upon other parameters. An after is not, however, a part of the fitting model. Instead it is a parameter that will be evaluated upon completion of the fit using the best fit values. The list of after parameters will be reported in the log file. Using an after parameter anywhere in your fitting model will result in Artemis reporting an error in the model. Afters can depend upon other afters, but you should take care in with the order that the afters appear in the list. The after parameters will be evaluated only once after the fit, thus circular or out-of-order dependencies will not be resolved.

The Guess, Def, Set page is divided into two sections. At the top is a listbox containing the list of all defined parameters. At the bottom is the edit area which contains the controls used to establish the parameters.

The parameter listbox

This area contains a four-column list of all the parameters defined in a project. The left-most column counts the parameters. The second column contains a tag identifying the type of the parameter. The third column contains the parameter name. The right-most column contains the parameter's math expression.

Parameters are coded by color and by the tag in the second column. Guess parameters are written in purple text and have the "g:" tag. Def parameters are written in green text and have the "d:" tag. Set parameters are written in black text and have the "s:" tag. Restraints are written in pink text and have the "r:" tag. Skip parameters are written in grey text and have no tag. After parameters are written in blue-grey text and have the "a:" tag.

There are a large number of mouse clicks and key sequences that serve a purpose in the listbox:

1. A left mouse click selects a parameter and displays it in the edit area.
2. A double click of the left mouse button selects a parameter, displays it in the edit area, and prompts you for the parameter annotation. See **Parameter annotations**.
3. A right mouse click selects a parameter, displays it in the edit area, and posts a contextual menu about that parameter. The menu has several

items in it. The "Move" submenu is used to reposition the current parameter in the list. The "Make" submenu serves to change the type of the parameter. The "Copy" item will replicate the anchored parameter, appending a few characters to the end of its name. The "Build restraint" item is discussed below. The "Annotate" menu item prompts for the parameter annotation. The "Find" menu item will search through all parameter and path parameter math expressions and show you how that parameter is used in the project. The "Grab" menu item is only enabled for guess parameters and will insert the best-fit value from a fit as the value for that parameter. Finally the "Discard" menu item will remove that parameter from the list after prompting for confirmation.

4. Control-d will define the parameter in the edit area.
5. Control-g will grab the current parameters best-fit value from a fit.
6. Control-e will show the editing area if it is hidden.
7. Control-k and control-j will move the selection up and down in the list. Note that these two key-sequences serve to move the anchor up and down in the Data and Path List when the Guess, Def, Set page is not showing.
8. Control-n will clear the selection and focus on the parameter name entry box so that you can create a new parameter.
9. Control-y will prompt you to then hit any of the g, d, s, r, k or e keys to set the type of the parameter. This is only way of setting the parameter type that does not involve the mouse.

Extended selection

Multiple items in the list of parameters can be selected using the control-click, shift-click, and click-drag sequences described for the Data and Paths List and for the log viewer. Only the anchored list item (i.e. the one surrounded by a dashed line and displayed in the edit area) can have its name and math expression edited.

The advantage of extended selection is that certain of the context menu options discussed above in item #3 can operate on many parameters at once. By doing extended selection then clicking the right mouse button somewhere in the selected region, the context menu will be posted with options for the group of selected parameters. Currently, groups of parameters can have their types set and can be discarded in this manner.

If you right-click outside the selected region, the extended selection will be cleared and the parameter clicked on will be anchored and selected.

The edit area

There are three rows of controls in the edit area. The top row has two entry boxes. The smaller one on the left is for entering the name of the parameter. The larger one on the right is for entering the parameter's math expression.

Below the entry boxes are a set of five radiobuttons for selecting the type of parameter being edited.

At the bottom of the edit area are five buttons for acting upon the parameter being edited. The "Undo edit" button clears the entry boxes and discards whatever changes were just made. The "New" button is used to define a brand new parameter. It clears the entry boxes, unselects parameters in the listbox, and gives focus to entry box for entering the parameter name. The "Grab" button becomes enabled after a fit is run. It inserts the best-fit value for a guess parameter. The "Discard" button deletes a parameter from the list. A dialog pops up confirming deletion. Finally, the "Hide" button removes the edit area from view to allow more parameters to be visible in the listbox. When the edit area is hidden, it is replaced by a button for restoring the edit area.

Here are the details of the behavior of these controls:

1. Hitting return in the parameter name entry box defines the parameter, inserts or updates it in the listbox, and puts focus on the math expression entry box. If a math expression has not yet been defined, the parameter will be defined as 0.
2. Hitting return in the math expression entry box defines the parameter, inserts or updates it in the listbox, and leaves focus on the math expression entry box.
3. Clicking on any of the radiobuttons defines the the parameter, inserts or updates it in the listbox, and leaves the focus unchanged.

Parameter annotations

An annotation is a short text string that is associated with the parameter. This string is written to the echo area whenever the parameter is selected in the listbox on the Guess, Def, Set page. The purpose of the annotation is to write a little hint about the role played by the parameter in the fitting model. If a guess parameter has no annotation when a fit is run, its annotation will be generated automatically. The automatic annotation for a guess parameter is its best fit value +/- its error bar. The automatic annotation for a def, after, or restrain parameter is its evaluated value after the fit.

Building restraints

One of the items in the context menu displayed when right-clicking on a parameter is for building restraints based on guess or def parameters. This tool provides a dialog for constructing one particular type of restraint – the type that

coerces a parameter to stay within a boundries for its value. The dialog prompts for a minimum and maximum value and for a term called the "amplifier". The math expression constructed is this one:

```
restrain param_res = penalty(param, min, max) * amp
```

The penalty function evaluates to 0 when `param` is between `min` and `max`, to `abs(min-param)` when `param` is less than `min`, and to `abs(param-max)` when `param` is greater than `max`. This is added in quadrature to reduced chi-square as the fit is evaluated.

The amplifier term determines the magnitude of the penalty. A large value for `amp` will force the fitted value of `param` not to stray too far outside its bounds. A small value will allow the fit more freedom to let `param` deviate from your initial guess.

See the **Ifeffit** FAQ, question 8.1 for more discussion of restraints, including discussion of other ways to set restraints that do not involve the `penalty()` function.

A cautionary note: restraints are not always appropriate. As an example, if a fit is returning a negative value for σ^2 , it may not be appropriate to apply a stiff restraint as a way of forcing that σ^2 to be a value that you expect. Often, a negative σ^2 is indicative of some other problem in the fitting model such as excessive structural disorder, a coordination number that is forced to be too small, the incorrect atomic species for a backscatterer, or some such. Using a restraint on σ^2 in a case like this would not fix the problem. Quite the opposite, it might foster a false sense of accomplishment by "fixing" the σ^2 "problem" without actually addressing the actual problem in the fitting model.

Highlighting

There is an option in the GDS menu for highlighting parameters. This prompts you for a text string. Any parameter names or math expressions that match that string will be marked with a green background. This is particularly useful for large parameter lists. The text string is interpreted as a perl regular expression and so any valid perl metacharacters can be used. (This includes regular expressions using `{ code }`) and other similar constructions, a practice the author of **Artemis** does not recommend, but does not prevent.)

Importing and exporting text files

For large, complex fitting models, it may be convenient to edit the parameter list with a text editor or even to write a program which generates the parameters and writes them to a text file. In that case, it is convenient to be able to import and export a textual representation of the parameter list. These files are of a simple format. Any line like these:

```

guess  a   5
set    b   6
def    c   a+b

```

can imported to and exported from the Guess, Def, Set page via the GDS menu. In an imported file, any line beginning with any of **guess**, **def**, **set**, **restrain**, **after**, or **skip** will be imported as a parameter. The second word on the line will be taken as the parameter name and the remaining words on the line will be concatenated to form the math expression. On export lines will follow this format:

```

type name = math_expression

```

Very little error checking is performed upon import to verify that the parameter is defined sensibly, so use this feature with caution.

6 ARTEMIS: ATOMS, The Crystallographic Front End to FEFF

ARTEMIS - ATOMS, The Crystallographic Front End to FEFF

The purpose of **Atoms** is to generate a **feff.inp** file from crystallographic data. The hard part of making a **feff.inp** file is creating the long list of atomic coordinates. **Atoms** thus makes the hard part of running **Feff** easy, at least for crystalline materials.

This page can be used to create input data for **Atoms** from scratch. It will also be used to display crystallography data imported from an **atoms.inp** file or a CIF file. To import an **atoms.inp** file or CIF file, use the normal file import dialog.

The title box

At the top is a text box for entering title lines identifying the crystallographic data. These lines will be written to the **feff.inp** file and to the top of the **Feff** interpretation page. This is a good place to cite the literature reference or to provide other important information about the crystal.

Crystal parameters

To the left side of the page are entry boxes for entering space group, lattice constants, and lattice angles of the crystal. A space group must always be provided. **Atoms** is very flexible about how the space group symbol is entered. You can use the Hermann-Maguin or Scheonflies symbols or the index of the space group from the International Tables. The algorithm that interprets the symbol is insensitive to white space and capitalization – **P m -3 m** and **PM-3M** are interpreted the same. For complete details about how the symbols are interpreted, see the **Atoms** documentation on Bruce's web site.

Lattice constants are entered in units of Angstroms, angles are entered as decimal numbers in degrees (and not in arc minutes – i.e. 89 and a half degrees is entered as 89.5 rather than 89’30’’). Many space groups have symmetries that make some lattice angles and constants the same. In those situations, it is only necessary to fill in the essential values. For instance, a cubic space group only requires a value for the **a** constant. **Atoms** will know to set the other lattice constants the same and to set the angles to 90 degrees. For lower symmetry groups, you must provide all the necessary information.

Below the lattice constants are entry boxes for **Rmax** and the shift vector and a menu for selecting the absorption edge of the **Feff** calculation. **Rmax** is the radial extent of the cluster that will be written to the **feff.inp** file. Some space groups are given in the International Tables with two different origins – i.e. the origin is placed at sites with two different point symmetries. The fractional coordinates of the sites are different for the two different settings of the crystal. In those cases, **Atoms** requires that you use a particular one of the two choices. If your input data has used the other origin choice, it should be fairly obvious. In that case, coordination numbers and distances to the coordination shells will usually be obviously wrong. When you use one of the space groups for which two origin choices exist, **Artemis** will issue a warning. If you suspect that the wrong origin choice has been used, insert the values for the shift vector that were reported in the warning message.

On occasion, crystals are reported in the literature using origins other than the standard one used in the International Tables. A famous example is germanium oxide. Here is the crystal data for GeO₂:

```

title GeO2 (hexagonal)
space p 32 2 1
a=4.98502      c=5.64800
rmax=6.0      core=Ge
shift  0 0 0.66667
atoms
  Ge    0.4513  0.0    0.0
  O     0.3969  0.3021  0.0909

```

For some reason, the crystallography reference for this material uses an origin that is shifted by 2/3 in the z direction relative to the origin used in the International Tables. To get **Atoms** to compute this structure correctly, the shift vector given above must be used.

The atoms list

To the right side of the page is the list of unique crystallographic sites. As new sites are created, they are inserted into the list. The sites are not edited directly, instead the editing area at the bottom of the screen is used and the list of all sites is displayed here. This works much the same as the Guess, Def, Set page.

To edit a site, left-click on its entry in the list. It’s element symbols, coordinates, and site tag will be displayed in the edit area. A right click on a site in

the list will post a context menu with several functions that can be performed on that site. You can re-order the list using the "Move" menu item. A site can be copied and the copy added to the list using the "Copy" menu item. The "Discard" menu item completely removes the site from the list. The list supports extended selection. When many sites are selected (i.e. highlighted in yellow), the "Discard" menu item will work on all the selected sites.

Sites can also be reordered using the keyboard. **Alt-k** and **Alt-j** can be used to move the selected site up or down in the list.

The edit area

At the bottom of the page is the collection of widgets used to actually create and edit unique crystallographic sites. The element box is used to insert the two-letter element symbol for the site. The site will not be created if this is not a valid symbol. The tag can be any 10-letter string used to identify the site. The tag is used to differentiate sites that contain the same element.

The boxes for the **x**, **y**, and **z** coordinates can be filled with floating point numbers or simple fractions. That is, 0.5 and 1/2 are both acceptable. These coordinates are fractional positions in the unit cell and are not Cartesian coordinates.

Once you have created all sites in your crystal, click the "Run Atoms" button. This will process the crystallographic data, create the **feff.inp** file, display the **feff.inp** page.

Atoms template files

The **feff.inp** data that is generated when the "Run Atoms" button is pressed is determined by the contents of a special template file. **Artemis** is distributed with a number of template files serving different purposes. The structure of the **feff.inp** data is set by the value of the "atoms->template" preference. The default value is "feff", which tells **Artemis** to use the template file suitable for running **Feff6**.

If you want to run some other version of **Feff**, you should set the "atoms->template" preference variable to the appropriate value. Templates are provided with **Artemis** for writing **Feff7** and **Feff8** input files. **Feff8** input files can be written which are suitable for XANES or non-self-consistent EXAFS calculations.

Sometimes, it is useful to modify template files for writing out specialized **feff.inp** data. If these modified template files are placed in **~/horae/atp/** (unix) or **C:\Program Files\Ifeffit\horae\atp** (windows), **Artemis** will be able to find them.

Final note

A full explanation of how the **Atoms** algorithms works is beyond the scope of this document page.

7 ARTEMIS: The FEFF Input File

ARTEMIS - The **FEFF** input file

This page displays the **Feff** input data, which includes some control parameters and a long list of atomic coordinates. This page is no more sophisticated than a text box which serves as a primitive editor and a button at the bottom for running **Feff**. Explaining **Feff** is beyond the scope of this document.

When **feff** is finished, you will be presented with a dialog asking how many paths to import. The choices are none, the first path, the first 10 paths, and all paths. The number in the third option is configurable in the preferences dialog. Should you ever need to rerun **Feff** after starting a project, "none" is usually the right answer. The other options may result in one or more paths being defined twice in the project – a confusing situation.

If **Feff** fails to run to completion, **Artemis** will try to recognize the problem and post a suggestion for how to solve the problem. If **Artemis** does not recognize your problem, explain it to Bruce so he can add that problem to **Artemis**'s database of troubleshooting solutions.

8 ARTEMIS: Interpretation of the FEFF Calculation

ARTEMIS - Interpretation of the **FEFF** calculation

This page provides a concise overview of the **Feff** calculation. At the top of the page is a summary of some of the statistics of the calculation. Below that is a chart showing the details of each path from the calculation. For each path, the degeneracy, the half path length and the amplitude factor are shown. The last column shows a tokenized summary of the scattering path – this allows you to see at a glance which atoms were involved in the path.

The information and context menus available on this page allow you to organize, understand, and manipulate the paths in this **Feff** calculation. Pretty much all functions involving the paths *except* writing math expressions for the path parameters are available on this page.

The interpretation chart

The colors and fonts used in the chart convey information:

Bold, black font

These are paths that have been imported into the project and are included in the fit.

Bold, brown font

These are paths that have been imported into the project but are excluded in the fit.

Normal, black text

These are paths that have not been imported into the project but which are available to be imported.

Normal, grey text

These are paths that are unavailable for importation into the project. These can be made available by re-running the **Feff** calculation. After the **Feff** run, it is best to choose the "import no paths" to avoid reimporting paths already in the project. After that, these paths will be written in normal, black text, indicating that they are available for import.

Light brown background

The light brown background is used to indicate single scattering paths.

Light blue background

The light blue background is used to indicate collinear or nearly collinear multiple scattering paths.

Context menus

There are interesting and useful context menus on every part of this page. These menus are available by right clicking.

Right clicking anywhere in the text box at the top of the page will pop up a menu with options for viewing files from the **Feff** calculation.

Right clicking in the interpretation chart will post a menu of options relevant to the path on the line on which you clicked. Each of the four kinds of paths given by the four fonts described above has its own menu.

For paths that are imported in the fit, the menu offers options for plotting the path, displaying that path's page, including or excluding the path in the fit, selecting or deselecting that path for plotting, making that path the default for evaluation of def parameters after a fit, displaying the text of the file containing the path, or discarding the path. The choices for including or excluding and for selecting or deselecting depend on the state of that path in the Data and Paths List. Also some options might be greyed out depending on the state of that path.

For paths that have not been imported into the project, the context menu allows you to import the path with the option of displaying its page or leaving the display on the **Feff** interpretation. For paths that are unavailable for import, a message saying so is posted when one of those lines is right-clicked.

The interpretation chart allows for extended selection of lines in the chart. You can select additional paths by holding the control key while clicking with the left mouse button. Holding the shift key while left clicking selects all line between the anchor (the one outlined with a dashed line) and the one you click on. You can also click and drag to select all the lines you drag over. When more than one line is selected, the content of the context menu change to reflect functionality that makes sense for many paths. Extended selection in the interpretation

chart is therefore a good way of including/excluding, selecting/deselecting, or plotting a large number of paths.

The context menu that pops up when many lines are selected may be a little surprising. Its contents depend upon the state of the anchored line, which in this case is the one that you right-click on to post the menu. The options in the context menu will be suitable to the state of the anchored selection regardless of the states of the other selected lines. If you choose a menu item that does not make sense for some of the selected lines, those lines will be ignored.

Here is a concrete example. Suppose that you select a number of lines, some of which are included in the fit and some of which have not been imported in the fit. If you then right click on one of the included paths, you will get options appropriate to included paths. If you then ask to plot the selected paths along with the data, the included paths will be plotted and the imported paths will be ignored. If, instead, you click on one of the paths that has not been imported yet, the context menu will give you the option of importing the selected paths. In that case, the paths that have already been imported will be ignored.

Trouble shooting

On occasion you might see that lines in the **Feff** interpretation do not properly report on the contents of the path. When this happens, site tags are replaced by this string: `<?>`. There are a couple common reasons you might see the `<?>` tags:

1. You have done some advanced voodoo with **Feff**, editing the `files.dat` or `paths.dat` files then rerunning the last module to produce specialized output.
2. You have discovered a bug in the algorithm **Artemis** uses to harvest information from the **Feff** calculation. IN that case, you should send the `feff.inp` file or the **Artemis** project file to Bruce so he can fix the problem.

Note that the appearance of the `<?>` tags is probably not an indication that **Feff** has misbehaved. The **Feff** calculation has to run to completion and generate its normal output before this problem can manifest itself. The **Feff** calculation is almost certainly usable to analyze the data. The **Feff** interpretation page is **Artemis**'s attempt to organize information about the **Feff** calculation in some user-friendly format. That this organizational effort failed is not necessarily an indication that **Feff** failed.

9 ARTEMIS: The Path Page

ARTEMIS - The path page

The path page is displayed whenever a **Feff** path is selected from the Data and Paths List. This page is used to establish the math expressions of the path parameters for this path.

At the top of the page is a line identifying which **Feff** calculation this path is from. Below that are three toggles. One is used to include or exclude the path from use in the fit. There are many other ways in **Artemis** to include and exclude paths other than to use this toggle. See [The Feff interpretation page](#), `artemis_intrp` and `artemis_menubar` for more discussion of this. Also Control-t is the same as clicking this toggle.

The second toggle is used to specify paths that you would like plotted after a fit (or sum of paths) is finished. By default, the data and the fit (or sum) is plotted after the fit (or sum) and no paths are plotted. Any paths selected for plotting will be added to the plot after the fit (or sum) is finished.

The third toggle is used to set which path is the default path for evaluation of Def parameters after the fit. It is possible to write math expressions which evaluate differently for different paths. An example might be a math expression using the `reff` parameter. For any such Def parameters, it is necessary to tell **Artemis** which path should be used for the reporting of those parameters in the log file. The default is to use the first path listed in the Data and Paths List.

Below that is a box which summarizes the path. This gives some statistics about the path as well as displaying a color-coded "map" of the scattering path. The central atom is always displayed in red text. Other atoms are in black text. The grey text shows the length and scattering angle of each leg of the path. In the case of a high-order multiple scattering path which has legs which have a non-zero Eulerian eta angle between them, the eta angle will be displayed as well. If that last sentence was gibberish, it suffices to know that paths of that sort are almost never observable in real EXAFS data.

At the bottom of the page is the list of path parameters. This is the most important section of the page because it is here that the details of the fitting model are realized. There is an entry box for each of the various types of path parameters. The math expression appropriate for each parameter should be entered in the entry box.

When a **Feff** calculation is imported into **Artemis**, a set of automatic parameters are generated, entered into the list on the Guess, Def, Set page, and entered into the path parameter boxes for each path imported. The default behavior of **Artemis** is to generate a set of parameters appropriate for a simple, single scattering, first shell fit. While it might be OK to immediately click the big green button, most fitting models will require substantial editing.

The right mouse button serves many important purposes on the path page. Clicking the right mouse button anywhere in one of the entry boxes will highlight the word underneath the cursor and post a menu. The entries in the menu are for defining the word as a parameter on the Guess, Def, Set page. For each parameter type there is the option of jumping or staying. In either case, the parameter is defined and added to the list on the GDS page. For jumping, the GDS page is then displayed. For staying, the current path page remains displayed.

Right clicking on one of the path parameter labels will post a menu of functions related to defining path parameter math expressions. The "Edit" option

will pop up a dialog used for entering a math expression and then optionally exporting its value to other paths. The "Clear" option does just that.

The various "Export" options are ways of constraining path parameters to be the same for other paths. The "Grab" options make the current path parameter the same as the path parameter in the previous or following path.

The " σ^2 " label has some additional options. These insert the syntactically correct text appropriate to using either the Correlated Debye or single frequency Einstein models for the σ^2 of the path.

To enable the display of spaces for the `dphase`, `k_array`, `amp_array`, or `phase_array` path parameters, you must click on the "Extended path parameters" button in the Paths menu.

10 ARTEMIS: The Log Viewer

ARTEMIS - The log viewer

When a fit is anchored in the Data and Paths list, the log file viewer is displayed in the main panel. The purpose of this page is to examine log files from the most recent fit or from previous fits. These log files can be read individually or reports can be generated based on their contents.

When this page is displayed, each fit is entered into the list box on the left side of the page. Double clicking the left mouse button on a fit in the listbox will display that fit's raw log file. Right clicking on a fit will post a menu with choices for displaying that fit's log file in raw, quick, or columnar form or for performing some other tasks related to that fit.

Much more interesting than displaying the log files, though, is to generate reports on the log files. Near the top of the page is a combo box for selecting among the parameters on the Guess, Def, Set page. Choosing one, then clicking on the "Write report" button will find extract that parameters best-fit value and uncertainty from each log file. This feature allows you to track the evolution of individual fitting parameters as you develop your fitting model.

The combo box containing the names of the fitting parameters is filled using the contents of the Guess, Def, Set page. Sometimes it may be useful instead to fill the combo box with the parameter names extracted from a log file. This would be useful, for instance, for examining a parameter that was used at one point, but is no longer on the GDS page or has been made into a skip parameter (and so is not included in the combo box by default). To do this, right click on a fit and select the "Get parameter list" item.

Some modifications can be made to the reports generated by the log viewer. Clicking on the "Compute the average value" button tells **Artemis** to compute the arithmetic mean and standard deviation of the parameter from the values extracted from the various log files. These will be displayed in the header of the report.

Clicking on the "Fit Einstein temperature" button will tell **Artemis** to fit σ^2 data to a model consisting of a single frequency oscillator plus a constant offset. The report header will then contain the best fit values and

uncertainties for the characteristic temperature and constant offset. This calculation will only happen if the figures of merit for the selected log files are reasonable temperatures and the best fit values for the chosen parameter are reasonable σ^2 values. This function makes a series of checks on the figures of merit and best fit values to determine if they seem to be data appropriate for this calculation. These heuristics can be tuned by setting parameters in the logview section of the preferences dialog.

The final item in the context menu that is displayed when right clicking on an item in the log files list is an option to restore that fitting model. Among the information that is saved every time a fit is made is a complete description of the fitting model, including which data file is being fit, the complete list of **Feff** path used, and all fitting, data, and path parameters. This feature allows you to revert **Artemis** to the state it was in when a past fit was made. When you do this reversion, **Artemis** will clear out the contents of the Data and Paths List and then recreate the project in the form of the selected fitting model. This is more than just a change of parameter values. **Artemis** keeps track of all data and **Feff** paths used throughout the course of the project and can restore even fits that are significantly different from the current fit.

Importing **Athena** project data | artemis.athena || Output files || **Artemis** project files ||

11 ARTEMIS: Plotting Data

ARTEMIS - Plotting data

Plots in **Artemis** are made using the selected items in the Data and Paths List, which are the ones highlighted in orange. See the main document section for an explanation of how to select items for plotting.

At the top of the plot panel are three big, red buttons. One is for making a plot in k-space, one is for R-space, and the third is for q-space (i.e. back-transformed k-space).

k-Weighting

Below the plot buttons are a set of radiobuttons for setting the k-weight to use in the plots. The k-weight chosen will be used to weight a plot in k-space or to weight data for Fourier transforming. The same k-weight is used for each selected item. The button marked "kw" needs some explanation. When this button is chosen, the k-weight to use in the plot will be determined from the data being plotted. If the arbitrary k-weight enabled for the data set, the value for the arbitrary k-weight will be used, otherwise the smallest k-weight value enabled will be used. There are two reasons to use the "kw" button. One is to plot using your arbitrary weight. The other is to make a plot of two or more data sets using a different k-weight for each data set.

Note that these k-weight controls are unrelated to the controls which set the k-weight used in the fit. K-weighting for fitting and plotting are controlled

independently.

Selecting What Gets Plotted

Below the k-weight radiobuttons are menus for choosing which part of the complex functions `chi(R)` or `chi(q)` to plot. Plots involving multiple parts of the complex functions (e.g. real+envelope) are not currently possible.

Below these menus are three checkbuttons used for plotting the Fourier transform window, the background function, and the residual. If the window button is pressed, the appropriate window function will be plotted in any plot. The background and residual functions are only plotted if one of the selected items is a fit. The background will only be plotted if a background corefinement was made for that fit. If a fit is not among the selected items, the background and residual will not be plotted. Note that a plot with more than one selected fit may be quite confusing if the background or residual buttons are depressed since the background and residual will be plotted for each fit.

The ranges over which the plot will be made in the three spaces are controlled by the three sets of entry boxes.

Extra Plotting Features

The two additional tabs in the plotting panel contain the controls for the following utilities:

Indicators

Indicators are vertical bars that can be placed at user-chosen locations in k-, R-, or q-space. These indicators will get displayed every time a plot is made. The idea is that indicators are a guide to the eye, drawing attention to a place of interest as the data being plotted changes.

Indicators selected in either k- or q-space will be plotted in both k- and q-space, but not in R-space. Likewise, indicators selected in R-space will not be plotted in k- or q-space.

Several characteristics of the indicators, including the number, the linetype, and the color, can be set in the Plot section of the preferences dialog.

The indicators play well with each of the plotting options described below.

Stacking

Stacking refers to a vertical displacement the various traces. This is most useful for plotting the various path contributions in k-space, but is sometimes useful in other kinds of plots as well. Stacking requires three parameters which are set in the stacking notecard. The first control is series of radio buttons for choosing whether stacking happens in k-space, always, or never. If the k-space option is chosen, then q-space plots of the real or imaginary parts will also be stacked. (Basically, the "k-space" choice refers to any wiggly function of wavenumber.)

The other two controls set the initial offset value and the increment between stases.

Inverting

Inverting is a useful tool for displaying the path contributions in $|\chi(\mathbf{R})|$ plots. When this is selected, the $|\chi(\mathbf{R})|$ from any paths included in the plot will be multiplied by -1 so that they stick down below the zero-axis. Hopefully this kind of plot help reduce clutter while still helping to show which paths contribute where. The radiobuttons on this notecard allow you choose between never inverting, inverting $|\chi(\mathbf{R})|$, or inverting both $|\chi(\mathbf{R})|$ and $|\chi(\mathbf{q})|$. The real and imaginary parts in R- or q-space are never inverted. $\chi(\mathbf{k})$ is also never inverted. Inverting is turned off whenever stacking is selected and would effect the current plot (i.e. you cannot stack and invert at the same time).

Data set offsets

This feature is useful for multiple data set plots. This is similar to stacking in that the parameter denotes a vertical offset for use in the plot. Each trace associated with a particular data set is plotted at the same level, but the data sets will be offset by the amount specified by this control. This provides a way of simultaneously visualizing all parts of a multiple data set fit. Negative values are recommended, with a negative offset, the traces will be plotted in the same order from top to bottom as in the plot legend.

Stacking is disabled when data set offsets are used. Inverting is used with data set offsets, although I think this results in confusing plots.

Palettes || Using the Data and Paths List || =head1 ARTEMIS: Editing Math Expressions

ARTEMIS - Editing math expressions

The math expression editing dialog is a way of setting path parameter math expressions for many paths at once. It works on a given path parameter, e.g. it sets ϵ_0 or σ^2 for many paths but does not touch other path parameters. This dialog is available in two different context menus. If you right click on a path parameter label on the path page and selection "Edit for many paths", then the dialog will pop up for editing that parameter. If you right click on an entry on the **Feff** interpretation page and select the "Edit path parameters" cascade, then select a path parameter, the dialog will pop up for editing that parameter.

Operation of the dialog

The dialog is fairly simple. At the top is a text entry box for typing in your math expression. Below that are various radiobuttons for specifying how to apply the math expression to the various paths in your project. The options are:

1. Add the math expression to every path in the current **Feff** calculation.

2. Add the math expression to every path in the each **Feff** calculation.
3. Add the math expression to every path in the each **Feff** calculation associated with the current data set.
4. Add the math expression to selected paths (i.e. the ones highlighted in orange in the Data and Paths list).

Tokens

You can write your math expressions using token. Tokens are short character strings which will be replaced by path-specific information as the math expression is applied to each path. The tokens are:

%i

The path index from the **Feff** calculation. This is actually computed from the name of the '**feffNNNN.dat**' file from the **Feff** calculation. For instance, if the file is '**feff0029.dat**', then **%i** will expand to 29.

%I

The path index from the **Feff** calculation, padded to fill four characters. For instance, if the file is '**feff0029.dat**', then **%I** will expand to 0029.

%r

The effective path length (or **reff**) from the **Feff** calculation for the path.

%d

The degeneracy of the path.

%D

A template for the Debye function. This always expands to the string "debye(temp,thetad)" and may need be edited after the fact to use the correct variable names. This is offered because the author finds it hard to remember the order of the arguments to the Debye function.

%E

A template for the Einstein function. This always expands to the string "eins(temp,thetae)" and may need be edited after the fact to use the correct variable names. This is offered because the author finds it hard to remember the order of the arguments to the Einstein function.

12 ARTEMIS: Automated First Shell Theory

ARTEMIS - Automated first shell theory

Sometimes thinking about a fitting model is more than a problem merits. You just want a quick 'n' dirty stab at the first shell – perhaps to measure the

centroid of the distribution, perhaps to tell if a sample is 4- or 6-coordinated. Whatever.

Artemis is not extremely well suited to rapid-fire, first shell analysis. By design, **Artemis** tends to force the user to slow down and think hard about every step. **Artemis** is powerful, but she ain't simple.

The quick first shell (QFS) theory tool is an attempt at addressing this shortcoming. It works like this:

1. Import some data. Set the Fourier transform and fitting parameters to suitable values. Specifically, be sure to set the fitting range such that it encloses the first peak of the data.
2. Select "Quick first shell theory" from the Theory menu. This will display the QFS dialog.
3. The QFS dialog provides spaces for selecting the parameters for a simple first shell theory. These include the atomic species of the absorber and the scatterer, the absorption edge of the experiment, the approximate distance between the absorber and scatterer, and the coordination geometry to use in the **Feff** calculation.

Currently the following coordination geometries are available:

- 4-coordinate crystal
- 6-coordinate crystal
- octahedral molecule
- tetrahedral molecule
- square-planar molecule

The QFS theory is probably not highly sensitive to the choice of coordination geometry. Since the unknown sample is probably not well described by any of these geometries, they are all merely approximations for use in a quick 'n' dirty fit.

4. Once you have set up the parameters for the QFS theory, click the "Do it!" button. This will step through the following without pausing:
 - a. Build an input file for the **Feff** calculation
 - b. Run **Feff**
 - c. Import the first path from the **Feff** calculation

d.

Create a set of guess parameters for the amplitude, the σ^2 , the e_0 , and the ΔR . Also created are set parameters for the third and fourth cumulants, but they are set to zero. These higher cumulant set parameters are created to make it easy to consider higher cumulants in subsequent fits merely by changing them from set to guess.

If you have a mixed first shell, you might choose to repeat steps 2 through 4 two or more times.

At the end of this sequence, you are left with **Artemis** in its normal state. You may need to adjust the parameters used in the fit. The QFS dialog is really just a tool for initially setting up the project. It in no way changes the normal operation of **Artemis**.

If you import data from an **Athena** project file, the species of the absorber and the edge will be set correctly when you start the dialog.

The Menubar || The preferences dialog ||

13 REFERENCES

Here are the relevant URLs:

IFEFFIT

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

PGPLOT

<http://www.astro.caltech.edu/~tjp/pgplot/>

Perl

<http://www.perl.com>

perl/Tk

<http://www.lehigh.edu/~sol0/ptk/>

14 MISSING FEATURES

You betcha!

15 WHAT'S IN A NAME?

Artemis was the goddess of the hunt, an apt metaphor doing EXAFS analysis. **ARTemis** is also a pun on the nature of EXAFS analysis that works in English and in the romance languages.

16 AUTHOR

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Iffffit is copyright (c) 1992 - 2006 Matt Newville
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