HAMA_Readme

hamaFortran.exe is a program designed to calculate the wavelet transform of EXAFS spectra and to reconstruct the spectra from the wavelet transform.
Model spectra or real EXAFS spectra may be processed. (A short description of the model function see below.)
Morlet or Cauchy mother wavelets may be used for the analysis.

Accompanying files:

Wgnuplot.exe is used for the visualization of the spectra, Fourier transforms, wavelets.
ModelParameters.txt contains the model function parameters. This file can be easily changed by any text editor.

Output files:

1. **function.txt** ASCII file contains two columns: k-values and corresponding weigthed signal (or model) values.
2. **Fourier.txt** ASCII file contains Fourier transform of the function under investigation (two columns: frequency and amplitude).
3. **meshr.txt** ASCII file contains the R-coordinates (two columns: number of points-R-coordinate).
4. **meshk.txt** ASCII file contains the k-coordinates (two columns: number of points-k-coordinate).
5. **parameters.txt** file contains all information used for the calculation (see parameters.txt file description).
6. **recon.txt** ASCII file contains three columns: k-coordinates, reconstructed signal from wavelet transform, initial signal.
7. **wavelet.txt** ASCII file contains two columns: number of point and value of scaled wavet function. It is used to demonstrate the scaling procedure. For three scaling parameter values the scaled wavelet functions are presented: 0, Rmax/2, Rmax.
8. **FFT_w.txt** ASCII file contains Fourier transform of a mother wavelet (two columns: frequency and amplitude).

The wavelet transform file is specified by the user in IGOR or ORIGIN format.

The IGOR-format file is a real array of size (3**kaxis*+1)*(*raxis*+1). In the *RedimensionWaves* command is to set New Rows: (3**kaxis*+1) and New Columns: (*raxis*+1).

The ORIGIN-format file cointains three columns *X* (*k*-values), *Y* (*R*-values) and *Z* (wavelet-values).

Then user can choose a working regime. There are the following regimes:

- to work with a model function (see Model function description),

OR

- to work with a real EXAFS spectrum,

AND

- to use Morlet mother wavelet (see Morlet wavelet),

OR

- to use Cauchy mother wavelet (see Cauchy wavelet).

After choice of the regime, the calculations are done sequentially in the following steps:

1. Weighted signal or model is plotted.
2. Fast Fourier transform of the function under investigation is calculated and plotted.
3. Choice of the *R*-region under interest limits is done by the user (➔input *Rmin* and *Rmax in dialog*).
4. Mother wavelet function is plotted to demonstrate a scaling procedure.
5. Direct wavelet transform is calculated using the trapezoidal-rule for the integration.
6. Inverse wavelet transform is calculated.

Model function description

The model function is given below. This is a sum of two sinuses modulated by Gaussian.

$$signal = part1 + part2$$

$$part1 = ampli1 * \frac{1}{\sqrt{2\pi}\,sigma1} \exp^{-\frac{(k-centrum1)^2}{2sigma1^2}} * \sin\left(frequency1 * [k - phase1]\right)$$

$$part2 = ampli2 * \frac{1}{\sqrt{2\pi}\,sigma2} \exp^{-\frac{(k-centrum2)^2}{2sigma2^2}} * \sin\left(frequency2 * [k - phase2]\right)$$

All parameters are given in the **ModelParameters.txt** file. You can change very easily the parameters using any text-editor .

Parameters.txt file description

The file parametes contains the following information

- Input file name given by User,
- Number of points in the experimental spectrum or model function,
- The first k-value
- The last k.value
- k-step value
- Parameters of a mother wavelet function
- Output file name given by User
- K-poins number where WL transform is calculated (3 times initial number)
- R-points number
- Min k-value on new interval
- Max k-value on new interval
- R-min value
- R-max value

Morlet wavelet

$$\psi(t) = \frac{1}{\sqrt{2\pi}\sigma}\left(\exp(i\kappa t) - \exp\left(-\frac{\kappa^2}{2}\right)\right)\exp\left(-\frac{t^2}{2\sigma^2}\right)$$

κ and σ are the program parameters kappaMorlet and sigmaMorlet.

Chauchy wavelet

$$\psi(t) = \left(\frac{i}{i+k}\right)^{n+1}$$

n is the program parameter nResolut.

Recommendations for the use of the Morlet wavelet:

κ is the frequency of the sine- and cosine functions. It is a free wavelet parameter which indicates how much oscillations of the sine wave are covered by a Gaussian envelope with the half-width σ=1. So, for beginning it is useful to set σ=1.
One property of κ is obviously. For a great number of κ the R dependency of the WT will be similar to the FT. The choice of e.g. κ=15 is useful to obtain an overview-WT over the whole spectrum.
For a good resolution of the WT for a certain critical distance R_{crit} it is recommended to choose $\kappa = 2R_{crit}$. Then the user may try to go to lower values of κ to get better resolution on the k-axis.