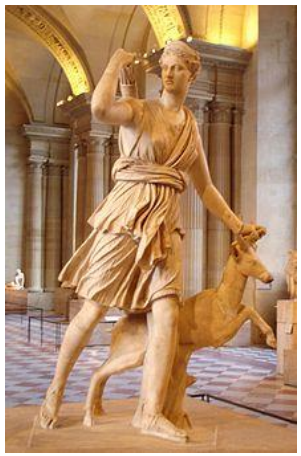
Parallel Session on Artemis



X-Ray Absorption Fine Structure

XAFS

Santiago J. A. Figueroa
Researcher
Beamline coordinator XAFS2
santiago.figueroa@lnls.br

5th School on X-Ray Spectroscopy Methods

Campinas, 23 de Agosto de 2016

Planning

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?

Parallel Session on Artemis

1.Artemis, some aspects of the program

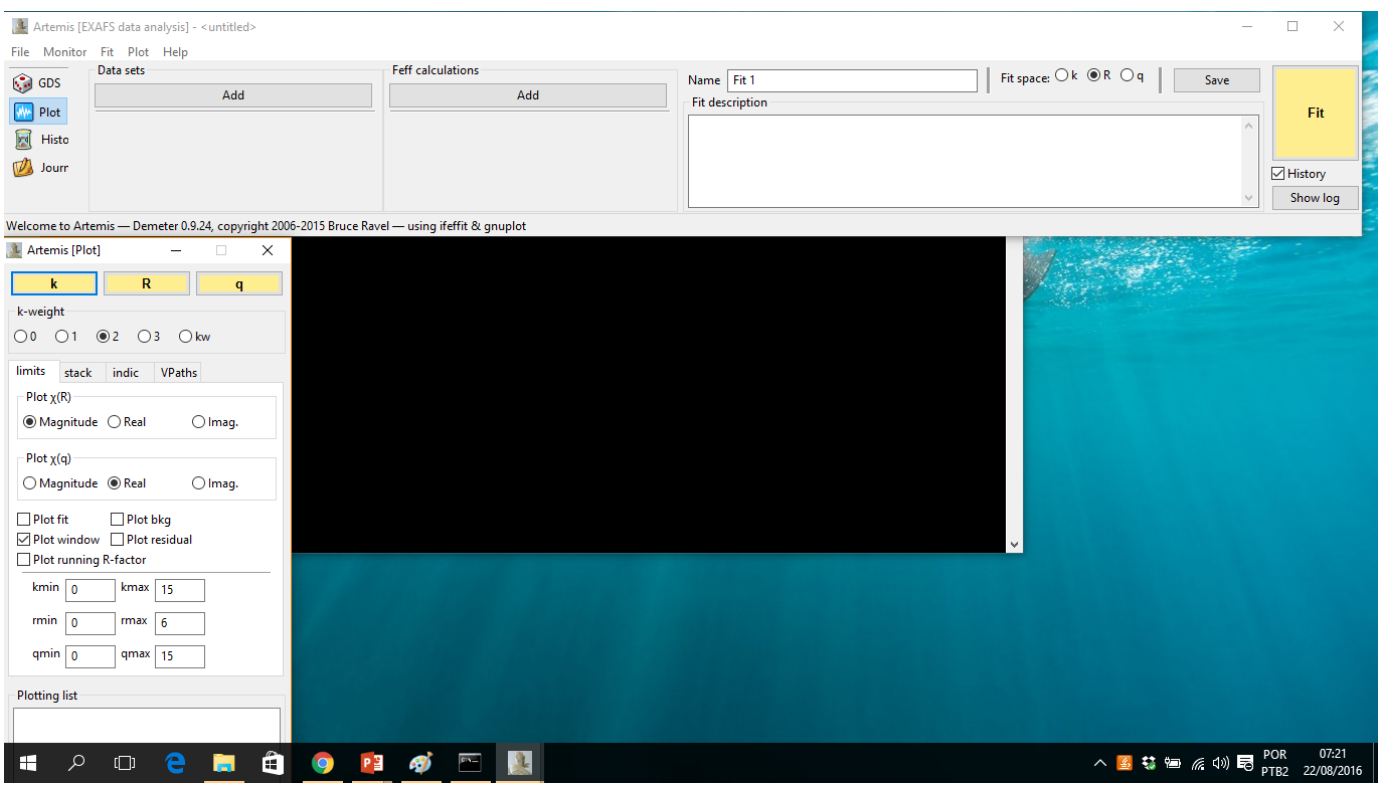
2. Starting Artemis

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.



https://bruceravel.github.io/demeter/documents/Artemis/startup/index.html

Parallel Session on Artemis

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.

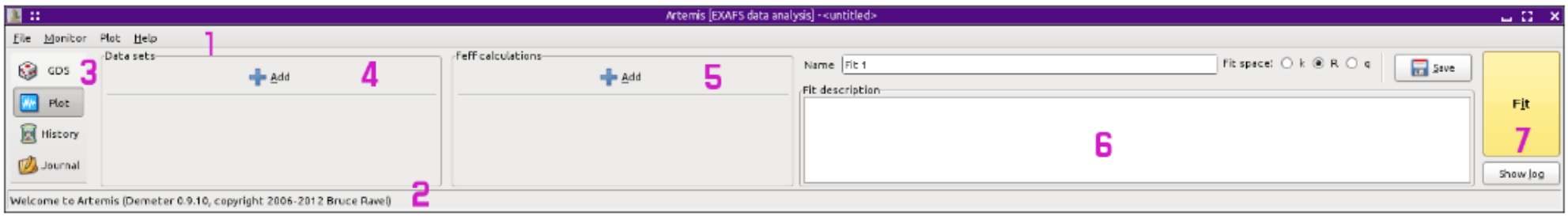


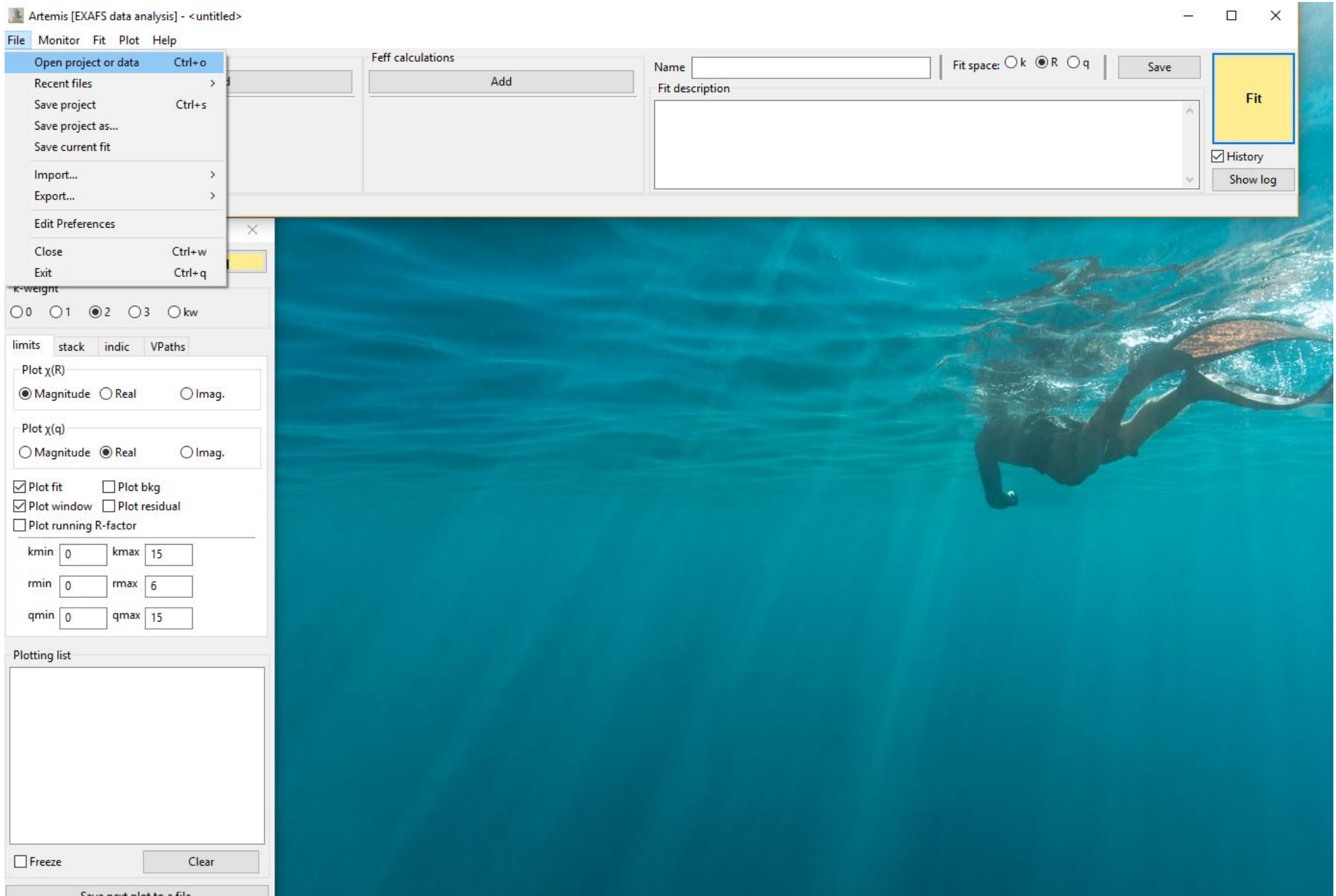
Fig. 2.2 The main window.

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.

https://bruceravel.github.io/demeter/documents/Artemis/startup/main.html

Parallel Session on Artemis

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



Parallel Session on Artemis

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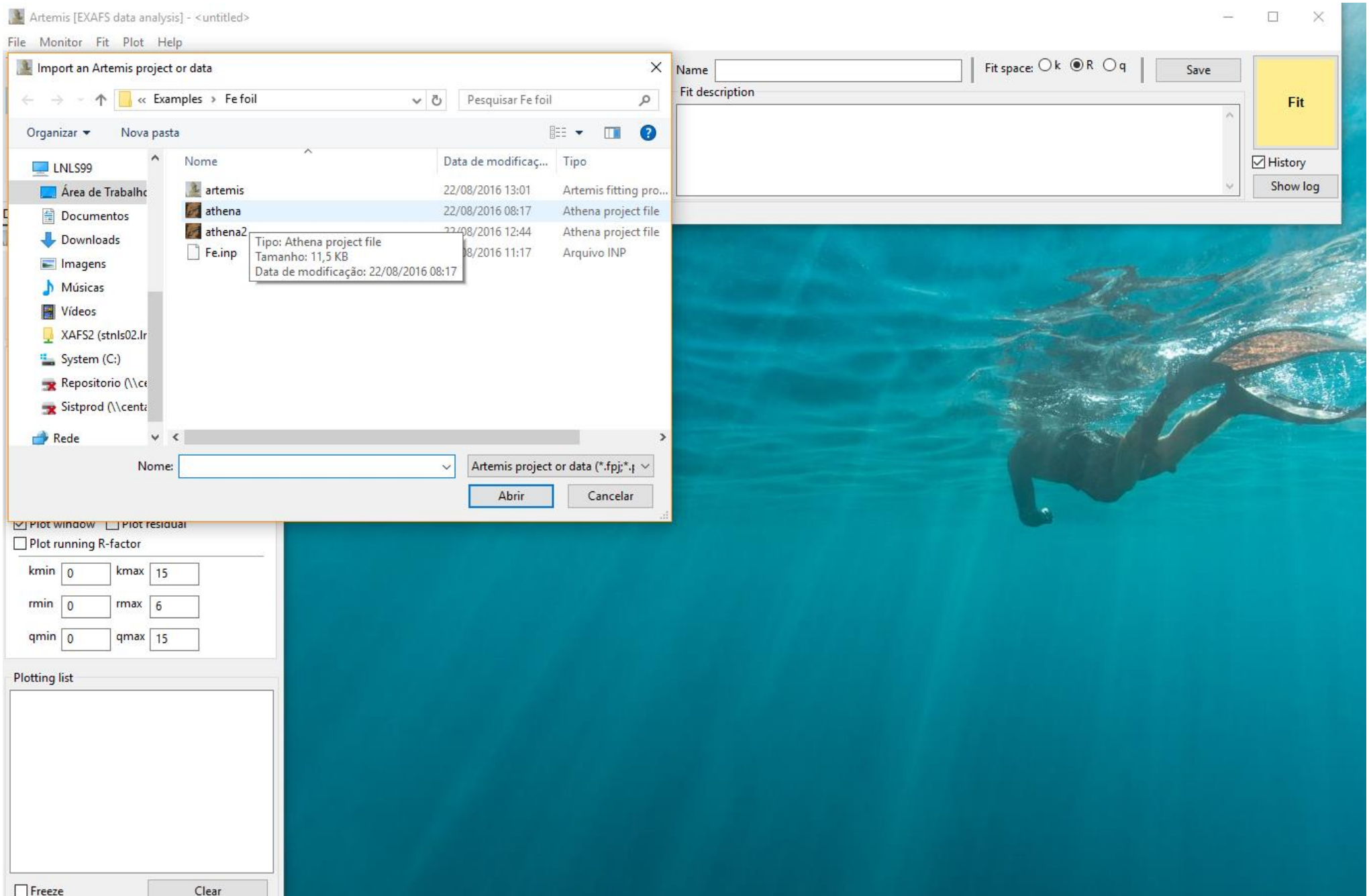

Parallel Session on Artemis

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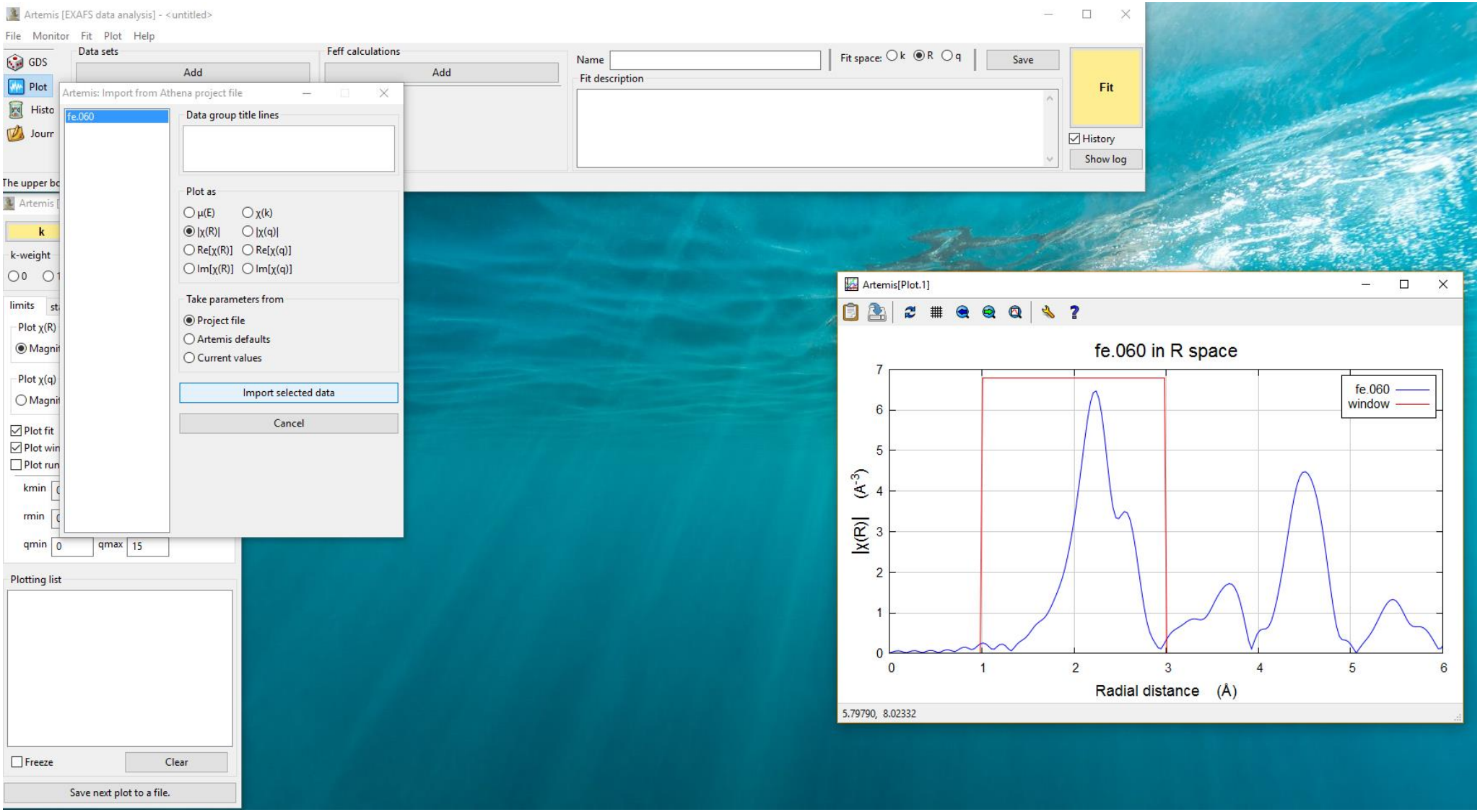

Parallel Session on Artemis

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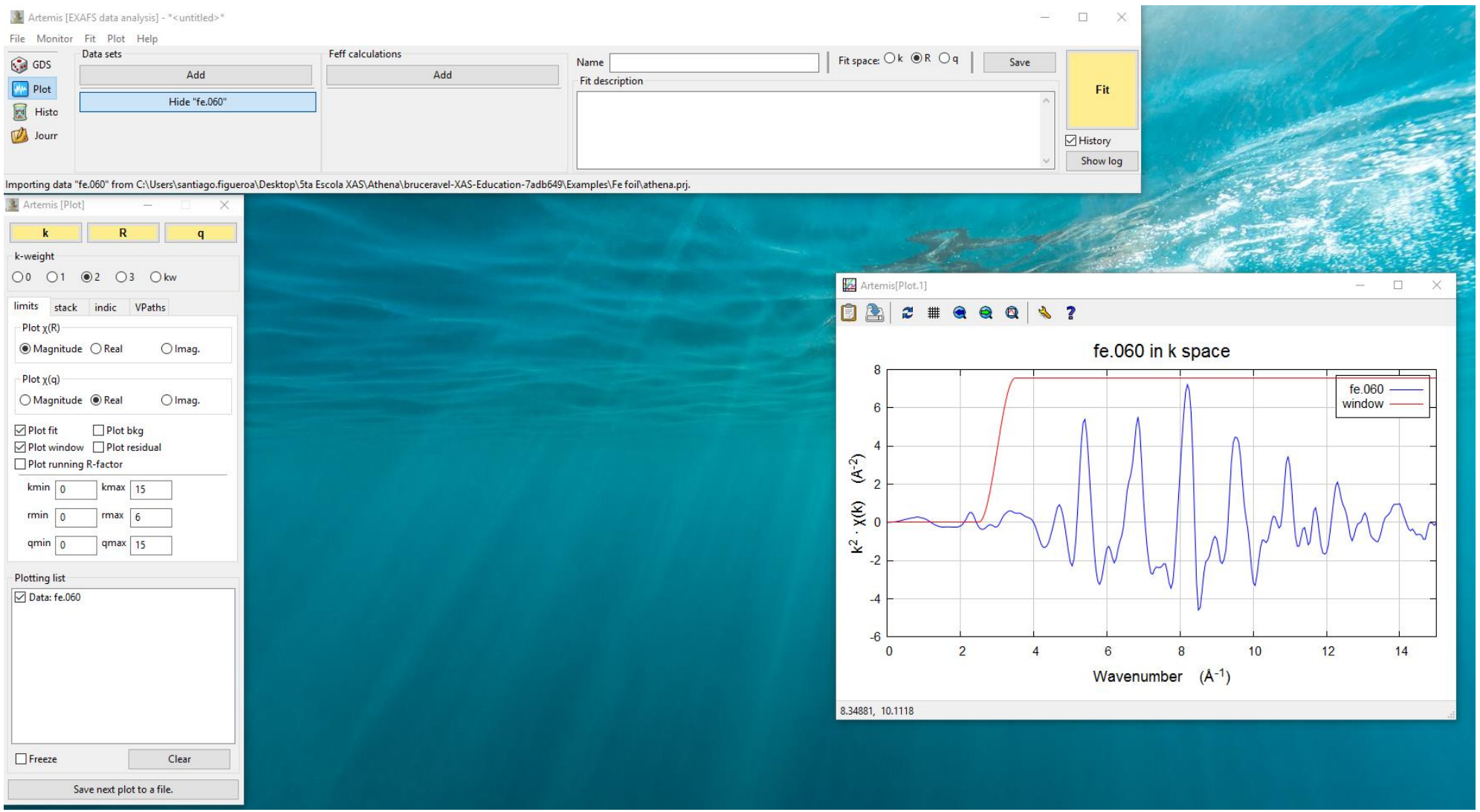

Parallel Session on Artemis

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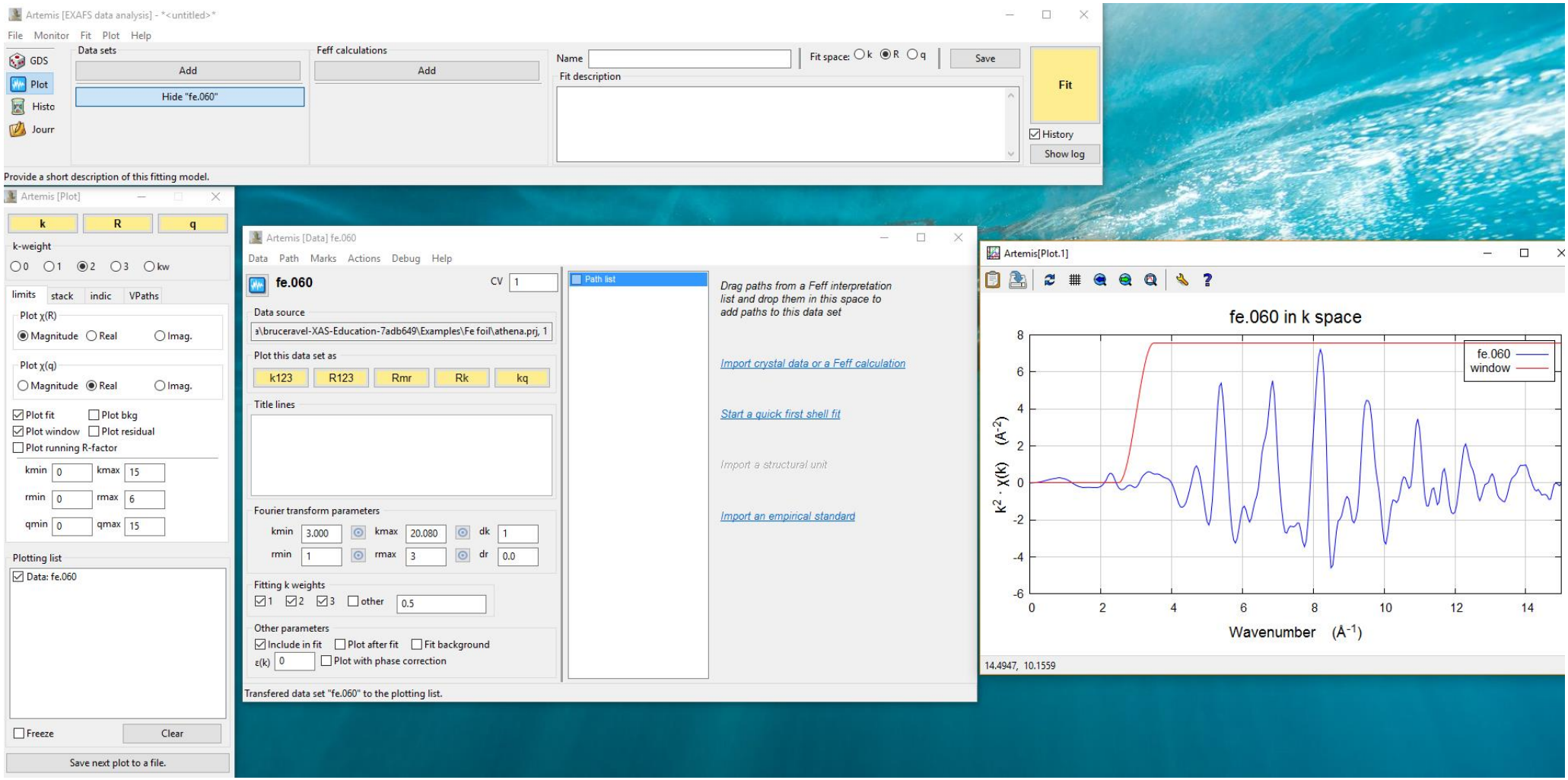

Parallel Session on Artemis

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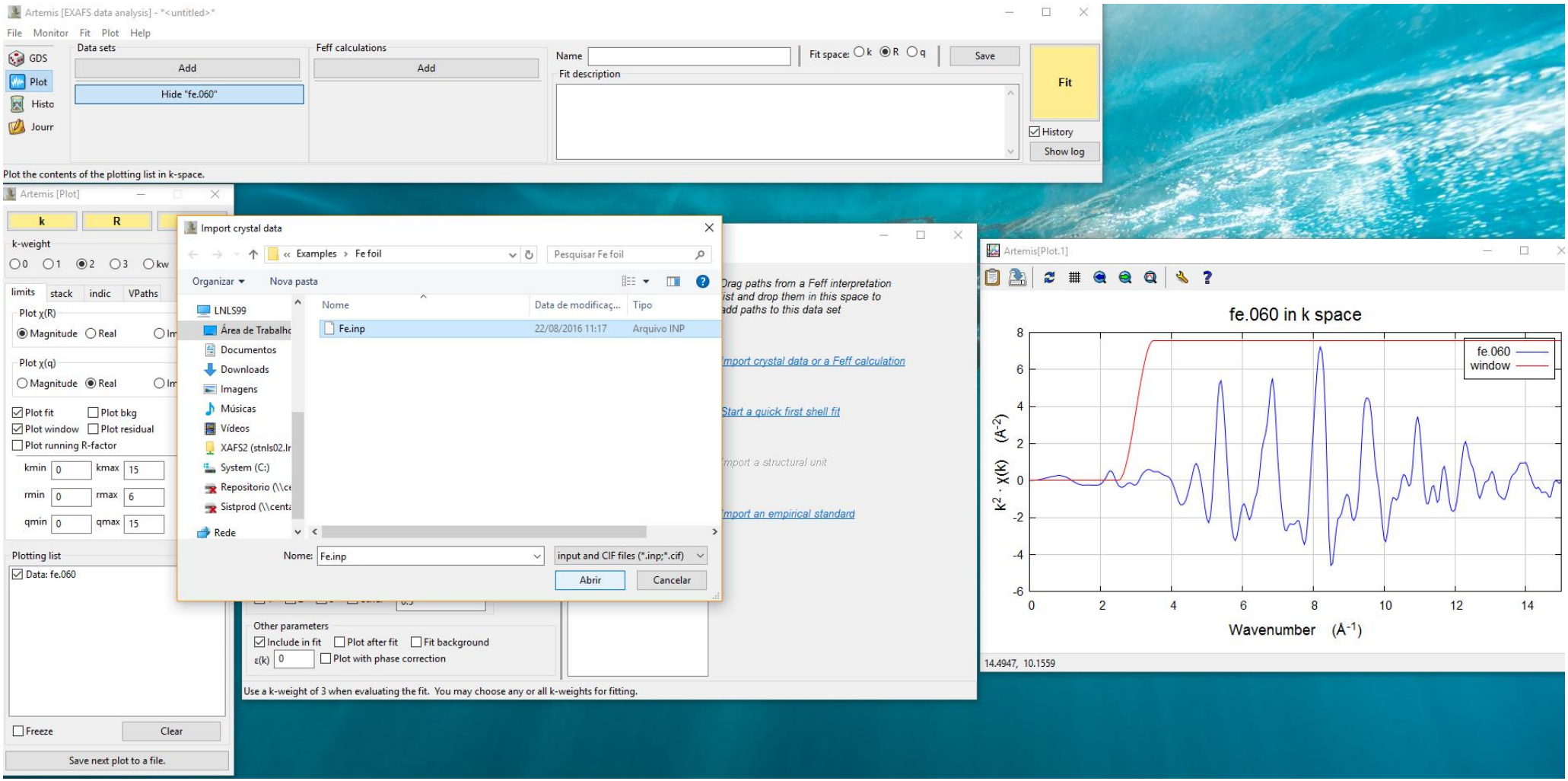
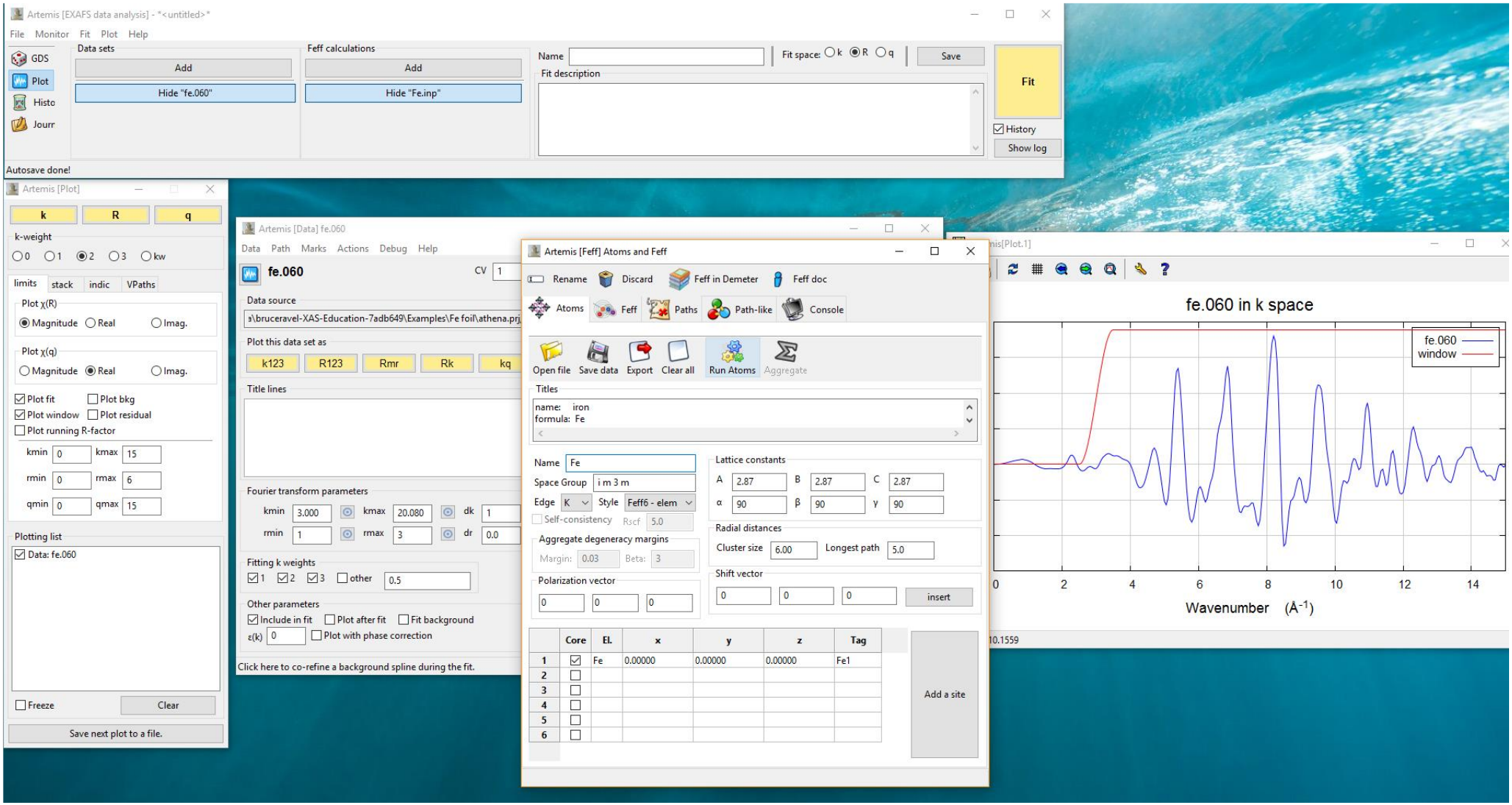


WEBATOMS: http://cars9.uchicago.edu/~newville/adb/search.html

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

Parallel Session on Artemis

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



Parallel Session on Artemis

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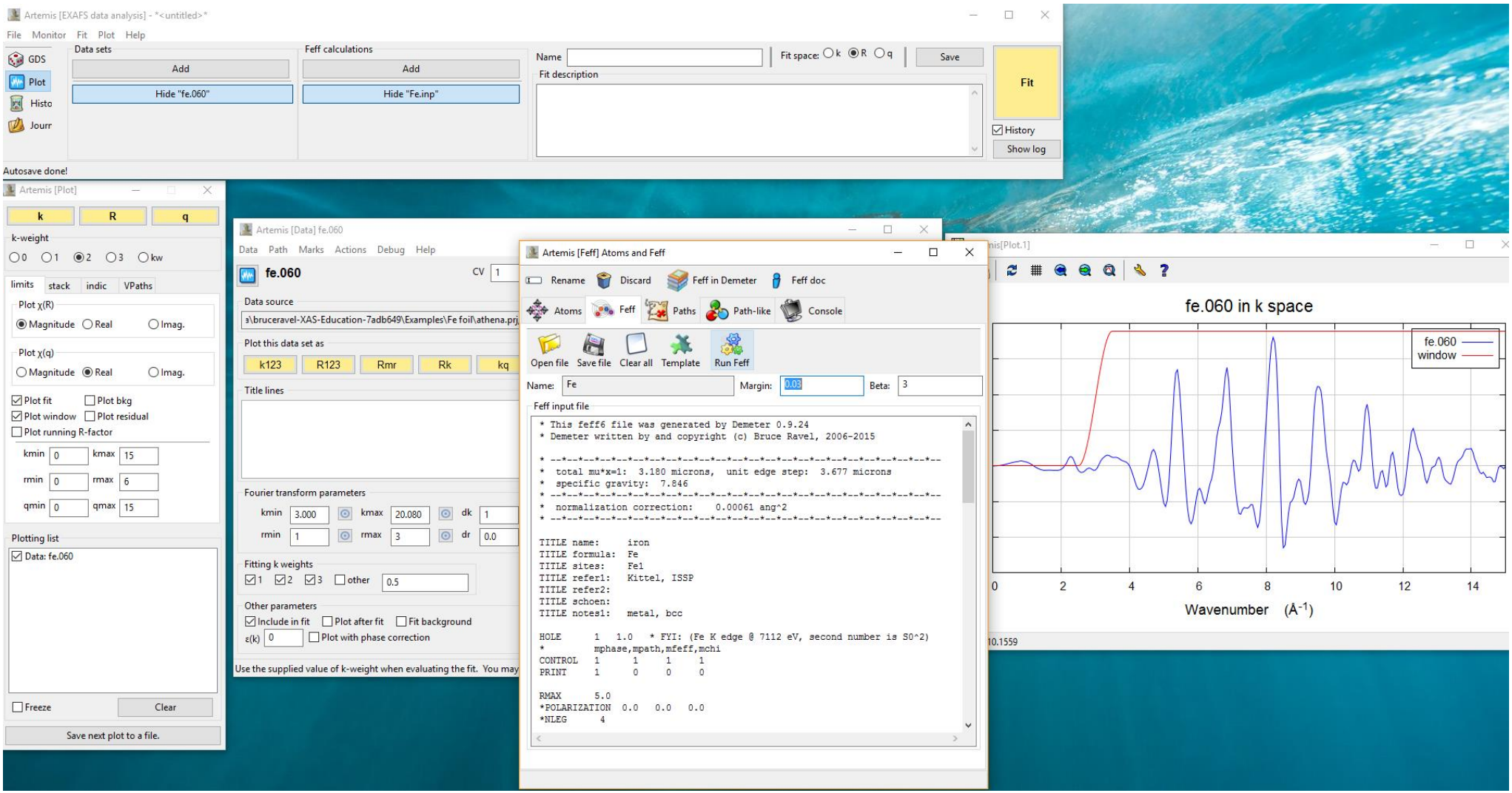

Parallel Session on Artemis

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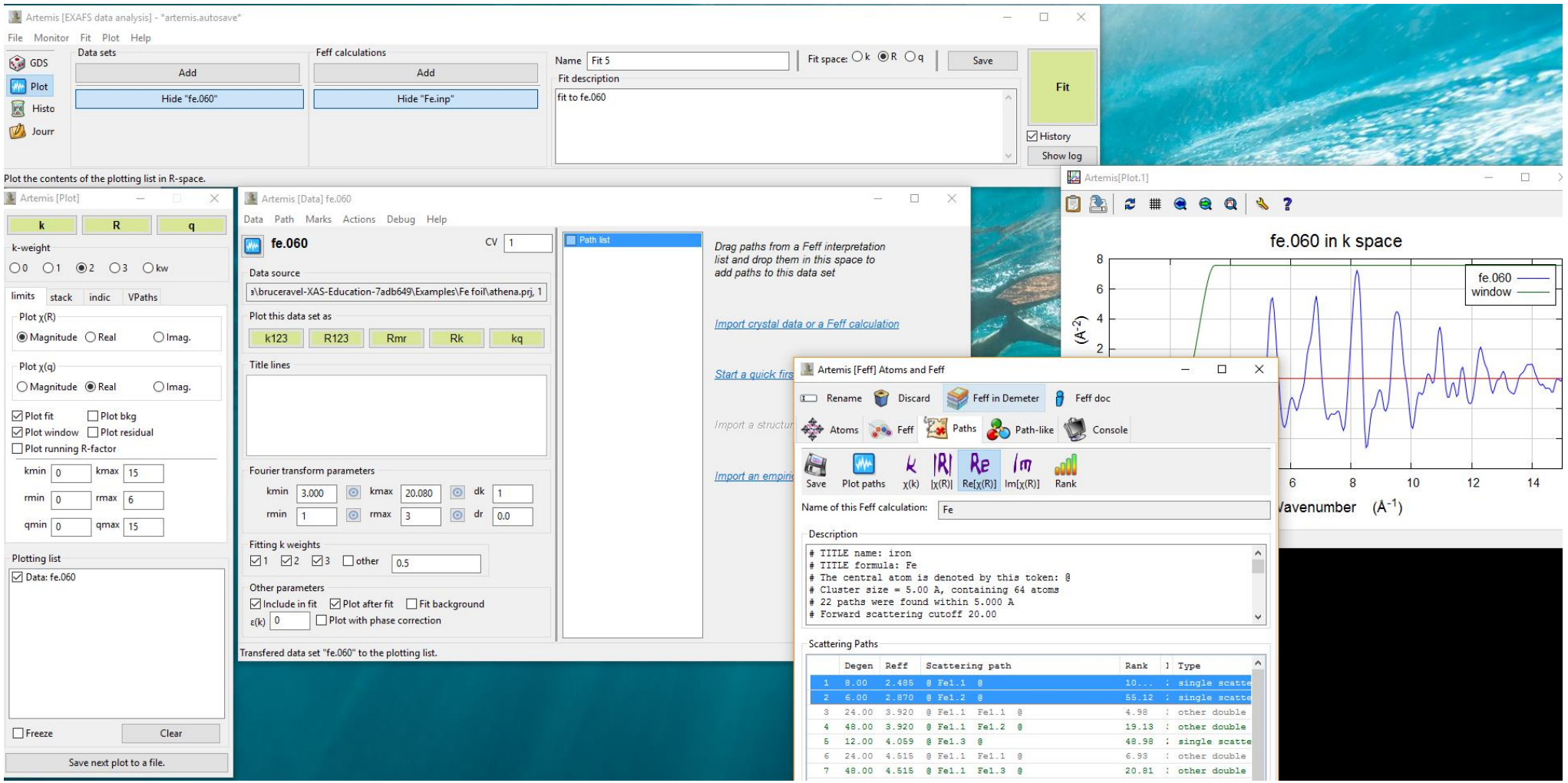

Parallel Session on Artemis

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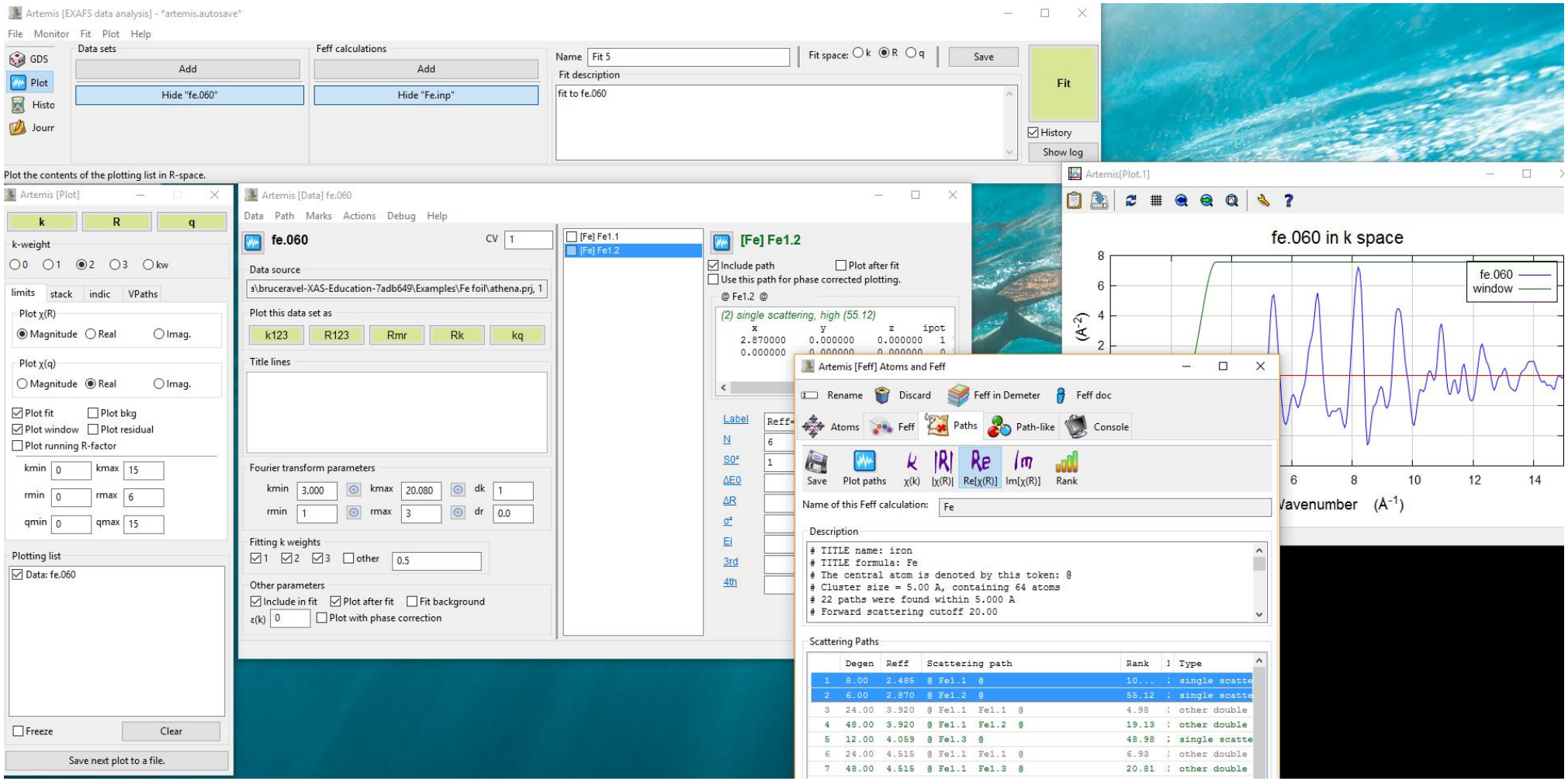

Parallel Session on Artemis

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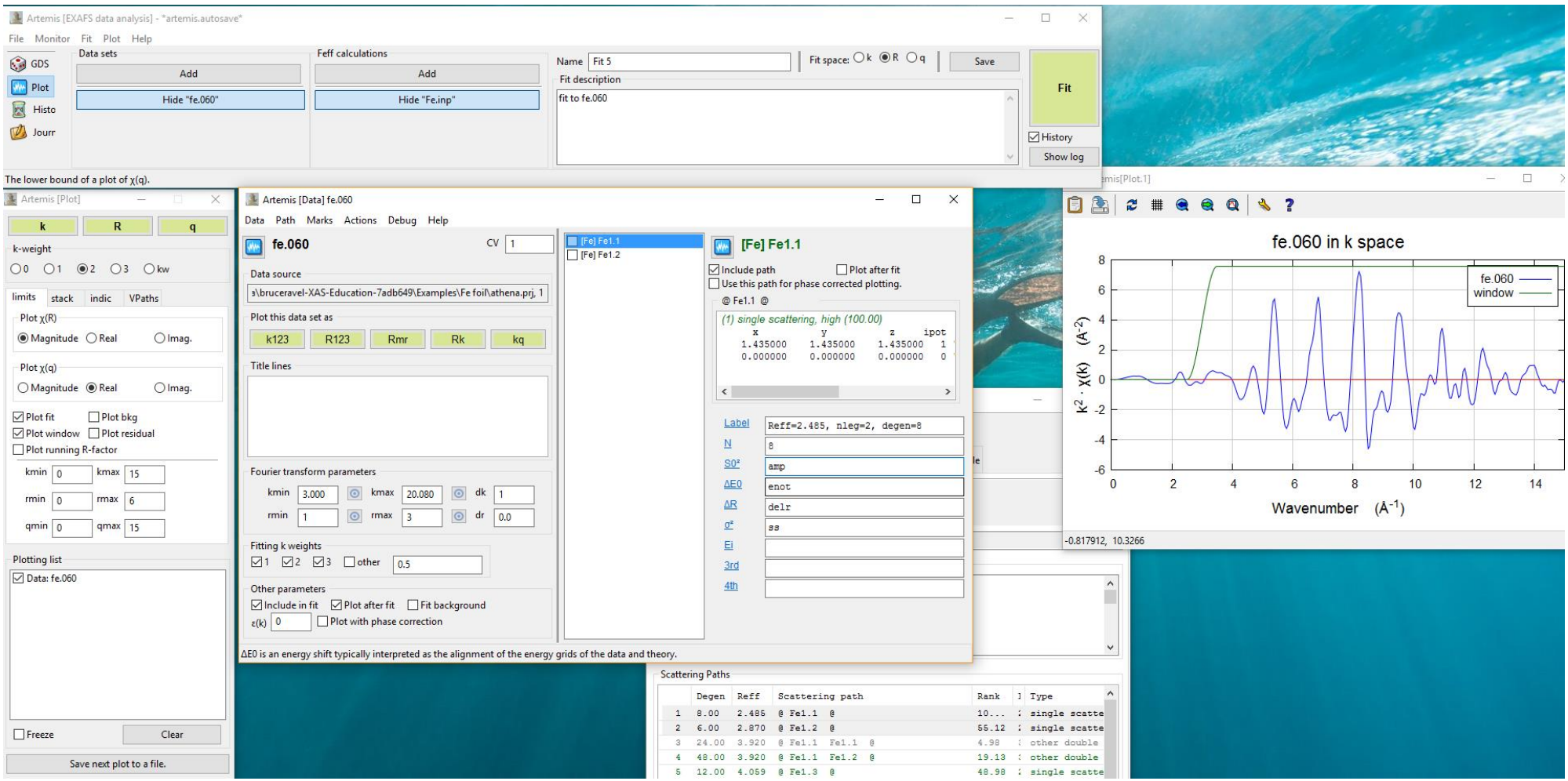

Parallel Session on Artemis

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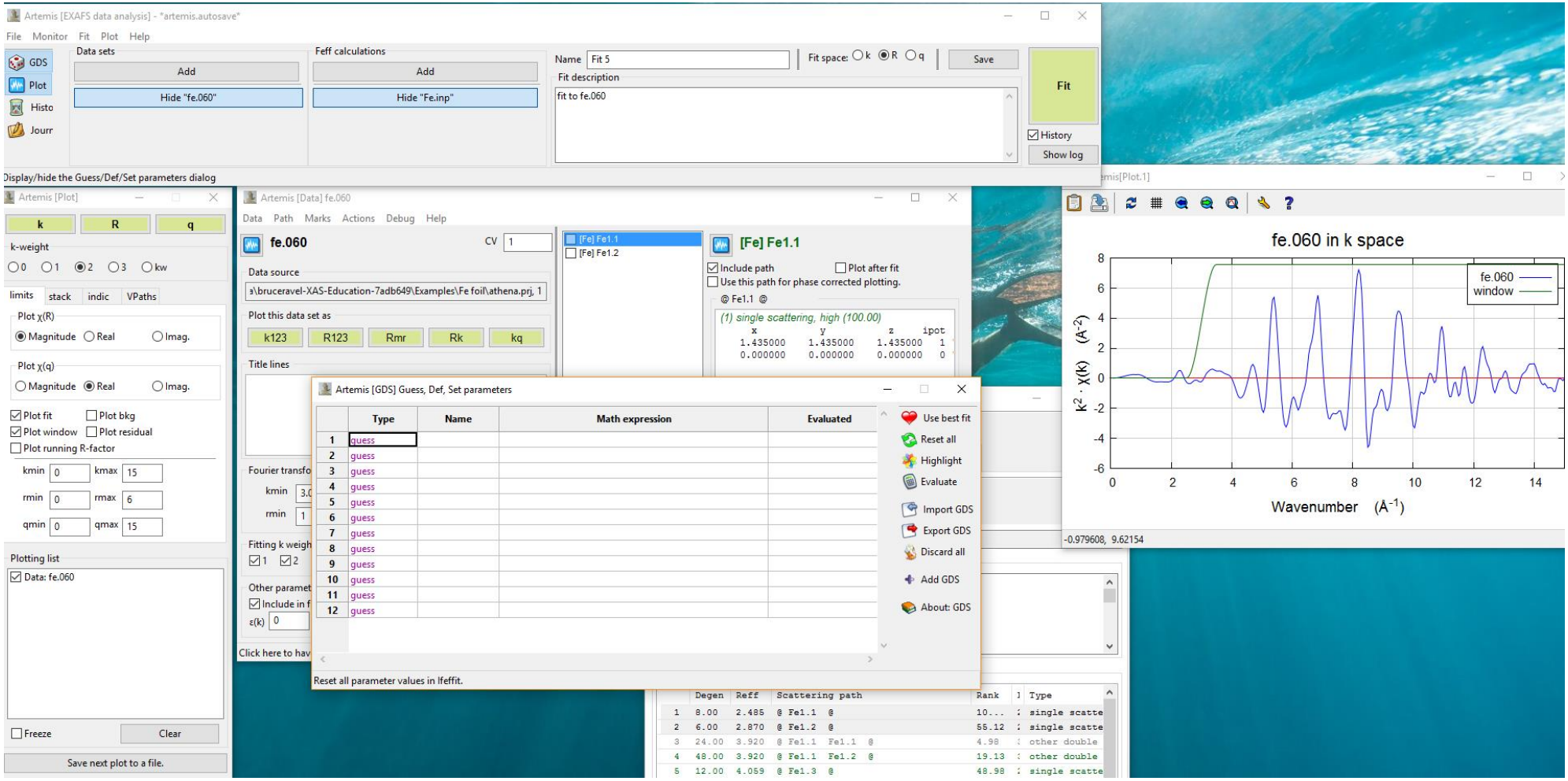
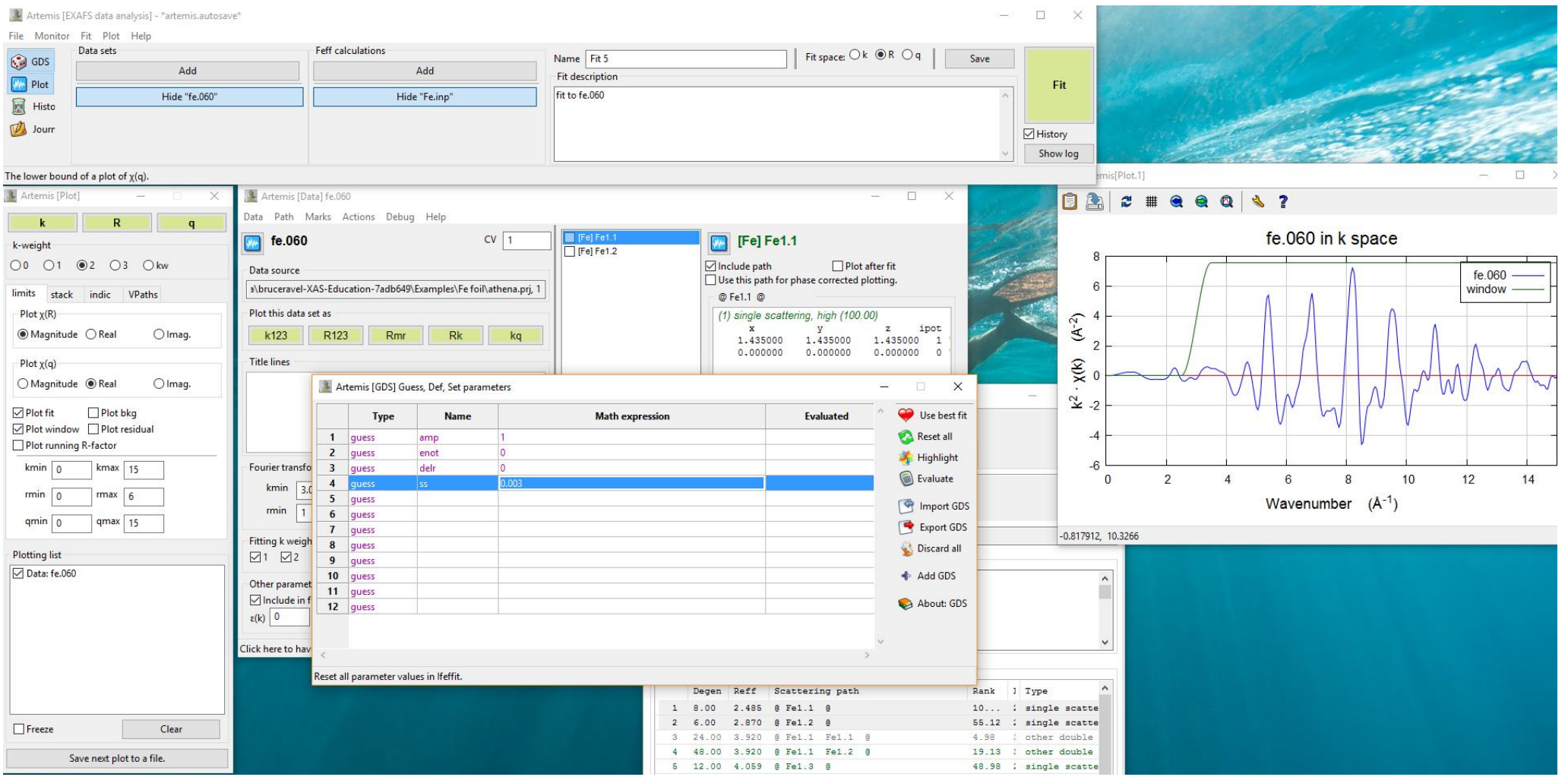
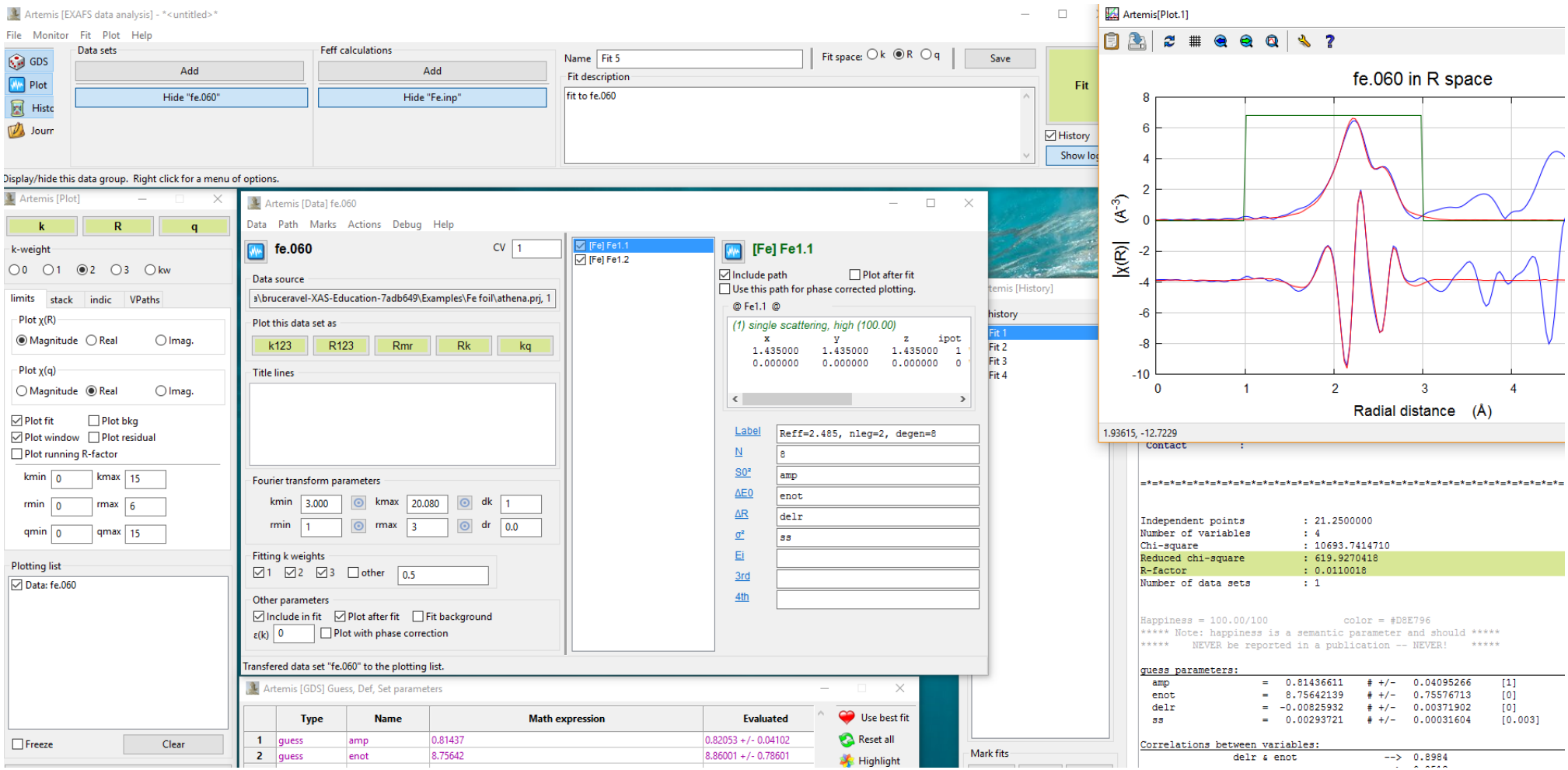
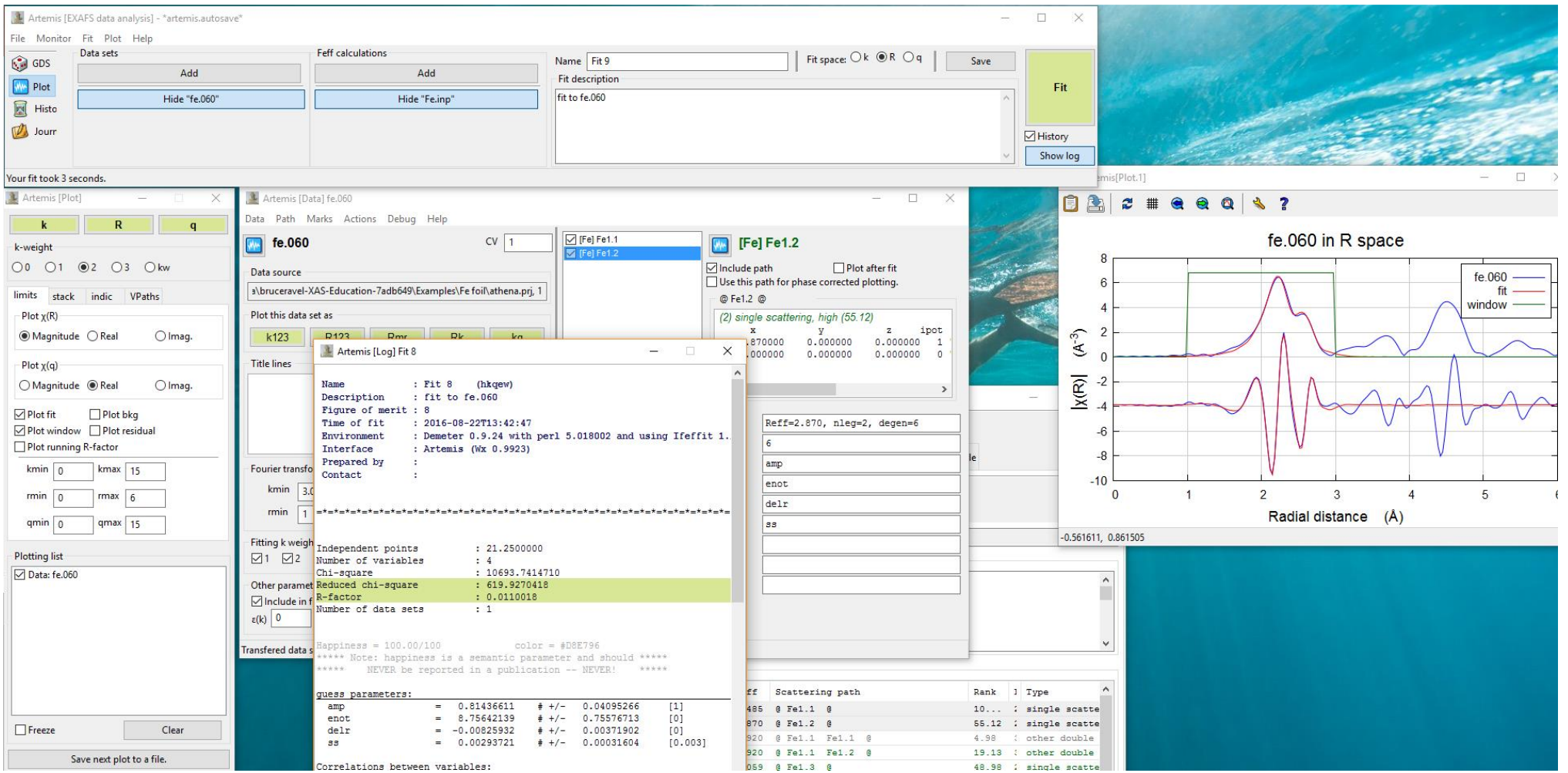



Artemis [EXAFS data analysis] - *artemis.autosave*
File Monitor Fit Plot Help
GDS
Plot
Histo
Jourr
Data sets
Add
Hide "fe.060"
Feff calculations
Add
Hide "Fe.inp"
Name Fit 5
Fit space: k R q
Save
Fit description
fit to fe.060
Fit
History
Show log
The lower bound of a plot of χ(q).
Artemis [Plot]
k R q
k-weight
limits stack indic VPaths
Plot χ(R)
Magnitude Real Imag.
Plot χ(q)
Plot fit Plot bkg
Plot window Plot residual
Plot running R-factor
kmin kmax rmin rmax qmin qmax
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
Data source
a\bruceravel-XAS-Education-7adb649\Examples\Fe foil\athena.prj, 1
Plot this data set as
k123 R123 Rmr Rk kq
Title lines
[Fe] Fe1.1
[Fe] Fe1.2
[Fe] Fe1.1
Include path Plot after fit
Use this path for phase corrected plotting.
@ Fe1.1 @
(1) single scattering, high (100.00)
x y z ipot
1.435000 1.435000 1.435000 1
0.000000 0.000000 0.000000 0
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
Use best fit
Reset all
Highlight
Evaluate
Import GDS
Export GDS
Discard all
Add GDS
About: GDS
Reset all parameter values in Ifeffit.
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
fe.060 in k space
fe.060
window
k² · χ(k) (Å⁻²)
Wavenumber (Å⁻¹)
-0.817912, 10.3266

Parallel Session on Artemis

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




Artemis [EXAFS data analysis] - *artemis.autosave*
File Monitor Fit Plot Help
GDS
Plot
Histo
Jourr
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
limits stack indic VPaths
Plot χ(R)
Magnitude Real Imag.
Plot χ(q)
Magnitude Real Imag.
Plot fit
Plot bkg
Plot window
Plot residual
Plot running R-factor
kmin kmax rmin rmax qmin qmax
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
Plot this data set as
k123
Title lines
Fourier transfo
Fitting k weigh
Other paramet
Include in f
Transfered data s
[Fe] Fe1.1
[Fe] Fe1.2
[Fe] Fe1.2
Include path
Plot after fit
Use this path for phase corrected plotting.
@ Fe1.2 @
(2) single scattering, high (55.12)
x y z ipot
Reff=2.870, nleg=2, degen=6
6
amp
enot
delr
ss
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 : 619.9270418
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:
Scattering path
Rank
Type
single scatte
other double
fe.060 in R space
fe.060
fit
window
|χ(R)| (Å^-3)
Radial distance (Å)
-0.561611, 0.861505

Laboratório Nacional de Luz Síncrotron

CNPEM

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

Parallel Session on Athena

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/

Thanks for your attention!

Obrigado pela sua atenção!

Questions, please email me:

santiago.figueroa@lnls.br

More info about Ifeffit and XAFS:

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

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

http://xafs.org/Tutorials

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

http://cars.uchicago.edu/ifeffit/Documentation

Acknowlegments: Bruce Ravel, Matt Newville and all the people that help to develop Ifeffit and Feff.