XAESA

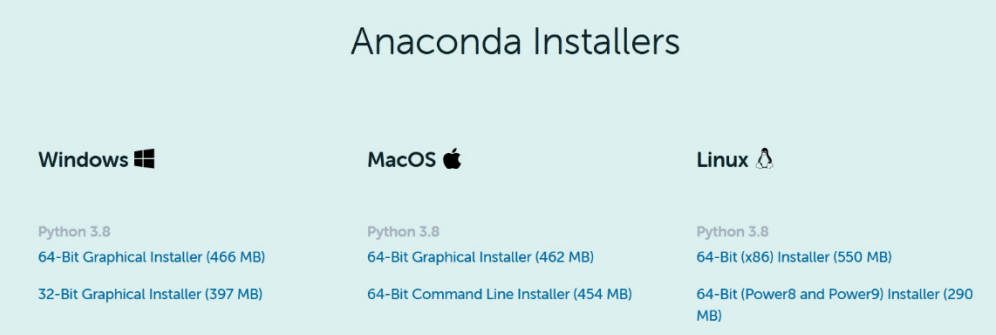
User Manual

Version 1.2

How to install XAESA

1) Install Python from

https://www.anaconda.com/products/individual



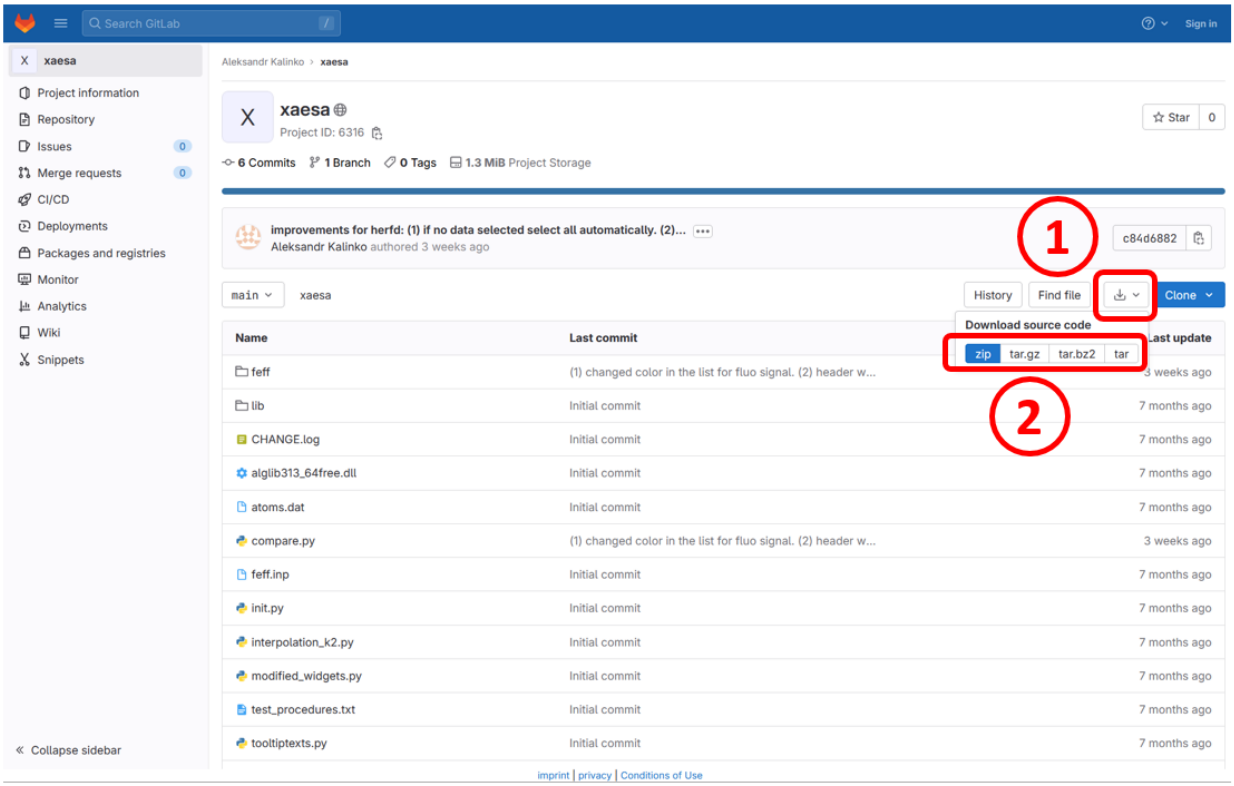
Select the version you need. For example, for Windows 10/11 select:

https://repo.anaconda.com/archive/Anaconda3-2020.07-Windows-x86_64.exe

Save and install.

2) Download XAESA code from

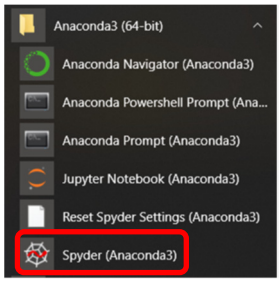
https://gitlab.desy.de/aleksandr.kalinko/xaesa



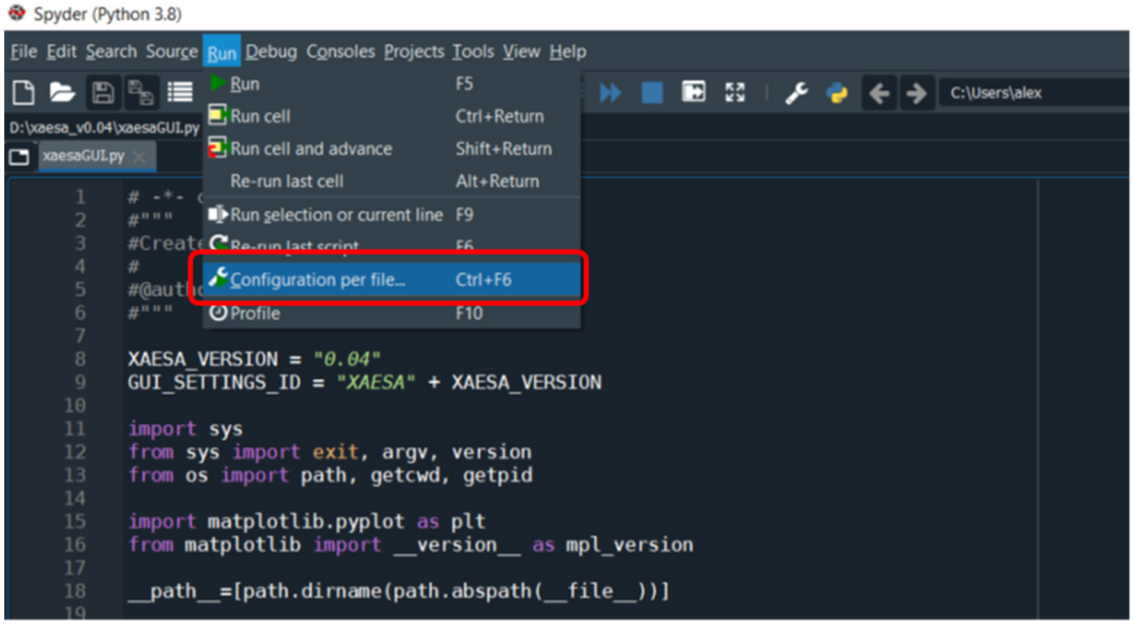
as a ZIP archive and unzip it in any directory.

How to run XAESA

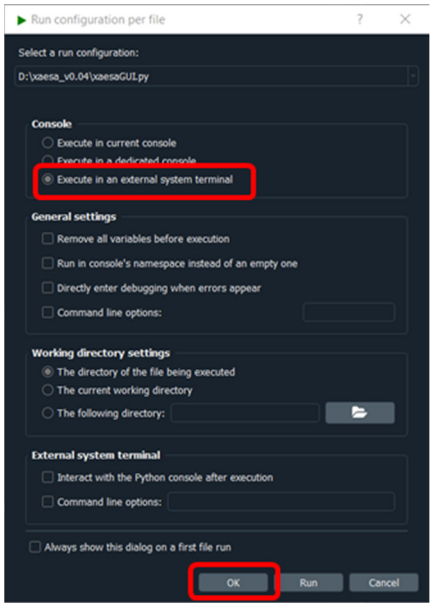
1) Open menu **Start, Anaconda3** and select **Spyder (Anaconda3)**



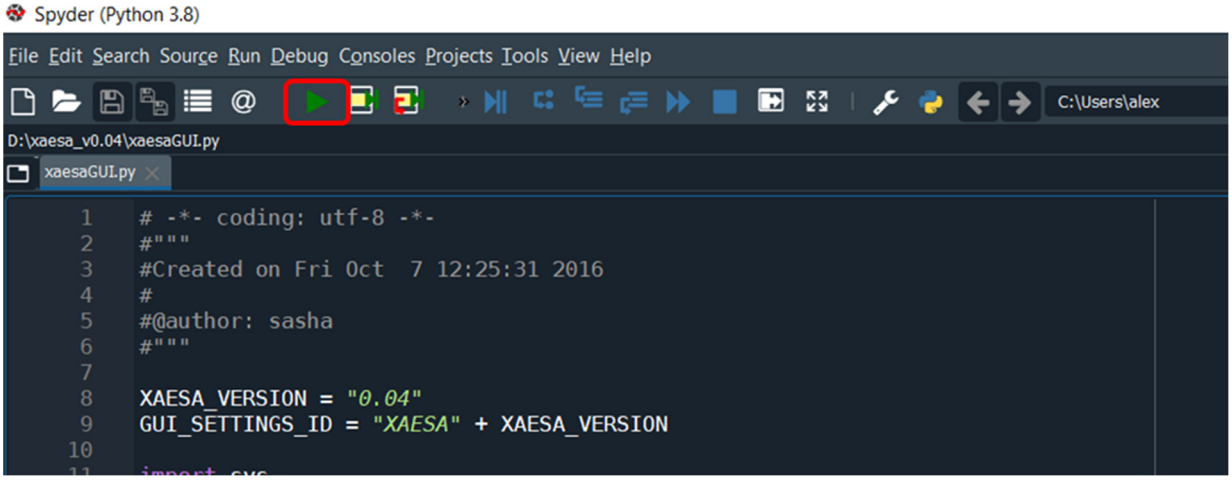
2) Open **xaesaGUI.py**, go to the menu **Run**, select **Configuration per file**



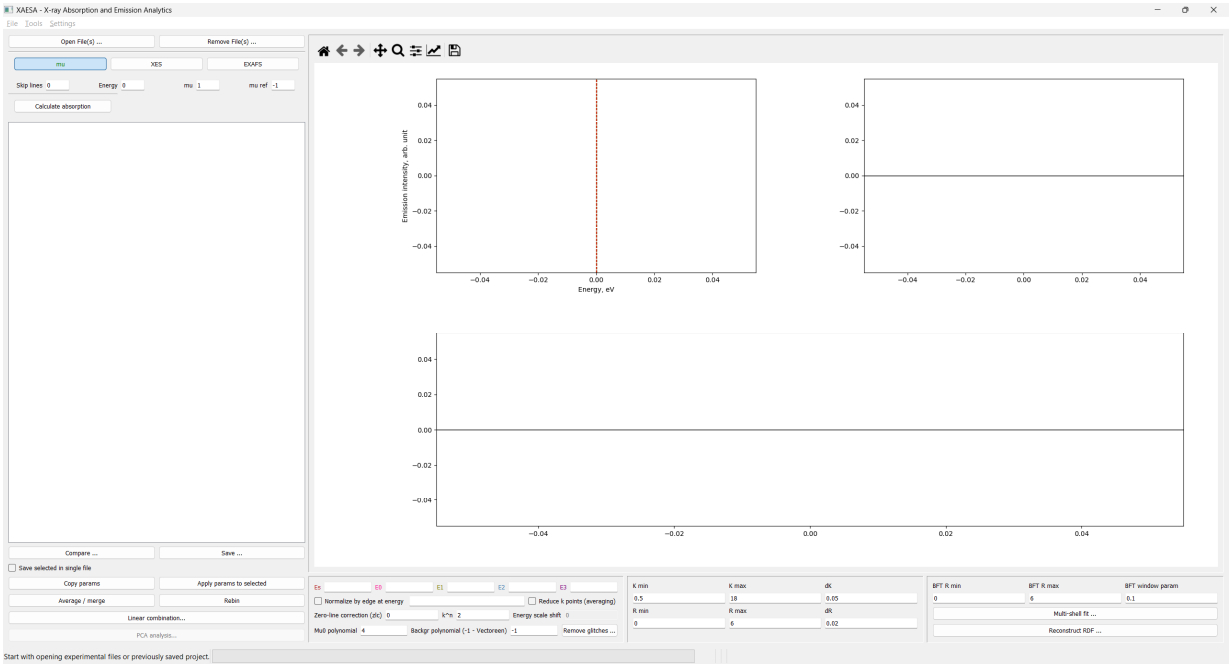
3) Select **Execute in an external system terminal** and click **OK**



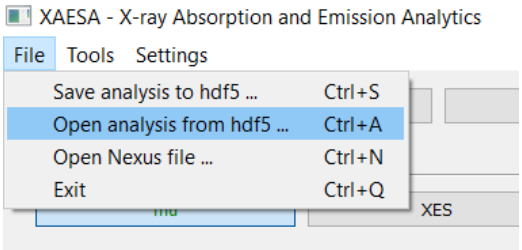
4) To run XAESA, click on 



5) XAESA will open in the external window



XAESA keeps all data in an HDF5 format file (*.hdf5), which can be saved and opened in the menu **File**:

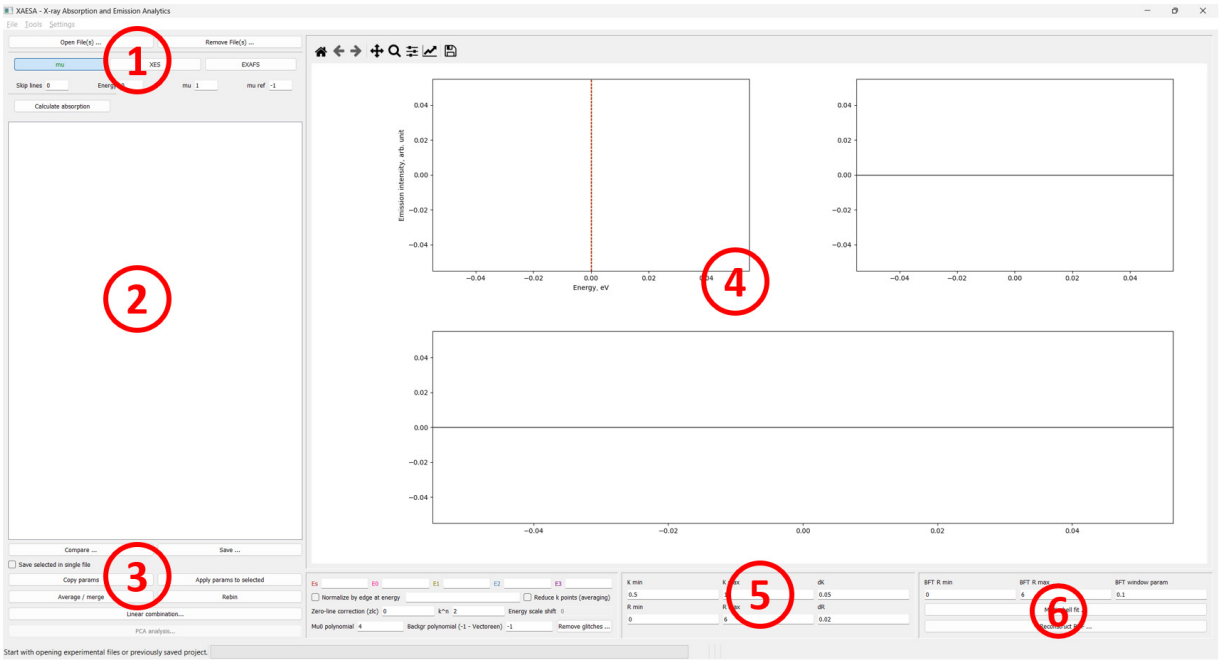


If necessary, it can be opened and manipulated using a viewer HDFView, which can be downloaded from here

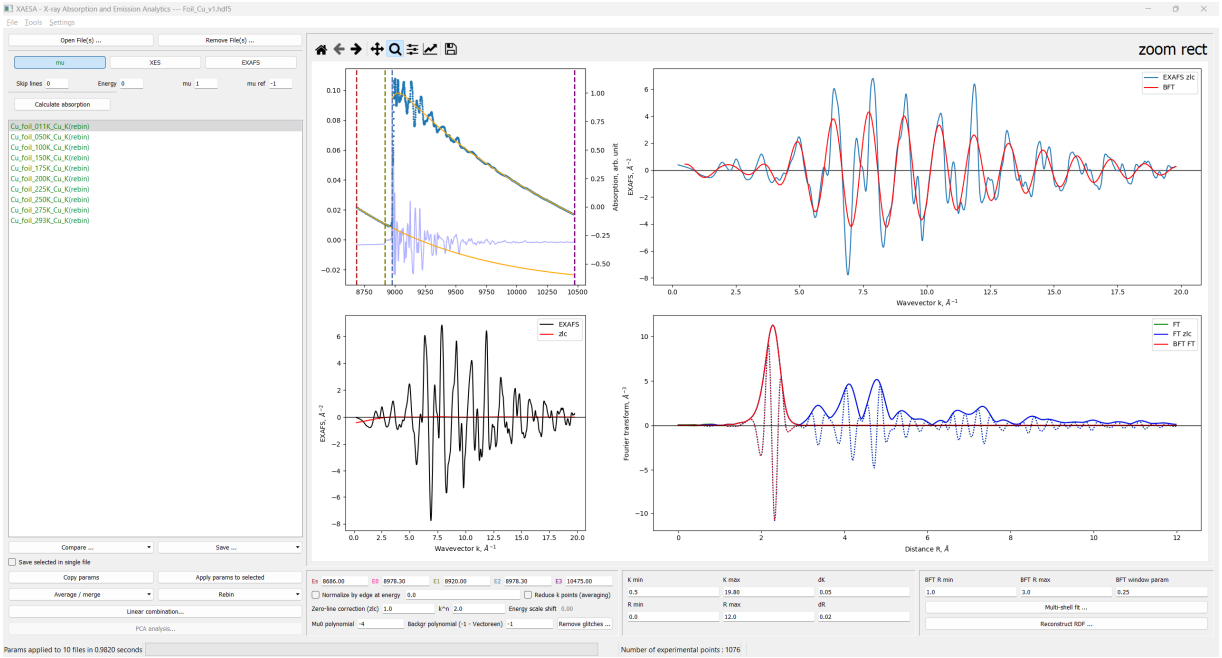
https://www.hdfgroup.org/downloads/hdfview/

The main parts of the XAESA screen

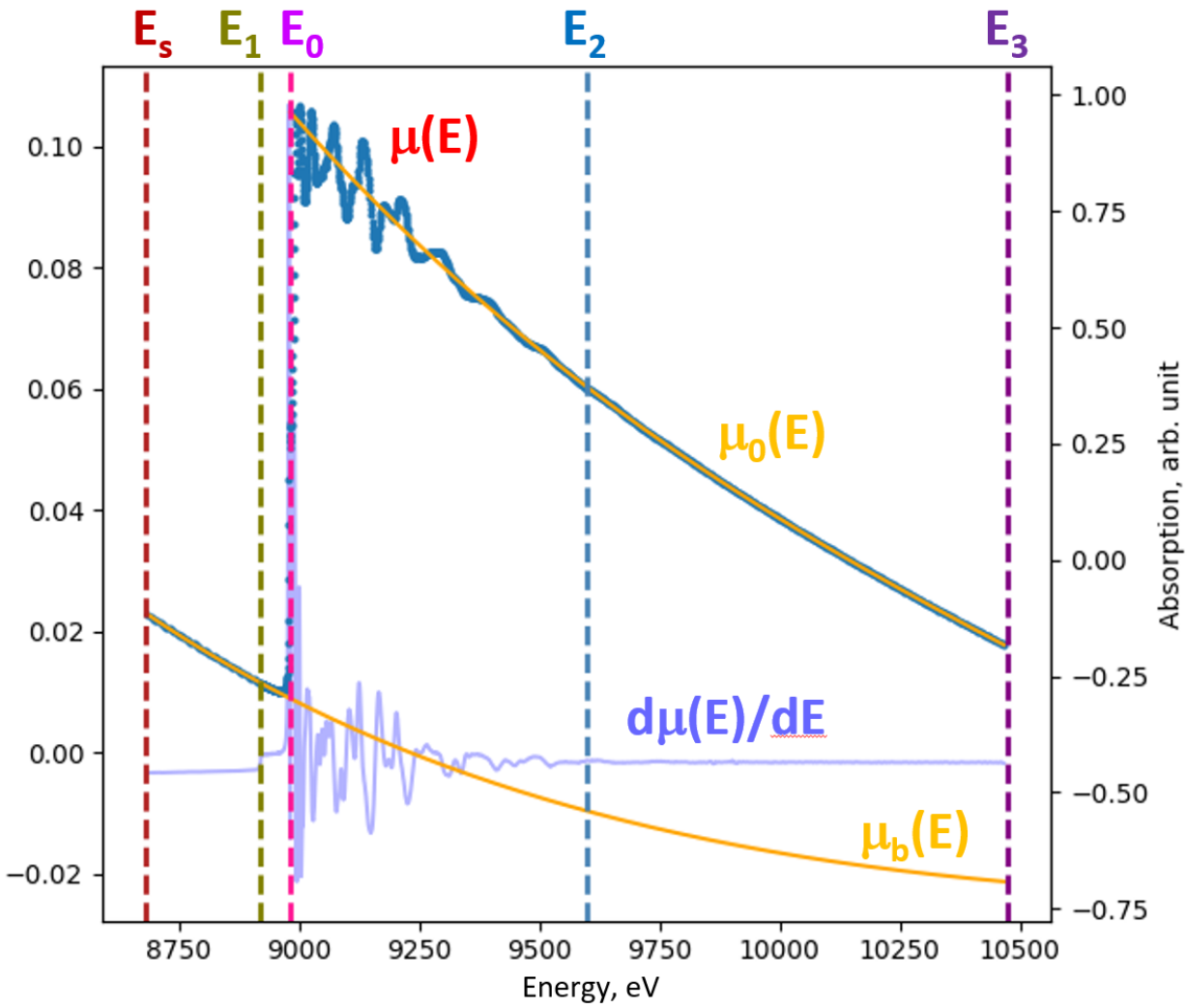
1) Menus to open experimental files in different formats.
2) Window with a list of opened files.
3) Menus to manipulate data.
4) Main graphical screen showing all data analysis.
5) Menus with parameters for data analysis.
6) EXAFS fitting using multi-component or regularization model.



Example of the analysis for the Cu K-edge in copper foil:



Definition of the main parameters for EXAFS extraction



EXAFS $\chi(E)$ is defined as

$$\chi(k)=(\mu(E)-\mu_b(E)-\mu_0(E))/\mu_0(E)$$

where photoelectron wavenumber k is defined as $k=(2m_e/\hbar^2\,(E-E_0))^{½}$.

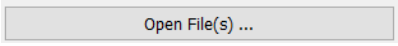
There are several important points to remember:

1) $\mu_0(E)$ can be corrected using the zero-line correction (zlc) parameter.
2) Normalization of EXAFS $\chi(k)$ can be done at specified energy.
3) EXAFS $\chi(k)$ can be multiplied by k^n (n=0,1,2,3).
4) Glitches can be removed, if present.

The Fourier transform (FT) of EXAFS $\chi(k)k^n$ is calculated from K_{min} to K_{max} with a step dK using the 10% Gaussian window. The FT range is defined by R_{min} and R_{max} with a step dR.

The inverse FT (back-FT) is calculated from BFT R_{min} to BFT R_{max} using the Hanning window with a BFT window parameter.

How to load data

There are several possibilities for how experimental or theoretical spectra can be loaded into XAESA using the button 

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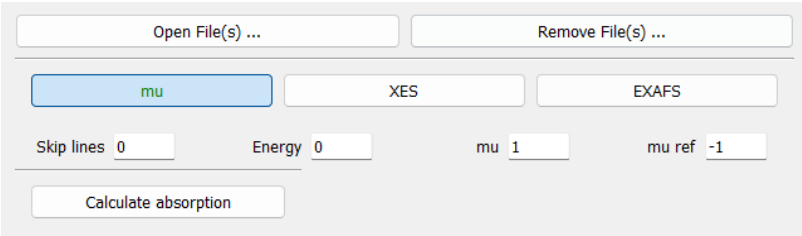
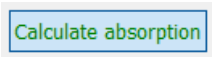
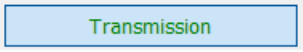
1) X-ray absorption coefficient μ(E) stored in a multi-column ASCII file can be loaded by, first, specifying the columns for the energy E and the absorption coefficient μ(E), and, next, by pressing the button 

:



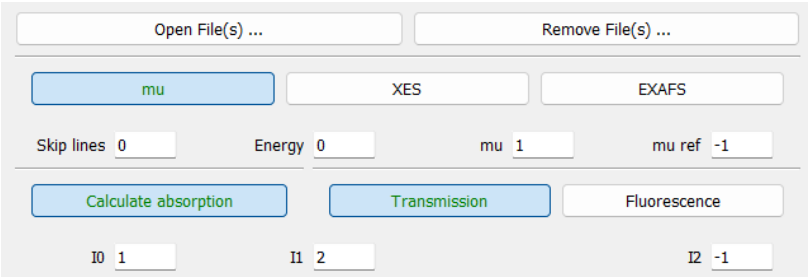
If necessary, one can skip several lines from the beginning of the file. N.B. All lines starting with "#" will be skipped automatically.

2) When experimental data are stored as signals from ionisation chambers, one needs to select 

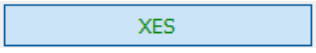
, the experimental mode (

or 

) and specify the columns for I0 and I1:



X-ray absorption coefficient will be automatically calculated as μ(E)=ln(I0(E)/I1(E)) for transmission or μ(E)=I1(E)/I0(E) for fluorescence.

3) X-ray emission spectrum (XES) can be loaded by selecting 

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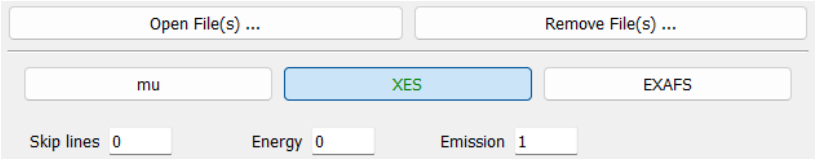
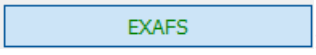
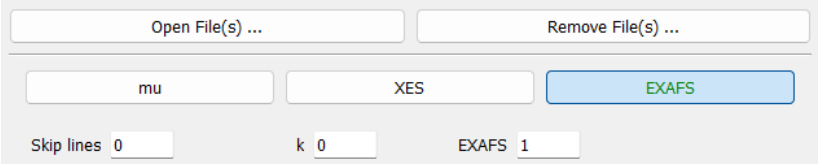
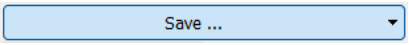


4) EXAFS spectrum χ(k) can be loaded by selecting 

:



How to export data

Absorption coefficient μ(E), XANES μ(E), EXAFS $\chi(k)k^n$, FT(R), and BFT $\chi(k)k^n$ spectra can be exported in an ASCII format by pressing the button 

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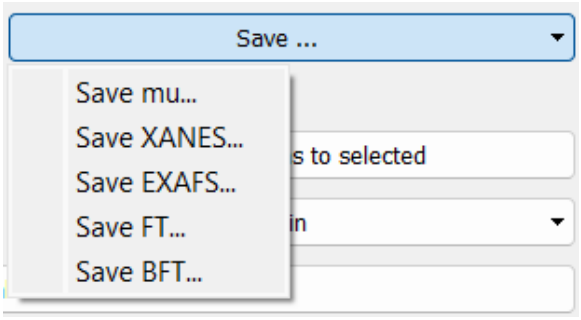
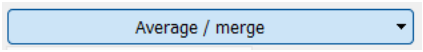
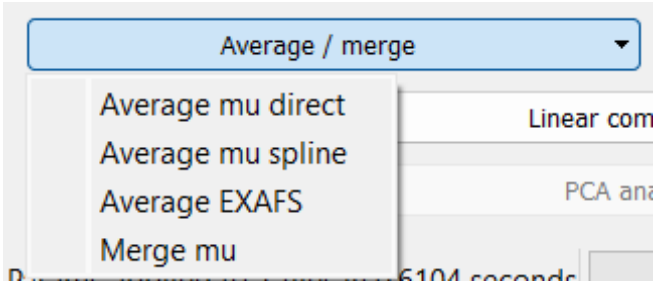


How to average/merge data

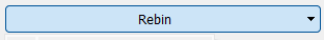
To average or merge several spectra, press the button 

and choose what to do:

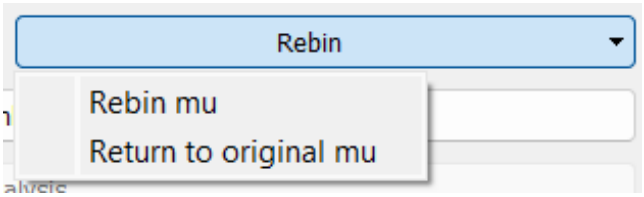


How to rebin data

Often original experimental spectra contain too many points, especially, at large energies. In this case, one can reduce the total number of points using the rebinning procedure.

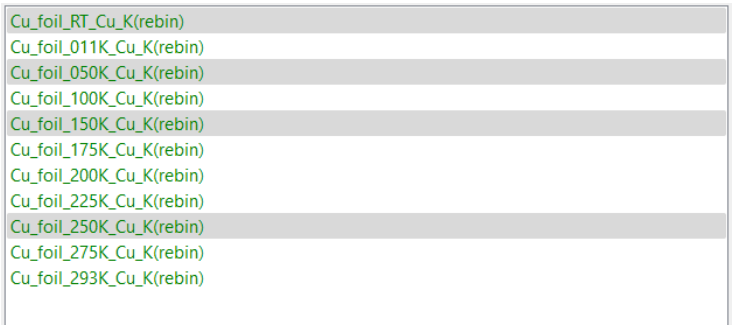
To do this, press the button 

and choose what to do:

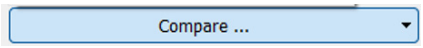


How to compare data sets

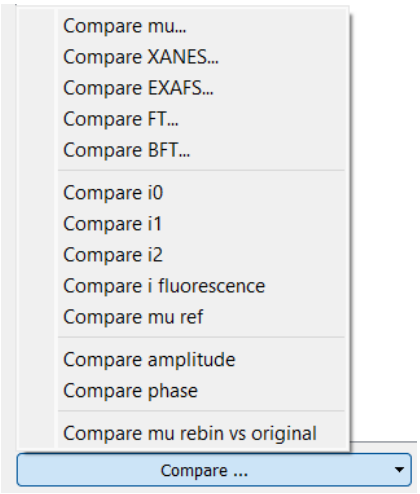
To compare several data sets, first select them in the window with a list of opened files:



This can be done by pressing CTRL + Mouse click.

Next, press the button 

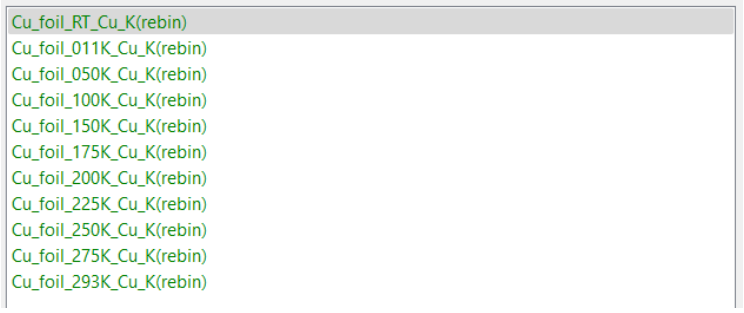
and choose what data to compare from the list:

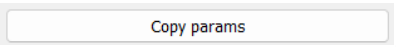


How to apply the parameters to another set(s) of data

The parameters of the analysis for a data set can be copied to Clipboard and applied to another data set(s). This is very convenient when many spectra should be analysed using the same set of parameters.

To do this, select a data set in the window with a list of opened files:



Press the button 

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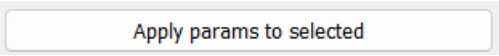
Next, select one or more data sets in the window with a list of opened files by pressing CTRL + Mouse click:

Press the button 

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How to perform a multi-shell fit

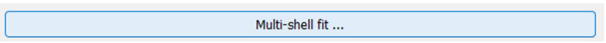
A multi-shell fit is based on an EXAFS equation:

$$\chi(k) = S_0^2 \sum_{i=1}^{M} \frac{N_i}{kR_i^2} f_l(\pi,k,R_i) \exp\left(-2\sigma_i^2 k^2 + \frac{2}{3}C_{4i}k^4 - \frac{4}{45}C_{6i}k^6\right) \exp\left(-\frac{2R_i}{\lambda(k)}\right) \times \sin\left(2kR_i - \frac{4}{3}C_{3i}k^3 + \frac{4}{15}C_{5i}k^5 + \phi_l(\pi,k,R_i) + 2\delta_c^l(k) - l\pi\right)$$

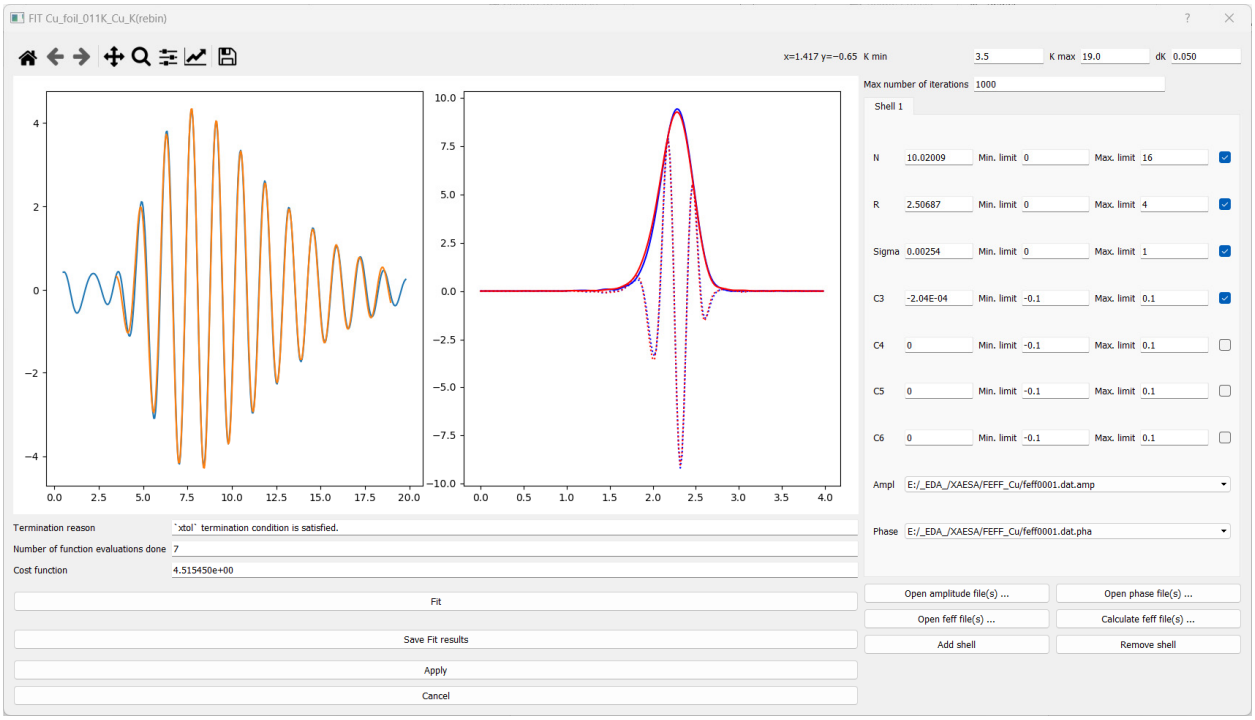
where

M - the number of coordination shells,
N_i - the coordination number of the *i*-shell,
R_i - the radius of the *i*-shell (the interatomic distance),
σ_i^2 - the mean square radial displacement (MSRD) (or the Debye-Waller factor) between the absorber and back-scatterer atoms located in the *i*-shell,
C_{ji} - the cumulants of the distribution, which account for anharmonic effects and non-Gaussian disorder,
S_0^2 - the scale factor, which accounts for the multielectron effects,
$\lambda(k)$ - the mean free path of the photoelectron,
$f_l(\pi,k,R_i)$ - the backscattering amplitude of the atoms in the *i*-shell,
$\phi_l(\pi,k,R_i)$ - the backscattering phase of the atoms in the *i*-shell,
$\delta_c^l(k)$ the absorbing atom phase shift,
l - the angular momentum of the photoelectron (l = 1 for K, L_1-edges and l = 2 or 0 for $L_{2,3}$-edges).

Note that $f_l(\pi,k,R_i)$, $\phi_l(\pi,k,R_i)$, $\delta_c^l(k)$, and $\lambda(k)$ functions must be calculated in advance using, for example, a FEFF code. As a result of such calculation, a set of feff*****.dat files should be obtained for all required shells.

To perform a multi-shell fit, press the button 

and the new window will open:

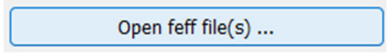


The window shows the experimental EXAFS spectrum by blue lines and the best-fitted EXAFS spectrum by orange and red lines in *k*- and *R*-space, respectively.

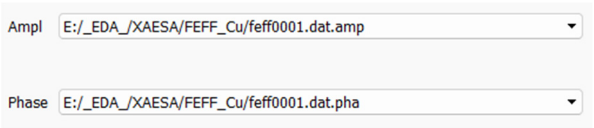
In this window, the parameters of the fit should be specified.

First, choose the required number of shells using two buttons:

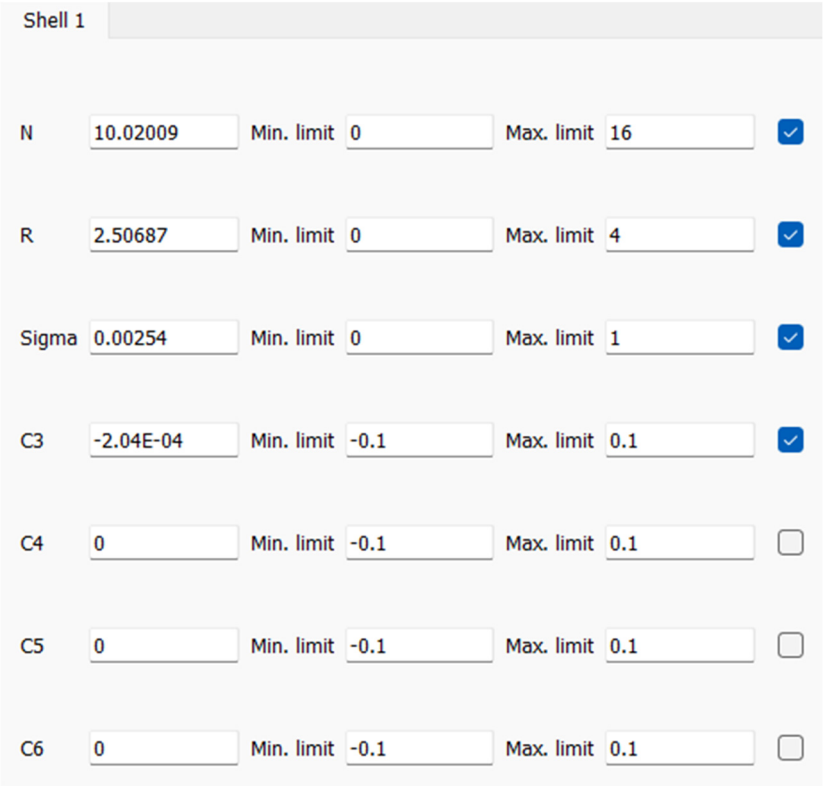
Next, for each shell:

- choose the feff*****.dat file with the information on the neighbouring atoms located in that shell using the button 

and select the required amplitude and phase shift functions from the dropdown lists:

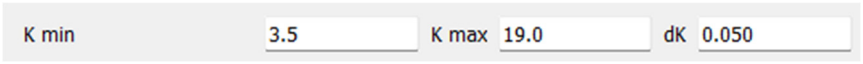


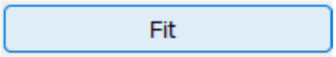
- set the initial, minimum and maximum allowed values for each structural parameter (N, R, σ^2 (≡ Sigma), Cj (j=3,4, 5,6) in the shell:



Use checkboxes at the right to fix (unchecked) or vary (checked) the required parameter.

Finally, the range of the fit in *k*-space should be set:



To start fitting, press the button 

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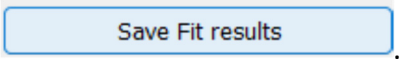
The results of the fit can be saved by pressing the button 

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How to reconstruct a radial distribution function (RDF)

This method allows one to reconstruct a radial distribution function (RDF) using the regularization-like method.

The EXAFS model is defined by the equation

$$\chi(k) = S_0^2 \int_{R_{\min}}^{R_{\max}} \frac{G(R)}{kR^2} F(\pi, k, R) \sin(2kR + \Phi(\pi, k, R)) \mathrm{d}R$$

where the coordination number is defined as

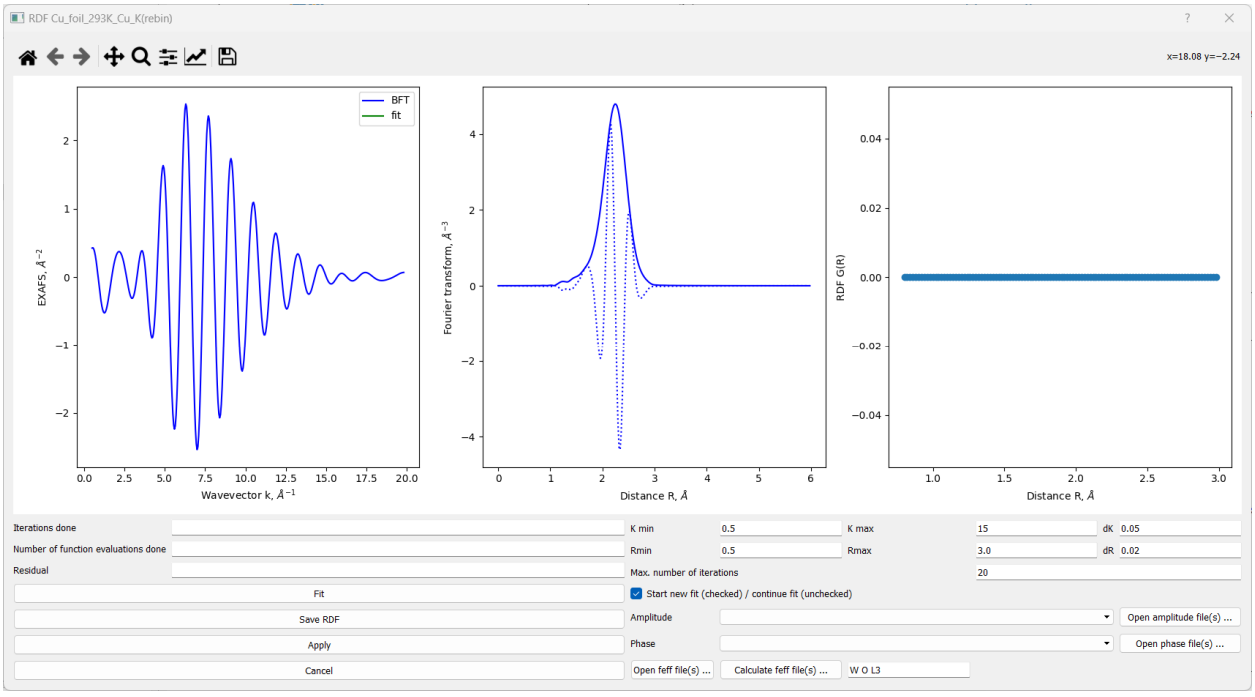
$$N = \int_{R_{\min}}^{R_{\max}} G(R) \mathrm{d}R$$

.

The method can be only used to fit the first coordination shell contribution containing atoms of one type. This method is useful when the first shell is distorted so that there is a distribution of close distances which cannot be resolved within the multi-shell model.

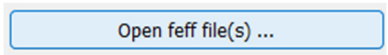
To perform a multi-shell fit, press the button 

and the new window will open:

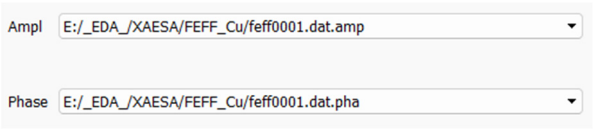


The window shows the experimental EXAFS spectrum by blue lines and the best-fitted EXAFS spectrum by green lines in *k*- and *R*-space, respectively. In addition, the true RDF is shown in the right panel by filled circles.

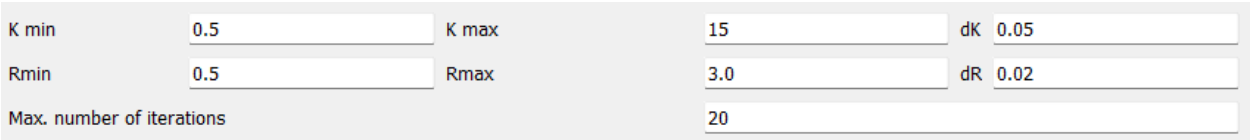
In this window, the parameters of the fit should be specified.

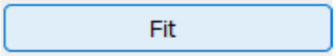
First, choose the feff*****.dat file with the information on the neighbouring atoms located in that shell using the button 

and select the required amplitude and phase shift functions from the dropdown lists



Next, set the range of the fit in *k*-space, the range of the RDF g(R) in *R*-space and the maximum number of iterations:



To start fitting, press the button 

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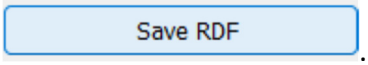
The results of the fit can be saved by pressing the button 

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