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X-Ray Absorption Fine Structure

XAFS

5th School on X-Ray Spectroscopy Methods



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- 1.Artemis, some aspects of the program
- 2.Example: fitting the signal for an iron foil fe.060
- 3.To do: following Bruce Ravel example on FeS₂
- 4.What do I do next?

1. Artemis, some aspects of the program

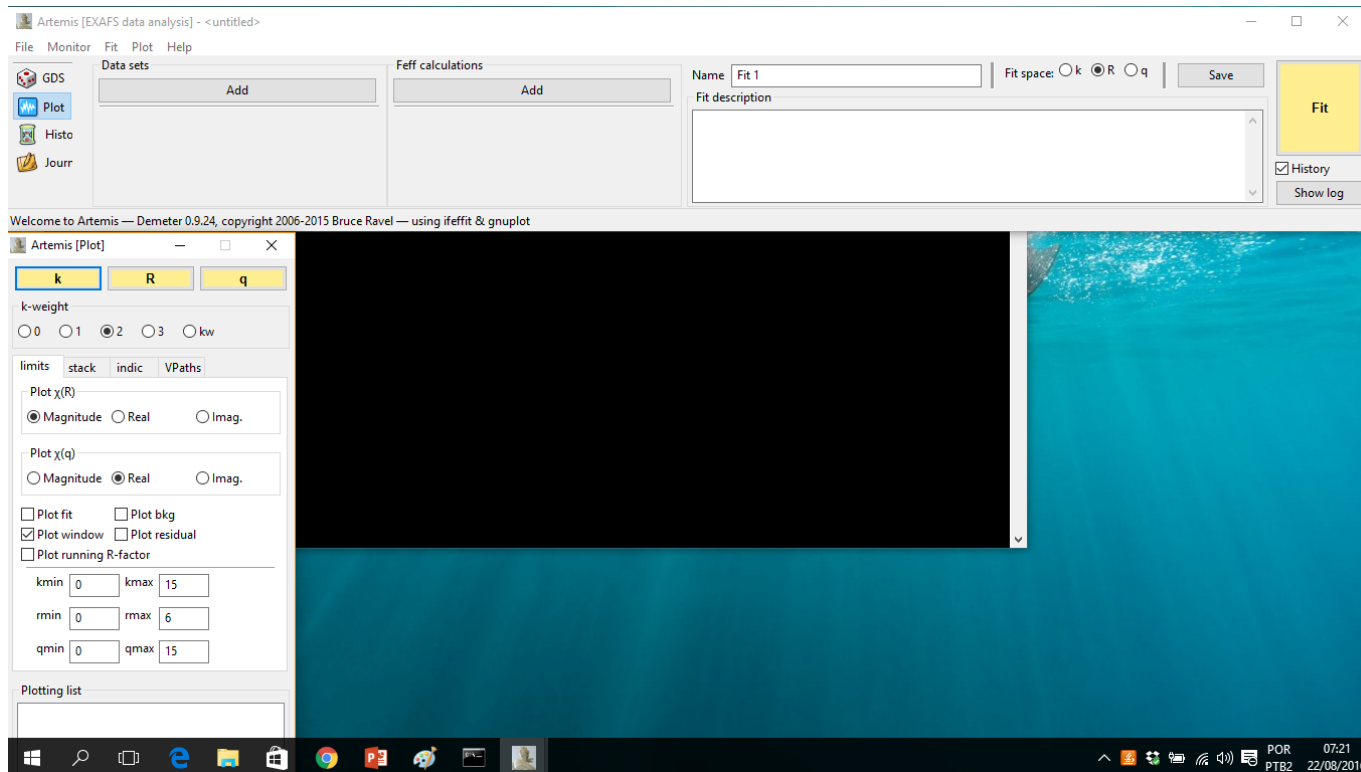
2. Starting Artemis

The ARTEMIS program is launched on Windows by double-clicking the ARTEMIS icon on the desk top, by selecting `artemis` from the DEMETER menu in the Start Menu, or by typing `dartemis` (that's pronounced 'ɑ:rtimis, with a *silent d*) at the command prompt. If you installed DEMETER using the standard installer package, you can also double-click on an ARTEMIS project file (i.e. one with a `.fpj` extension) to open it in ARTEMIS.

On a unix computer, ARTEMIS is launched by typing `dartemis` in the shell. Depending on how DEMETER was installed on your computer, there may be some kind of application launcher, such as a desktop icon, a panel or dashboard launcher, or an entry in some kind of application menu.

Todo: Describe how this is done on a Mac...

Once started, ARTEMIS displays two windows, as shown below.



1. Artemis, some aspects of the program

2.1. The main window

The main window provides an overview of the state of ARTEMIS as well as of your current fitting project. This window is divided into 7 areas.

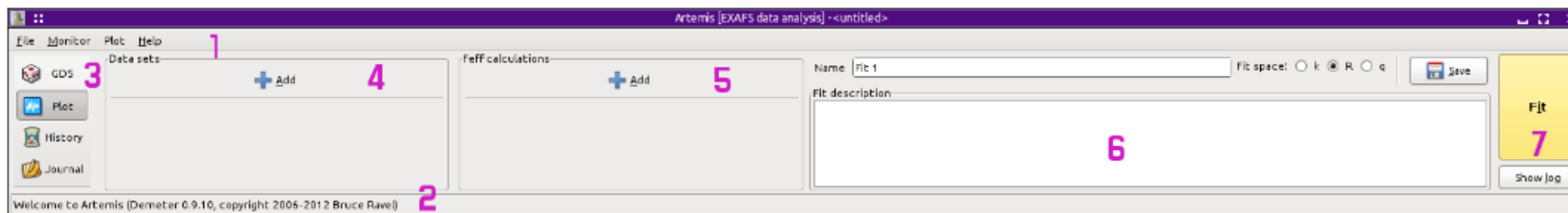
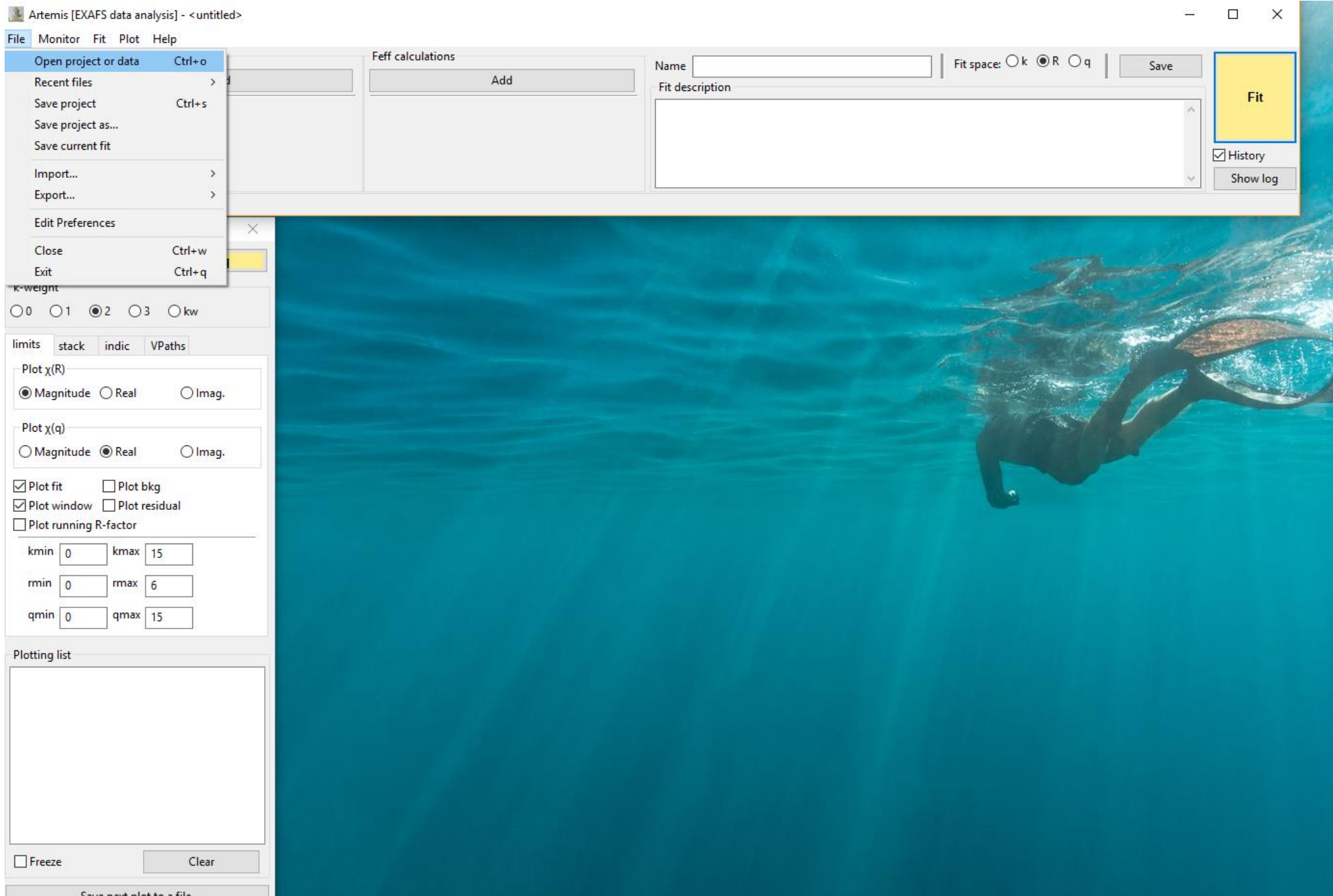


Fig. 2.2 The main window.

1. At the top is a menu bar. We will examine the contents of each menu below.
2. At the bottom is the status bar. This area is used to convey messages to you during the course of operating the program.
3. On the left is a stack of buttons used to show and hide various parts of ARTEMIS. Each of these will be described in detail later in the document.
4. To the right is the listing of data groups. The **Add** button is used to import a new data set into ARTEMIS. As data are imported, they will listed as a stack of buttons below the **Add** button.
5. Next comes the listing of FEFF calculations. The **Add** button is used to import new structural data set into ARTEMIS. This may be input data for FEFF, an `atoms.inp` file, or a CIF file containing crystal structure data. As FEFF calculations are started, they will listed as a stack of buttons below the **Add** button.
6. The wide area to the right of the FEFF calculations contains several controls for the current fitting project. The Name and Description boxes are used to describe the current state of your fitting project. The name should be a concise description of the current fit and is used as a label identifying a specific fit. The description is a lengthier, free-form bit of text describing the current fit in more detail. This text will be written to log files. ARTEMIS does a decent job of automatically generating text for both of these boxes, but providing your own text will help you to document the progression of your fitting project. This section also has controls for selecting the space in which your fit is evaluated and for saving a project file in a single click.
7. On the far right is the **Fit** button. As you might imagine, this button is clicked to initiate a fit. The color of this button will change to provide a heuristic evaluation of the quality of each fit. Below the **Fit** button is **Show log** button, used to show or hide a window containing the results from the most recent fit.

2. Example: fitting the signal for an iron foil fe.060



Artemis [EXAFS data analysis] - <untitled>

File Monitor Fit Plot Help

- Open project or data Ctrl+o
- Recent files >
- Save project Ctrl+s
- Save project as...
- Save current fit
- Import... >
- Export... >
- Edit Preferences
- Close Ctrl+w
- Exit Ctrl+q

Feff calculations

Add

Name Fit space: k R q Save

Fit description

History

k-weight

0 1 2 3 kw

limits stack indic VPaths

Plot $\chi(R)$

Magnitude Real Imag.

Plot $\chi(q)$

Magnitude Real Imag.

Plot fit Plot bkg

Plot window Plot residual

Plot running R-factor

kmin kmax

rmin rmax

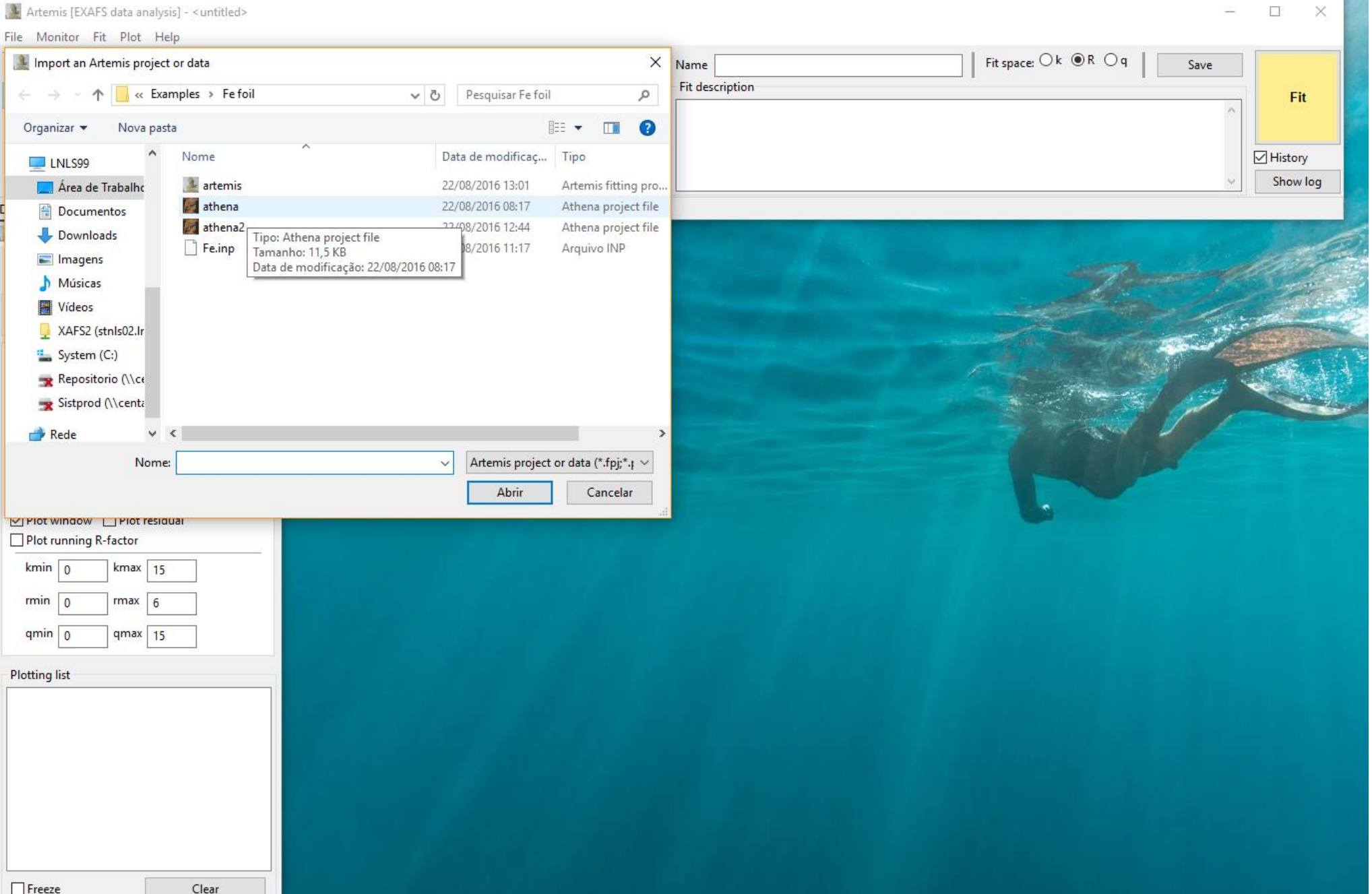
qmin qmax

Plotting list

Freeze

Save next plot to a file

2. Example: fitting the signal for an iron foil fe.060



The screenshot displays the Artemis software interface. The main window is titled 'Artemis [EXAFS data analysis] - <untitled>' and has a menu bar with 'File', 'Monitor', 'Fit', 'Plot', and 'Help'. A dialog box titled 'Import an Artemis project or data' is open, showing a file explorer view of the 'Examples > Fe foil' directory. The file list includes:

Nome	Data de modificaç...	Tipo
artemis	22/08/2016 13:01	Artemis fitting pro...
athena	22/08/2016 08:17	Athena project file
athena2	22/08/2016 12:44	Athena project file
Fe.inp	22/08/2016 11:17	Arquivo INP

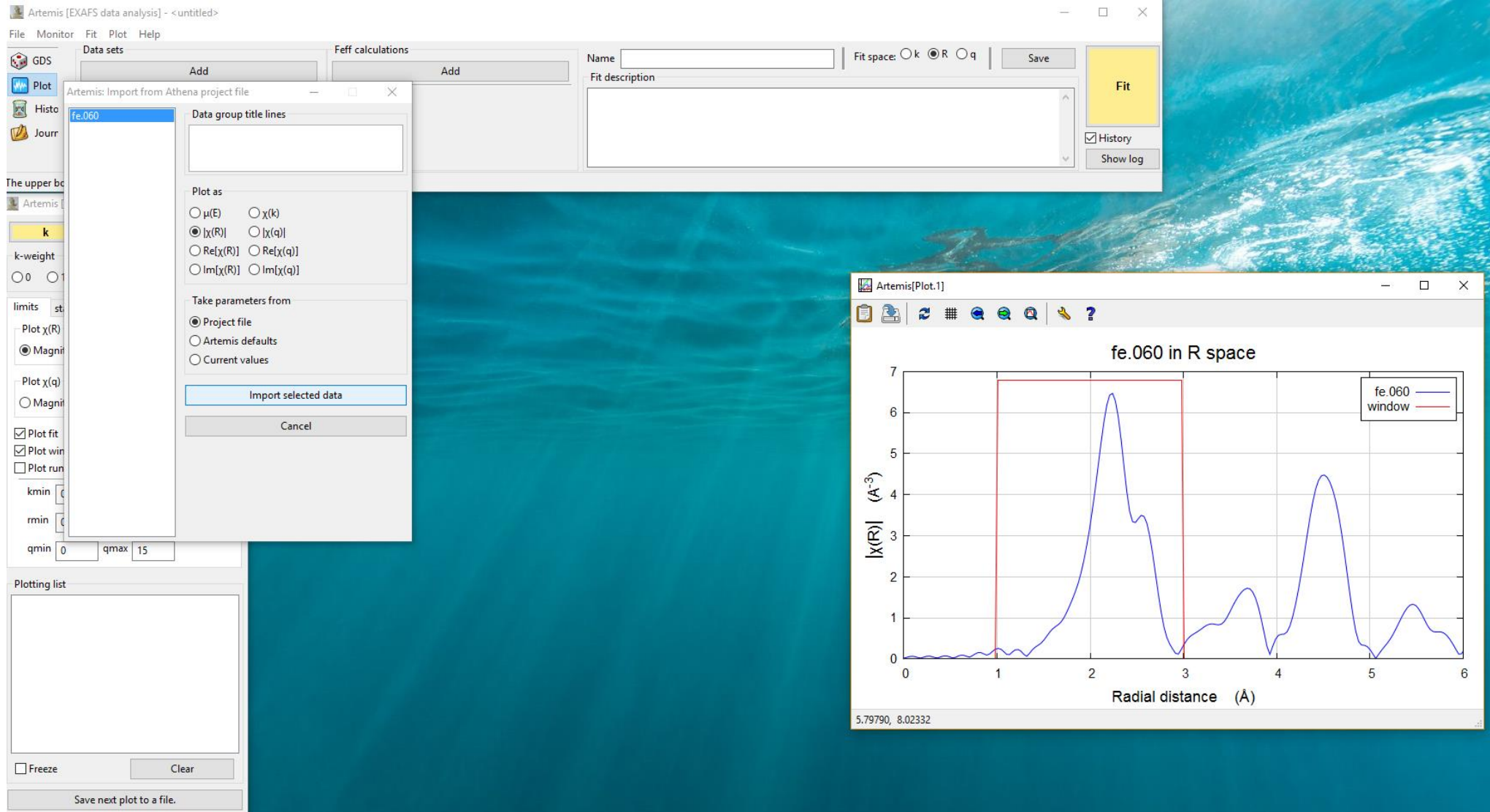
A tooltip for the 'athena' file shows: 'Tipo: Athena project file', 'Tamanho: 11,5 KB', and 'Data de modificação: 22/08/2016 08:17'. The 'Fit' window is also visible, with a 'Fit' button and a 'Show log' button. The background of the software interface features an underwater image of a diver.

Below the dialog box, the 'Plot window' and 'Plot residual' options are checked. The 'Plot running R-factor' option is unchecked. The plot parameters are:

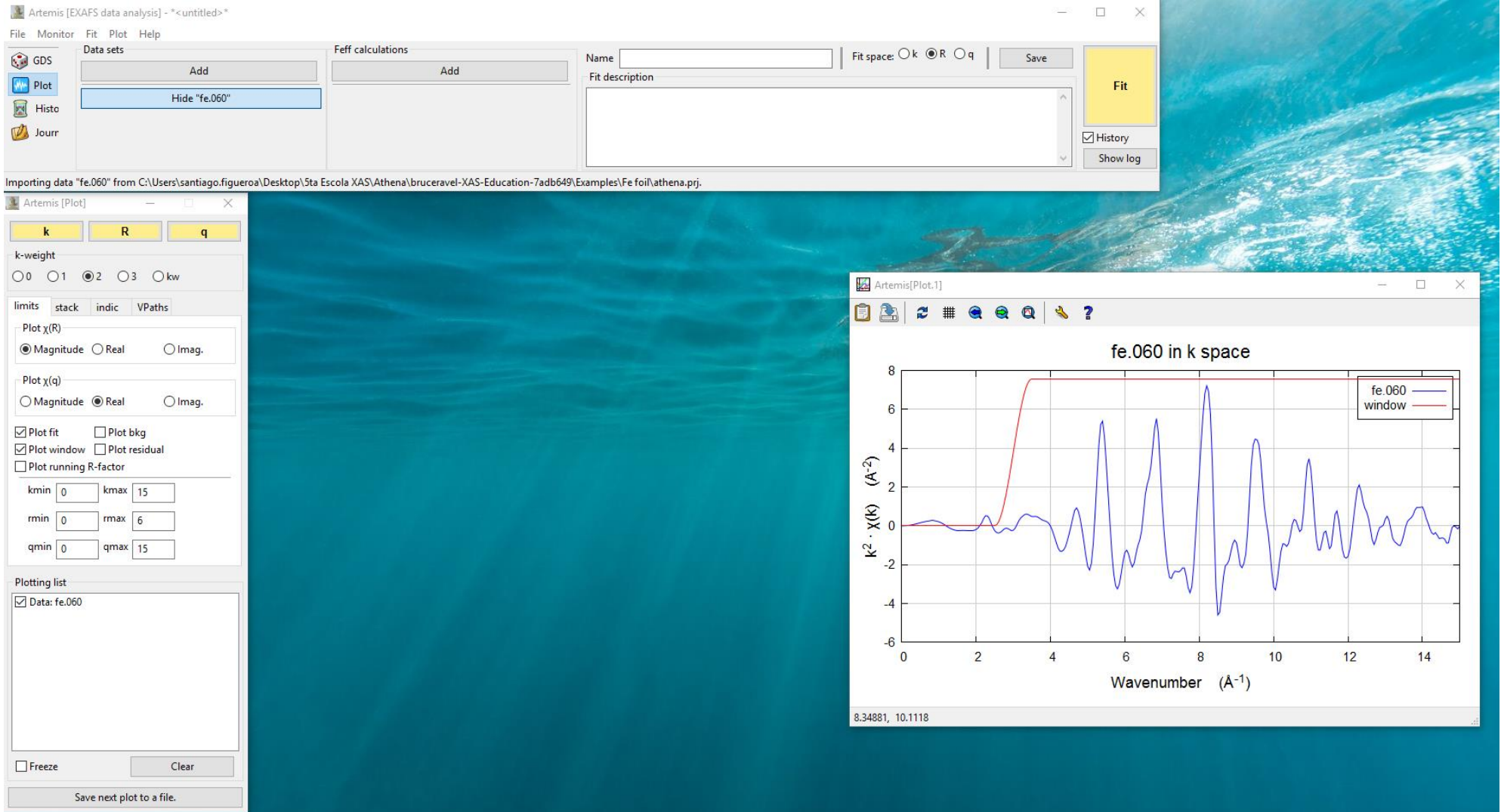
kmin	0	kmax	15
rmin	0	rmax	6
qmin	0	qmax	15

The 'Plotting list' is empty. At the bottom, there are 'Freeze' and 'Clear' buttons.

2. Example: fitting the signal for an iron foil fe.060



2. Example: fitting the signal for an iron foil fe.060



The screenshot displays the Artemis software interface for EXAFS data analysis. The main window is titled "Artemis [EXAFS data analysis] - *<untitled>*" and features a menu bar (File, Monitor, Fit, Plot, Help) and a toolbar with icons for GDS, Plot, Histo, and Jourr. The interface is divided into several panels:

- Data sets:** A panel on the left with an "Add" button and a list containing "Hide 'fe.060'".
- Feff calculations:** A panel with an "Add" button.
- Name and Fit space:** A section with a "Name" input field, a "Fit space" selector (radio buttons for k, R, q), and a "Save" button.
- Fit description:** A large text area for describing the fit.
- Fit button:** A prominent yellow "Fit" button.
- History and Log:** Checkboxes for "History" and "Show log".

Below the main window, a status bar indicates: "Importing data 'fe.060' from C:\Users\santiago.figueroa\Desktop\5ta Escola XAS\Athena\bruceravel-XAS-Education-7adb649\Examples\Fe foil\athena.prj."

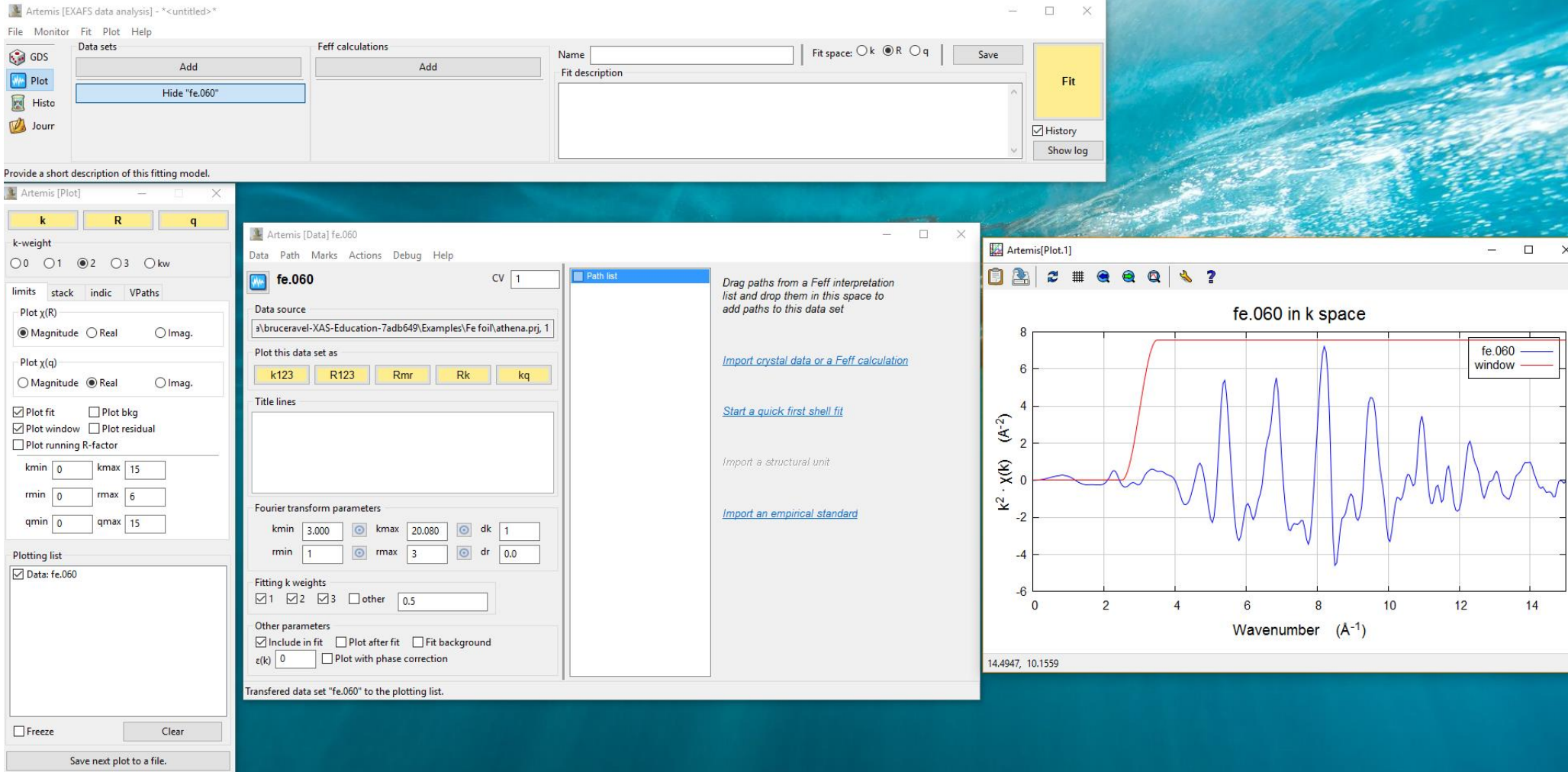
A secondary window titled "Artemis [Plot]" is open, showing a plot titled "fe.060 in k space". The plot displays the k-weighted signal $k^2 \cdot X(k)$ (in \AA^{-2}) on the y-axis (ranging from -6 to 8) against the Wavenumber (in \AA^{-1}) on the x-axis (ranging from 0 to 14). The plot shows a blue line representing the "fe.060" data and a red line representing the "window" function. The data exhibits characteristic oscillations, with a prominent peak around 8 \AA^{-1} . The window function is a step-like curve that rises from 0 at approximately 3 \AA^{-1} to a plateau of 8 \AA^{-2} by 4 \AA^{-1} .

The "Artemis [Plot]" window includes a control panel on the left with the following settings:

- k-weight:** Radio buttons for 0, 1, 2 (selected), 3, and kw.
- limits:** Tabs for "stack", "indic", and "VPaths".
- Plot x(R):** Radio buttons for Magnitude (selected), Real, and Imag.
- Plot x(q):** Radio buttons for Magnitude, Real (selected), and Imag.
- Plotting options:** Checkboxes for "Plot fit" (checked), "Plot bkg", "Plot window" (checked), "Plot residual", and "Plot running R-factor".
- Limits:** Input fields for kmin (0), kmax (15), rmin (0), rmax (6), qmin (0), and qmax (15).
- Plotting list:** A list with "Data: fe.060" checked.
- Buttons:** "Freeze" and "Clear" buttons.
- Footer:** "Save next plot to a file."

The status bar at the bottom of the plot window shows the coordinates "8.34881, 10.1118".

2. Example: fitting the signal for an iron foil fe.060



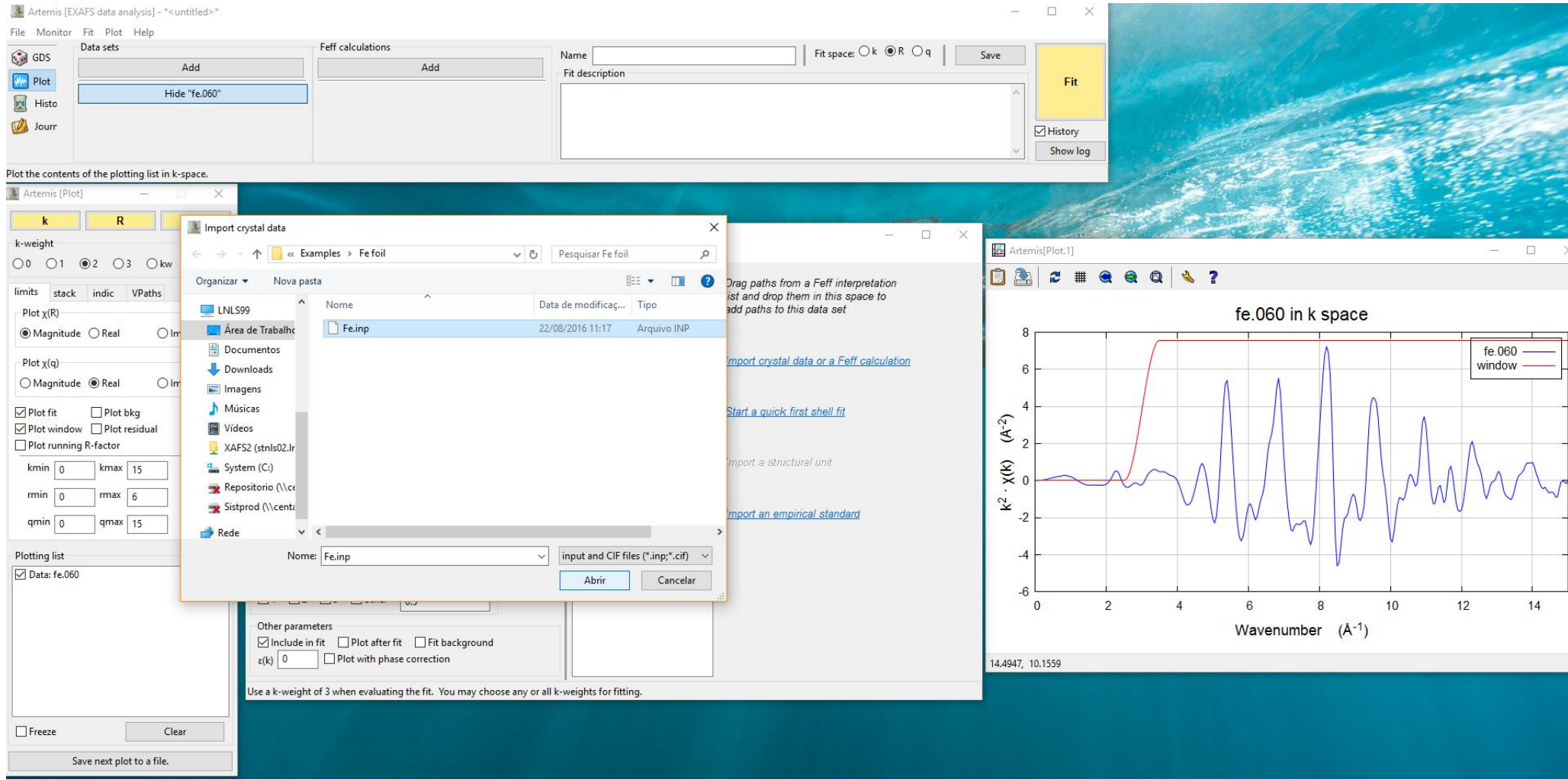
The screenshot displays the Artemis software interface for EXAFS data analysis. The main window is titled "Artemis [EXAFS data analysis] - *<untitled*>". It features a menu bar (File, Monitor, Fit, Plot, Help) and a toolbar with icons for GDS, Plot, Histo, and Jourr. The "Data sets" panel shows a list with "Hide 'fe.060'". The "Feff calculations" panel has an "Add" button. The "Fit" panel includes a "Fit" button, a "History" checkbox, and a "Show log" button. The "Fit space" options are k , R , and q .

A secondary window titled "Artemis [Plot]" is open, showing a plot of $k^2 \cdot X(k)$ versus Wavenumber (\AA^{-1}). The plot is titled "fe.060 in k space" and shows a blue line representing the data and a red line representing the fit. The x-axis ranges from 0 to 14, and the y-axis ranges from -6 to 8. The plot includes a legend for "fe.060" and "window".

A third window titled "Artemis [Data] fe.060" is open, showing the data source and fitting parameters. The data source is `\\bruceravel-XAS-Education-7adb649\Examples\Fe foil\athena.prj, 1`. The plot this data set as options are $k123$, $R123$, Rmr , Rk , and kq . The Fourier transform parameters are $kmin = 3.000$, $kmax = 20.080$, $dk = 1$, $rmin = 1$, $rmax = 3$, and $dr = 0.0$. The fitting k weights are 1 , 2 , 3 , and $other = 0.5$. The other parameters include $\epsilon(k) = 0$ and checkboxes for "Include in fit", "Plot after fit", "Fit background", and "Plot with phase correction".

A fourth window titled "Artemis [Plot.1]" is open, showing the plot of $k^2 \cdot X(k)$ versus Wavenumber (\AA^{-1}). The plot is titled "fe.060 in k space" and shows a blue line representing the data and a red line representing the fit. The x-axis ranges from 0 to 14, and the y-axis ranges from -6 to 8. The plot includes a legend for "fe.060" and "window".

2. Example: fitting the signal for an iron foil fe.060

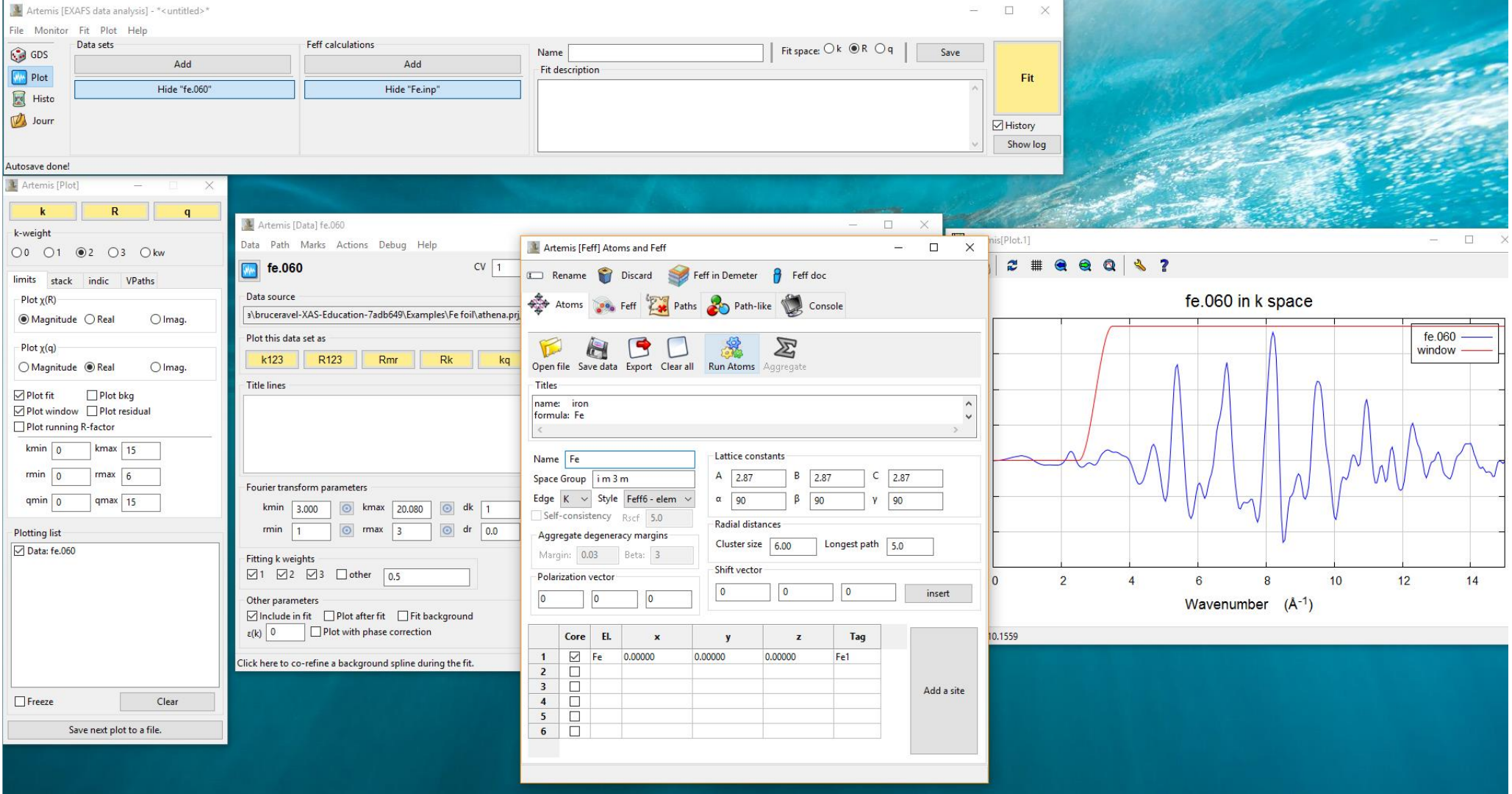


The screenshot displays the Artemis software interface for EXAFS data analysis. The main window shows a plot titled "fe.060 in k space" with the y-axis labeled $k^2 \cdot \chi(k)$ (in \AA^{-2}) and the x-axis labeled "Wavenumber (\AA^{-1})". The plot shows a blue line representing the data and a red line representing the fit window. The interface includes several control panels: "Data sets" with a "Hide 'fe.060'" button, "Feff calculations" with an "Add" button, and a "Fit" button. A dialog box titled "Import crystal data" is open, showing a file named "Fe.inp" selected from a directory. The dialog box also includes options for "Organizar", "Nova pasta", and "Pesquisar Fe foil".

WEBATOMS: <http://cars9.uchicago.edu/~newville/adb/search.html>

CIF Files: <http://www.iucr.org/resources/cif> or <https://icsd.fiz-karlsruhe.de/search/index.xhtml>

2. Example: fitting the signal for an iron foil fe.060



The screenshot displays the Artemis software interface for EXAFS data analysis. The main window shows the 'Artemis [EXAFS data analysis]' environment with various toolbars and panels.

Artemis [Data] fe.060 panel:

- Data source: `a:\bruceravel-XAS-Education-7adb649\Examples\Fe foil\athena.prj`
- Plot this data set as: `k123`, `R123`, `Rmr`, `Rk`, `kq`
- Fourier transform parameters: `kmin` 3.000, `kmax` 20.080, `dk` 1, `rmin` 1, `rmax` 3, `dr` 0.0
- Fitting k weights: `1`, `2`, `3`, `other` 0.5
- Other parameters: `Include in fit` (checked), `Plot after fit` (unchecked), `Fit background` (unchecked), `Plot with phase correction` (unchecked), `ε(k)` 0

Artemis [Feff] Atoms and Feff panel:

- Name: `Fe`
- Space Group: `i m 3 m`
- Edge: `K`, Style: `Feff6 - elem`
- Lattice constants: `A` 2.87, `B` 2.87, `C` 2.87, `α` 90, `β` 90, `γ` 90
- Radial distances: `Cluster size` 6.00, `Longest path` 5.0
- Shift vector: `0`, `0`, `0`

	Core	EL	x	y	z	Tag
1	<input checked="" type="checkbox"/>	Fe	0.00000	0.00000	0.00000	Fe1
2	<input type="checkbox"/>					
3	<input type="checkbox"/>					
4	<input type="checkbox"/>					
5	<input type="checkbox"/>					
6	<input type="checkbox"/>					

Artemis [Plot] panel:

- Plot $\chi(k)$ (checked), `Magnitude` (selected), `Real` (selected), `Imag.` (unchecked)
- Plot $\chi(q)$ (unchecked), `Magnitude` (selected), `Real` (selected), `Imag.` (unchecked)
- Plotting list: `Data: fe.060`

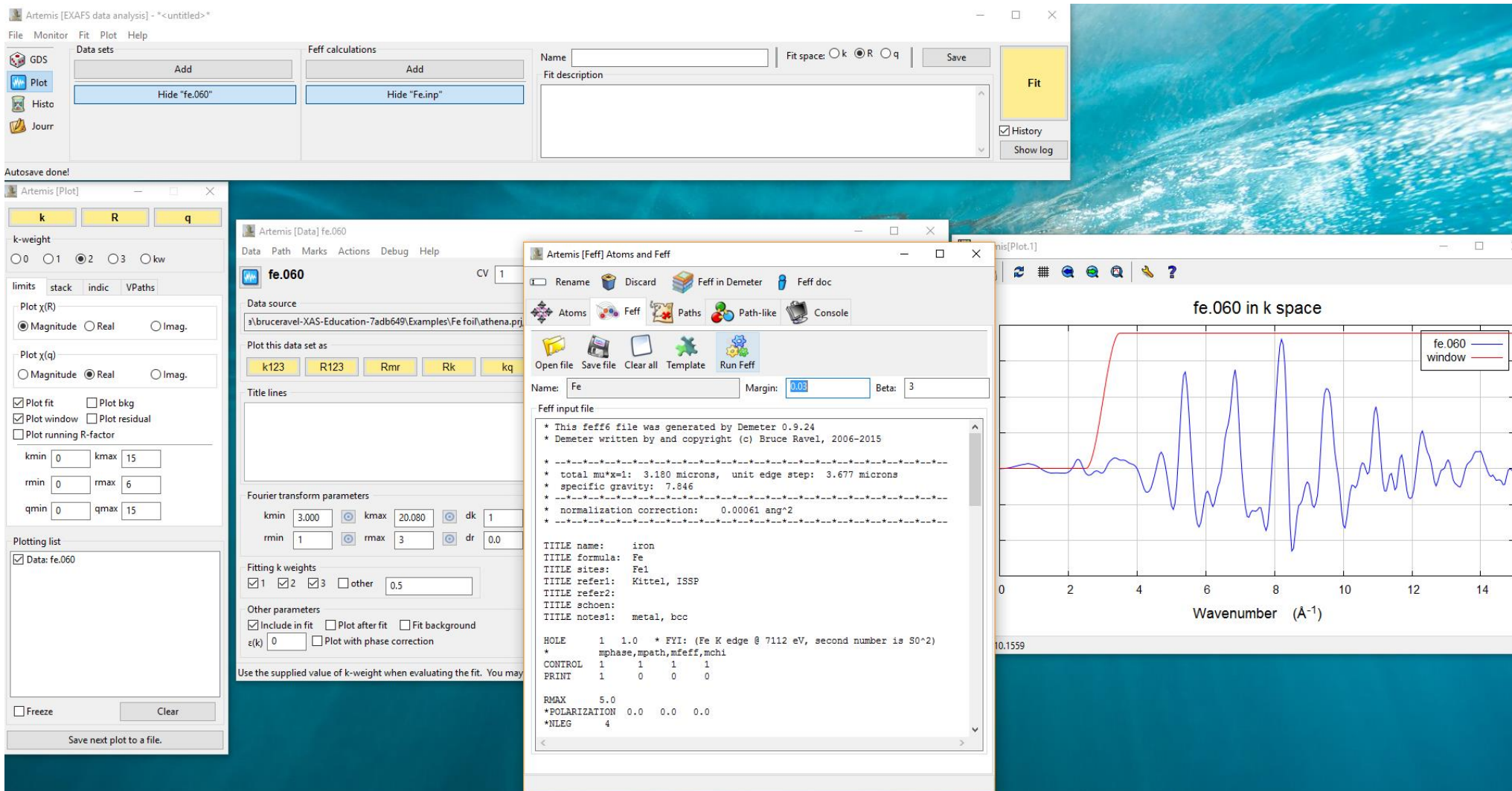
Artemis [Plot.1] panel:

Plot title: `fe.060 in k space`

Wavenumber (\AA^{-1})

Legend: `fe.060` (blue line), `window` (red line)

2. Example: fitting the signal for an iron foil fe.060



The screenshot displays the Artemis software interface for EXAFS data analysis. The main window shows the 'Data sets' and 'Feff calculations' panels. The 'Data sets' panel lists 'fe.060' and 'Fe.inp'. The 'Feff calculations' panel shows 'Fe' as the element being fitted. The 'Plot' window displays the EXAFS signal for 'fe.060 in k space' with a red fit line and a blue window line. The 'Feff [Feff] Atoms and Feff' window shows the input file content, including the title 'iron' and the Feff input file parameters.

Feff input file content:

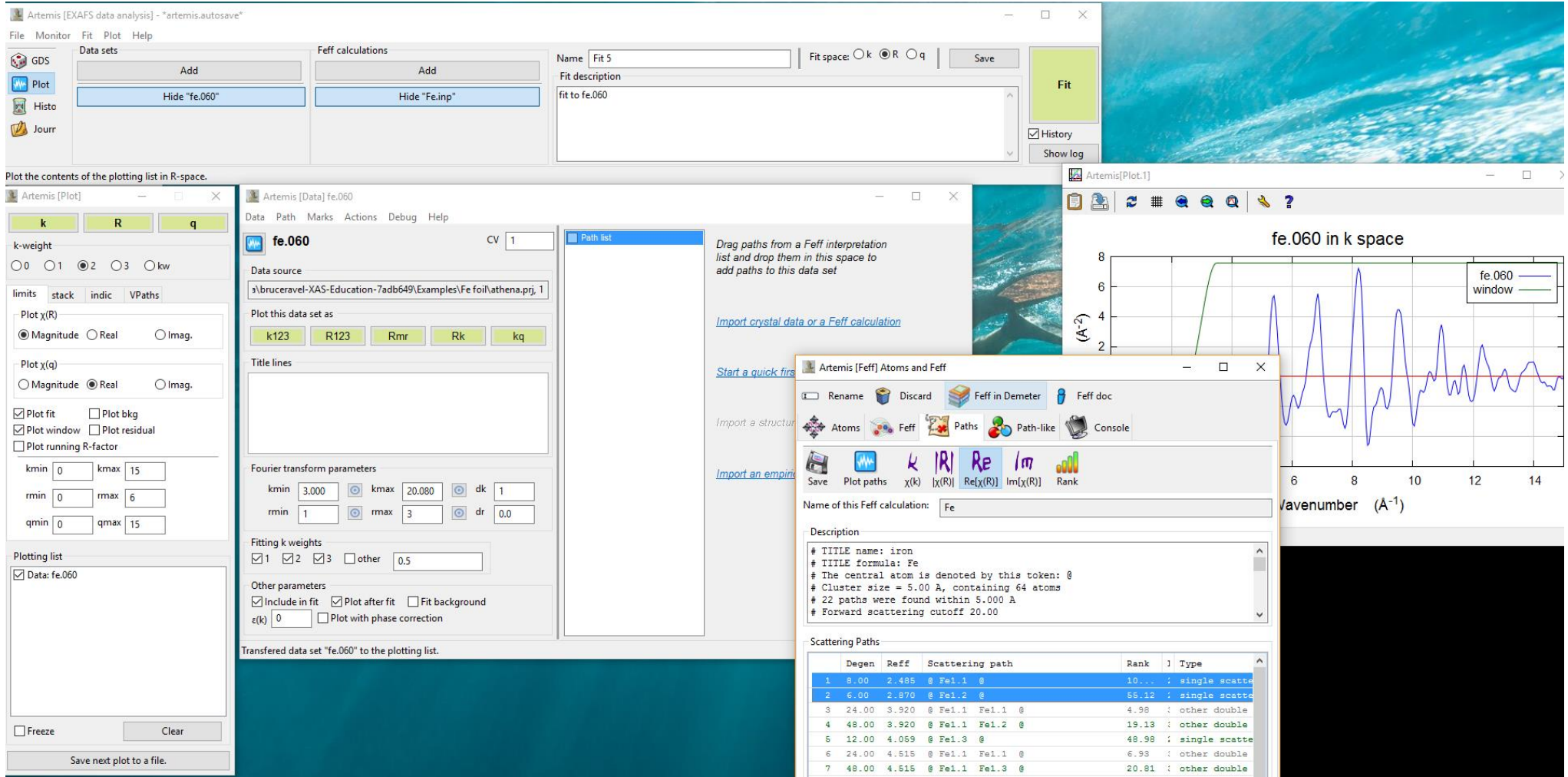
```

* This feff6 file was generated by Demeter 0.9.24
* Demeter written by and copyright (c) Bruce Ravel, 2006-2015
* -----
* total mu*x=1: 3.180 microns, unit edge step: 3.677 microns
* specific gravity: 7.846
* -----
* normalization correction: 0.00061 ang^2
* -----
TITLE name: iron
TITLE formula: Fe
TITLE sites: Fe1
TITLE refer1: Kittel, ISSP
TITLE refer2:
TITLE schoen:
TITLE notes1: metal, bcc

HOLE 1 1.0 * FYI: (Fe K edge @ 7112 eV, second number is S0^2)
* mphase,mphase,mfeff,mchi
CONTROL 1 1 1 1
PRINT 1 0 0 0

RMAX 5.0
*POLARIZATION 0.0 0.0 0.0
*NLEG 4
  
```

2. Example: fitting the signal for an iron foil fe.060



Artemis [EXAFS data analysis] - "artemis.autosave"

File Monitor Fit Plot Help

Data sets: Add, Hide "fe.060"

Feff calculations: Add, Hide "Fe.inp"

Name: Fit 5
Fit description: fit to fe.060
Fit space: k R q

Fit

History Show log

Plot the contents of the plotting list in R-space.

Artemis [Plot]

k R q

k-weight: 0 1 2 3 kw

limits: stack indic VPaths

Plot $\chi(R)$: Magnitude Real Imag.

Plot $\chi(q)$: Magnitude Real Imag.

Plot fit Plot bkg
 Plot window Plot residual
 Plot running R-factor

kmin: 0 kmax: 15
rmin: 0 rmax: 6
qmin: 0 qmax: 15

Plotting list: Data: fe.060

Freeze Clear

Save next plot to a file.

Artemis [Data] fe.060

Data Path Marks Actions Debug Help

CV: 1

Path list

Drag paths from a Feff interpretation list and drop them in this space to add paths to this data set

[Import crystal data or a Feff calculation](#)

[Start a quick first](#)

[Import a structure](#)

[Import an empirical](#)

Artemis [Feff] Atoms and Feff

Rename Discard Feff in Demeter Feff doc

Atoms Feff Paths Path-like Console

Save Plot paths $\chi(k)$ $\chi(R)$ $\text{Re}[\chi(R)]$ $\text{Im}[\chi(R)]$ Rank

Name of this Feff calculation: Fe

Description

```
# TITLE name: iron
# TITLE formula: Fe
# The central atom is denoted by this token: @
# Cluster size = 5.00 Å, containing 64 atoms
# 22 paths were found within 5.000 Å
# Forward scattering cutoff 20.00
```

Scattering Paths

Degen	Reff	Scattering path	Rank	Type
1	8.00	2.485 @ Fe.1 @	10.00	single scatter
2	6.00	2.870 @ Fe.2 @	55.12	single scatter
3	24.00	3.920 @ Fe.1 Fe.1 @	4.98	other double
4	48.00	3.920 @ Fe.1 Fe.2 @	19.13	other double
5	12.00	4.059 @ Fe.3 @	48.98	single scatter
6	24.00	4.515 @ Fe.1 Fe.1 @	6.98	other double
7	48.00	4.515 @ Fe.1 Fe.3 @	20.81	other double

Transferred data set "fe.060" to the plotting list.

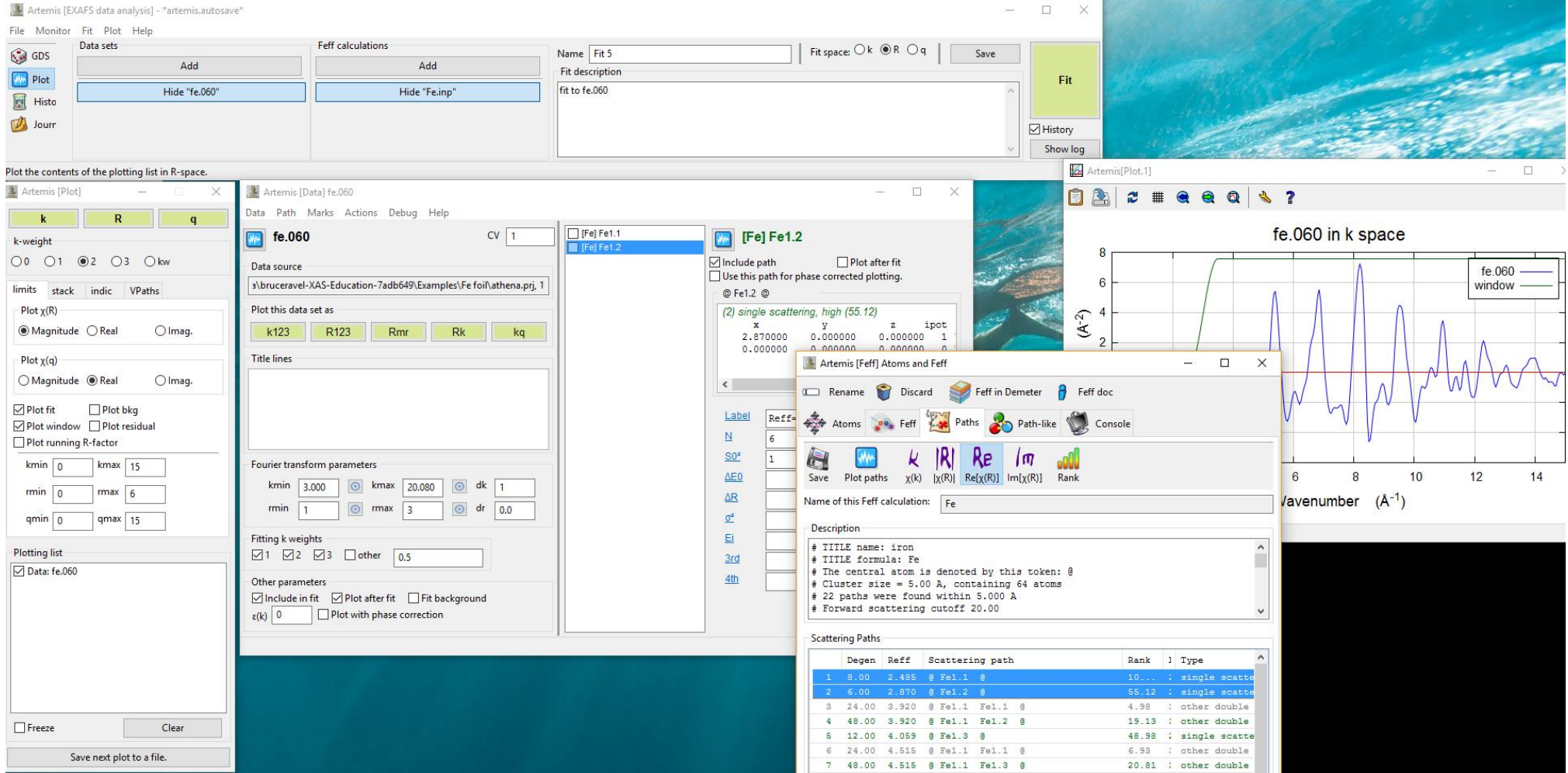
fe.060 in k space

(A⁻²)

Wave number (A⁻¹)

fe.060 window

2. Example: fitting the signal for an iron foil fe.060



The screenshot displays the Artemis software interface for EXAFS data analysis. The main window shows a plot titled "fe.060 in k space" with the x-axis labeled "k (Å⁻¹)" and the y-axis labeled "(A⁻²)". The plot shows a blue line representing the data and a green line representing the fit. A legend in the top right of the plot area identifies the blue line as "fe.060" and the green line as "window".

Several configuration panels are visible:

- Data sets:** Shows "fe.060" as the active data set.
- Feff calculations:** Shows "Fe1.2" as the active calculation.
- Plotting options:** Includes checkboxes for "Plot fit", "Plot window", "Plot residual", and "Plot running R-factor".
- Fourier transform parameters:** Includes fields for "kmin", "kmax", "dk", "rmin", "rmax", and "dr".
- Fitting k weights:** Includes checkboxes for "1", "2", "3", and "other", with a value of "0.5" for the "other" option.
- Other parameters:** Includes checkboxes for "Include in fit", "Plot after fit", "Fit background", and "Plot with phase correction".

An "Artemis [Feff] Atoms and Feff" dialog box is open, showing the "Description" and "Scattering Paths" sections. The description includes the title name "iron", the title formula "Fe", and details about the central atom and scattering paths. The scattering paths table is as follows:

Degen	Reff	Scattering path	Rank	Type
1	8.00	@ Fe1.1 @	10...	single scatter
2	6.00	@ Fe1.2 @	55.12	single scatter
3	24.00	@ Fe1.1 Fe1.1 @	4.98	other double
4	48.00	@ Fe1.1 Fe1.2 @	19.13	other double
5	12.00	@ Fe1.3 @	48.98	single scatter
6	24.00	@ Fe1.1 Fe1.1 @	6.93	other double
7	48.00	@ Fe1.1 Fe1.3 @	20.81	other double

2. Example: fitting the signal for an iron foil fe.060

The screenshot displays the Artemis software interface for XAFS data analysis. The main window is titled 'Artemis [EKAFS data analysis] - *artemis.autosave*'. It features a menu bar (File, Monitor, Fit, Plot, Help) and a toolbar with icons for GDS, Plot, Histo, and Jour.

The interface is divided into several panels:

- Data sets:** Shows 'fe.060' selected under 'Data sets' and 'Fe.inp' under 'Feff calculations'.
- Fit:** Shows 'Fit 5' with a description 'fit to fe.060'. It includes a 'Fit' button and checkboxes for 'History' and 'Show log'.
- Plot:** Displays a plot titled 'fe.060 in k space'. The y-axis is labeled $k^2 \cdot X(k) (\text{\AA}^{-2})$ and the x-axis is labeled 'Wavenumber (\AA^{-1})'. The plot shows a blue line for the data and a green line for the fit. A legend indicates 'fe.060' and 'window'.
- Parameters:** Shows fitting parameters for '[Fe] Fe1.1'. The 'Label' field contains 'Reff=2.485, nleg=2, degen=8'. Other parameters include 'N', 'S0²', 'enot', 'delr', 'Ei', '3rd', and '4th'.
- Scattering Paths:** A table at the bottom lists scattering paths with columns for 'Dege', 'Reff', 'Scattering path', 'Rank', and 'Type'.

Dege	Reff	Scattering path	Rank	Type
1	8.00	2.485 @ Fe1.1 @	10...	single scatte
2	6.00	2.870 @ Fe1.2 @	55.12	single scatte
3	24.00	3.920 @ Fe1.1 Fe1.1 @	4.98	other double
4	48.00	3.920 @ Fe1.1 Fe1.2 @	19.13	other double
5	12.00	4.059 @ Fe1.3 @	48.98	single scatte

The 'Plotting list' panel shows 'Data: fe.060' selected. The 'Fourier transform parameters' panel includes fields for 'kmin', 'kmax', 'dk', 'rmin', 'rmax', and 'dr'. The 'Fitting k weights' panel has checkboxes for '1', '2', '3', and 'other'.

2. Example: fitting the signal for an iron foil fe.060

The screenshot displays the Artemis software interface for EXAFS data analysis. The main window shows the 'Fit' panel with a 'Fit 5' session named 'fit to fe.060'. The 'Data sets' panel includes 'Hide "fe.060"' and 'Hide "Fe.inp"'. The 'GDS' panel shows the 'k-weight' set to 2 and various fitting options. A dialog box titled 'Artemis [GDS] Guess, Def, Set parameters' is open, showing a table of parameters:

Type	Name	Math expression	Evaluated
1	guess		
2	guess		
3	guess		
4	guess		
5	guess		
6	guess		
7	guess		
8	guess		
9	guess		
10	guess		
11	guess		
12	guess		

The plot window shows 'fe.060 in k space' with the y-axis labeled $k^2 \cdot \chi(k)$ (Å⁻²) and the x-axis labeled 'Wavenumber (Å⁻¹)'. The plot displays the experimental data (blue line) and the fit (green line). A table at the bottom of the interface shows the fit components:

Degen	Reff	Scattering path	Rank	Type
1	8.00	2.485 @ Fe1.1 @	10...	single scatte
2	6.00	2.870 @ Fe1.2 @	55.12	single scatte
3	24.00	3.920 @ Fe1.1 Fe1.1 @	4.98	other double
4	48.00	3.920 @ Fe1.1 Fe1.2 @	19.13	other double
5	12.00	4.059 @ Fe1.3 @	48.98	single scatte

Artemis [EXAFS data analysis] - *artemis.autosave*

File Monitor Fit Plot Help

Data sets: Add Hide "fe.060"

Feff calculations: Add Hide "Fe.inp"

Name: Fit 5
Fit description: fit to fe.060
Fit space: k R q

Fit

History Show log

The lower bound of a plot of $\chi(q)$.

Artemis [Plot]

k R q

k-weight: 0 1 2 3 kw

limits stack indic VPaths

Plot $\chi(R)$: Magnitude Real Imag.

Plot $\chi(q)$: Magnitude Real Imag.

Plot fit Plot bkg
 Plot window Plot residual
 Plot running R-factor

kmin 0 kmax 15
rmin 0 rmax 6
qmin 0 qmax 15

Plotting list
 Data: fe.060

Freeze

Save next plot to a file.

Artemis [Data] fe.060

Data Path Marks Actions Debug Help

fe.060 CV 1

Data source: s:\bruceravel-XAS-Education-7adb649\Examples\Fe foil\athena.prj, 1

Plot this data set as: k123 R123 Rmr Rk kq

Title lines

Fourier transform: kmin 3.0 rmin 1

Fitting k weight: 1 2

Other parameters: Include in fit $\epsilon(k)$ 0

Click here to have...

Artemis [GDS] Guess, Def, Set parameters

	Type	Name	Math expression	Evaluated
1	guess	amp	1	
2	guess	enot	0	
3	guess	delr	0	
4	guess	ss	0.003	
5	guess			
6	guess			
7	guess			
8	guess			
9	guess			
10	guess			
11	guess			
12	guess			

Reset all parameter values in lfeffit.

Degen	Reff	Scattering path	Rank	Type
1	8.00	2.485 @ Fe1.1 @	10...	single scatte
2	6.00	2.870 @ Fe1.2 @	55.12	single scatte
3	24.00	3.920 @ Fe1.1 Fe1.1 @	4.98	other double
4	48.00	3.920 @ Fe1.1 Fe1.2 @	19.13	other double
5	12.00	4.059 @ Fe1.3 @	48.98	single scatte

Artemis [Plot.1]

fe.060 in k space

$K^2 \cdot X(k)$ (\AA^{-2})

Wavenumber (\AA^{-1})

fe.060 window

-0.817912, 10.3266

2. Example: fitting the signal for an iron foil fe.060

The screenshot displays the Artemis software interface for EXAFS data analysis. The main window shows the 'Data sets' and 'Feff calculations' panels. The 'Data sets' panel includes 'Add' and 'Hide "fe.060"' buttons. The 'Feff calculations' panel includes 'Add' and 'Hide "Fe.inp"' buttons. The 'Fit' panel shows 'Fit 5' with a description 'fit to fe.060' and 'Fit space: k R q'.

The 'Artemis [Plot]' window shows the 'k' weight selected. The 'Artemis [Data] fe.060' window shows the data source and plotting options. The 'Artemis [GDS] Guess, Def, Set parameters' window shows a table of parameters:

Type	Name	Math expression	Evaluated
1	guess	amp	0.82053 +/- 0.04102
2	guess	enot	8.86001 +/- 0.78601

The 'Artemis[Plot.1]' window shows a plot of $|X(R)|$ (A⁻³) versus Radial distance (Å). The plot shows a blue line for the data and a red line for the fit. The fit is a single scattering model with parameters: Reff=2.485, nleg=2, degen=8. The plot also shows a green box highlighting the fit region.

The 'Contact' window shows the following statistics:

```

Independent points : 21.2500000
Number of variables : 4
Chi-square : 10693.7414710
Reduced chi-square : 619.9270418
R-factor : 0.0110018
Number of data sets : 1

Happiness = 100.00/100
**** Note: happiness is a semantic parameter and should ****
**** NEVER be reported in a publication -- NEVER! ****

guess parameters:
amp = 0.81436611 # +/- 0.04095266 [1]
enot = 8.75642139 # +/- 0.75576713 [0]
delr = -0.00825932 # +/- 0.00371902 [0]
ss = 0.00293721 # +/- 0.00031604 [0.003]

Correlations between variables:
delr & enot --> 0.8984
  
```

Artemis [EXAFS data analysis] - *artemis.autosave*

File Monitor Fit Plot Help

Data sets

Add

Hide "fe.060"

Feff calculations

Add

Hide "Fe.inp"

Name: Fit 9

Fit space: k R q

Save

Fit description: fit to fe.060

Fit

History

Show log

Your fit took 3 seconds.

Artemis [Plot]

k R q

k-weight: 0 1 2 3 kw

limits stack indic VPaths

Plot $\chi(R)$

Magnitude Real Imag.

Plot $\chi(q)$

Magnitude Real Imag.

Plot fit Plot bkg

Plot window Plot residual

Plot running R-factor

kmin 0 kmax 15

rmin 0 rmax 6

qmin 0 qmax 15

Plotting list

Data: fe.060

Freeze Clear

Save next plot to a file.

Artemis [Data] fe.060

Data Path Marks Actions Debug Help

fe.060 CV 1

Data source: s:\bruceravel-XAS-Education-7adb649\Examples\Fe foil\athena.prj.1

Plot this data set as: k123 R123 Dmx Dk km

Title lines

Artemis [Log] Fit 8

Name: Fit 8 (hkqew)

Description: fit to fe.060

Figure of merit: 8

Time of fit: 2016-08-22T13:42:47

Environment: Demeter 0.9.24 with perl 5.018002 and using Ifeffit 1.

Interface: Artemis (Wx 0.9923)

Prepared by:

Contact:

Independent points: 21.2500000

Number of variables: 4

Chi-square: 10693.7414710

Reduced chi-square: 619.9270415

R-factor: 0.0110018

Number of data sets: 1

Happiness = 100.00/100 color = #D8E796

***** Note: happiness is a semantic parameter and should *****

***** NEVER be reported in a publication -- NEVER! *****

guess parameters:

amp = 0.81436611 # +/- 0.04095266 [1]

enot = 8.75642139 # +/- 0.75576713 [0]

delr = -0.00825932 # +/- 0.00371902 [0]

ss = 0.00293721 # +/- 0.00031604 [0.003]

Correlations between variables:

Artemis [Plot.1]

fe.060 in R space

Legend: fe.060 (blue), fit (red), window (green)

Reff=2.870, nleg=2, degen=6

ff	Scattering path	Rank	Type
485	@ Fe1.1 @	10...	single scatte
870	@ Fe1.2 @	55.12	single scatte
920	@ Fe1.1 Fe1.1 @	4.98	other double
920	@ Fe1.1 Fe1.2 @	19.13	other double
059	@ Fe1.3 @	48.98	single scatte

3. To do: following Bruce Ravel example on FeS₂

Please access this site and follow the part that we don't have done yet...

<https://bruceravel.github.io/demeter/documents/Artemis/examples/fes2.html>

4. What do I do next?



It depends on you, but follow this can be an good option:

<https://speakerdeck.com/bruceravel>

<http://bruceravel.github.io/XAS-Education/>



Obrigado pela sua atenção!

Questions, please email me:

santiago.figueroa@lnls.br

More info about Iffeffit and XAFS:

<https://speakerdeck.com/bruceravel?page=2>

http://cars.uchicago.edu/iffefit/Mailing_List

<http://xafs.org/Tutorials>

<http://www.ixasportal.net/ixas/>

<http://cars.uchicago.edu/iffefit/Documentation>

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