Guide for wtEXAFS

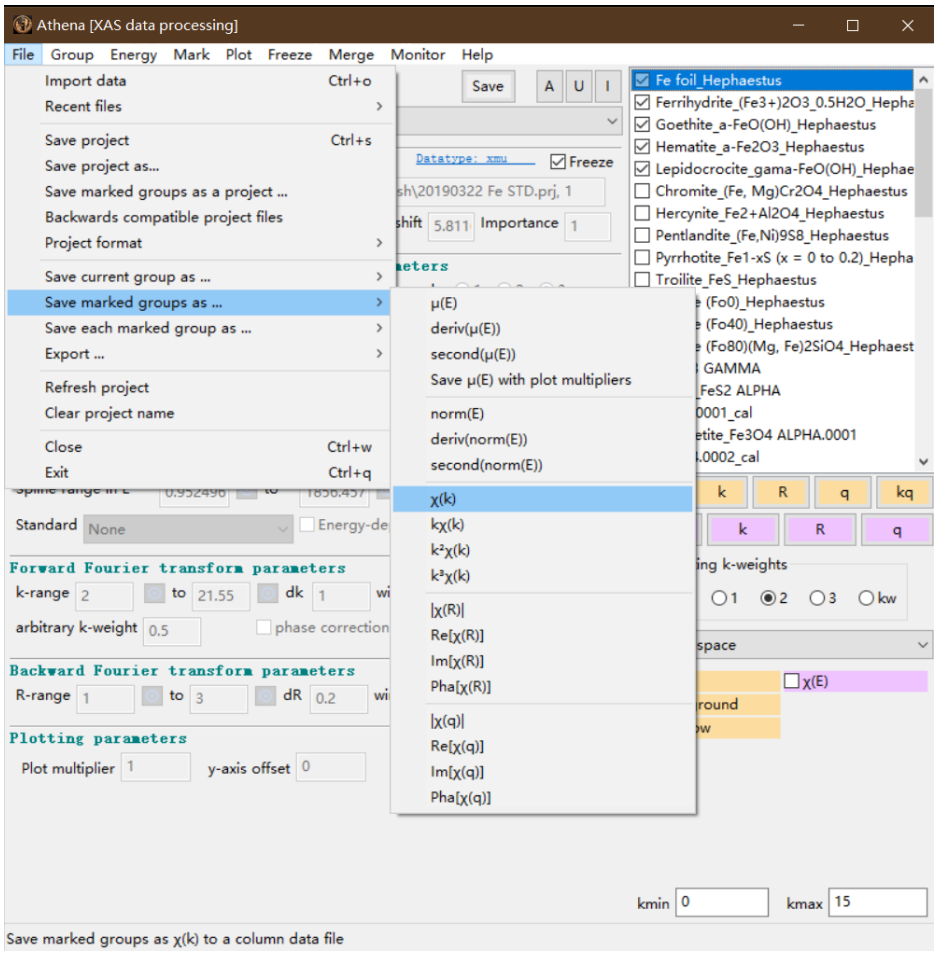
1. Start wtEXAFS

EXAFS is a powerful technique for detecting the local environment of atoms in different materials. EXAFS is a composite signal of electron waves, which is well suited for analysis using wavelet transform. Although it is difficult to gain quantitative results from wavelet transformation of EXAFS signal, wavelet transformation can still give more information to help us carry out k-space LCF, EXAFS modeling, and so on.

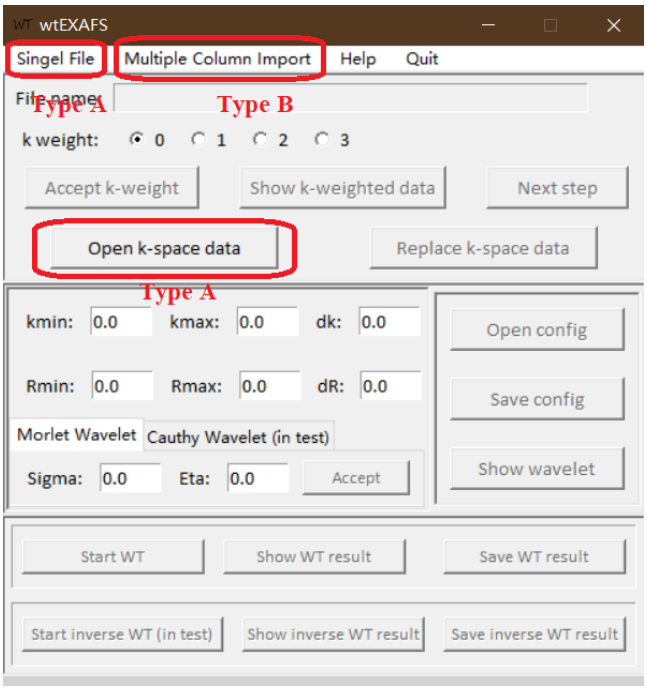
wtEXAFS is a Windows GUI for wavelet transformation of EXAFS. Let's start.

1.1 Import chi(k) data

- Firstly, it is highly recommended to import the *.chi file in wtEXAFS for wavelet transformation. And *.chi file can be extracted from ATHENA (Ravel and Newville, 2005) as shown:



- The main window of wtEXAFS is displayed as follows and data can be imported by clicking the button highlighted by red box. There are two ways to import data, namely Type A and Type B:



- Type A -- Single file mode:
  - Open *.txt/.chi file containing at least two column, one column is k, the other column is chi(k):

model.txt - 记事本

文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)

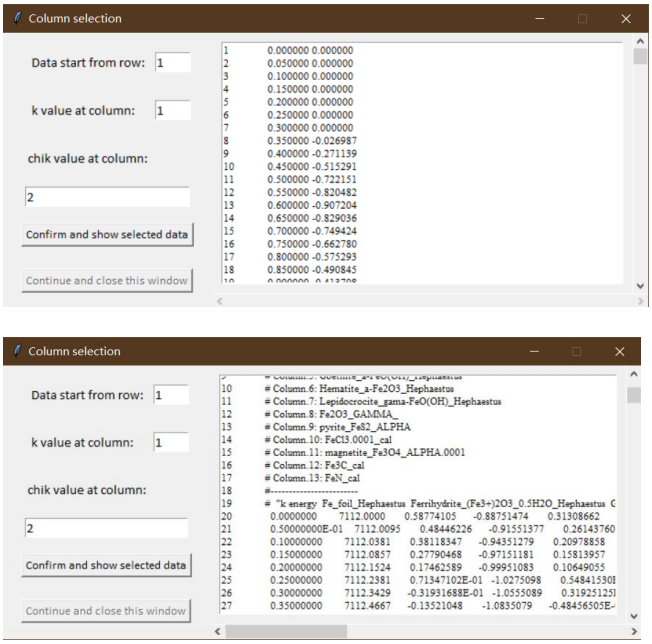
```
0.000000 0.000000
0.050000 0.000000
0.100000 0.000000
0.150000 0.000000
0.200000 0.000000
0.250000 0.000000
0.300000 0.000000
0.350000 -0.026987
0.400000 -0.271139
0.450000 -0.515291
0.500000 -0.722151
0.550000 -0.820482
0.600000 -0.907204
0.650000 -0.829036
0.700000 -0.749424
0.750000 -0.662780
0.800000 -0.575293
0.850000 -0.490845
0.900000 -0.413708
0.950000 -0.347966
1.000000 -0.292486
1.050000 -0.242646
1.100000 -0.191963
1.150000 -0.134659
1.200000 -0.067808
1.250000 0.004466
1.300000 0.073148
1.350000 0.126150
1.400000 0.154205
1.450000 0.164314
1.500000 0.156104
1.550000 0.143429
1.600000 0.135881
```

model.chi - 记事本

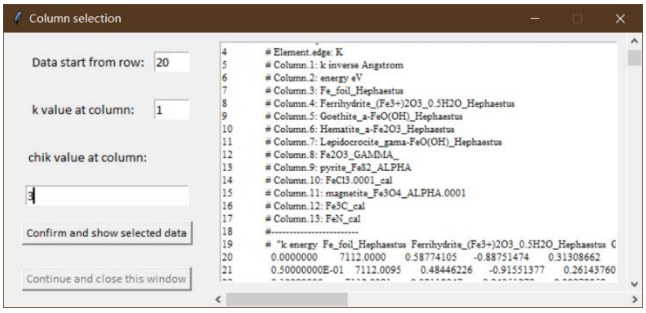
文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)

```
# XDI/1.0 Demeter/0.9.26
# Demeter.output_filetype: multicolumn chi(k)
# Element.symbol: Fe
# Element.edge: K
# Column.1: k inverse Angstrom
# Column.2: energy eV
# Column.3: Fe_foil_Hephaestus
# Column.4: Ferrihydrite_(Fe3+)2O3_0.5H2O_Hephaestus
# Column.5: Goethite_a-FeO(OH)_Hephaestus
# Column.6: Hematite_a-Fe2O3_Hephaestus
# Column.7: Lepidocrocite_gama-FeO(OH)_Hephaestus
# Column.8: Fe2O3_GAMMA_
# Column.9: pyrite_FeS2_ALPHA
# Column.10: FeCl3.0001_cal
# Column.11: magnetite_Fe3O4_ALPHA.0001
# Column.12: Fe3C_cal
# Column.13: FeN_cal
#-------------------------
#  "k energy  Fe_foil_Hephaestus  Ferrihydrite_(Fe3+)2O3_0.5H2O_Hephaestus  G
pyrite_FeS2_ALPHA  FeCl3.0001_cal  magnetite_Fe3O4_ALPHA.0001  Fe3C_ca
  0.0000000       7112.0000      0.58774105      -0.88751474       0.31308662
  0.50000000E-01  7112.0095      0.48446226      -0.91551377       0.26143760
  0.10000000      7112.0381      0.38118347      -0.94351279       0.20978858
  0.15000000      7112.0857      0.27790468      -0.97151181       0.15813957
  0.20000000      7112.1524      0.17462589      -0.99951083       0.10649055
  0.25000000      7112.2381      0.71347102E-01  -1.0275098        0.54841530E-
  0.30000000      7112.3429      -0.31931688E-01 -1.0555089        0.31925125E-
  0.35000000      7112.4667      -0.13521048     -1.0835079        -0.48456505E-01
0.22601724
  0.40000000      7112.6096      -0.23848927     -1.0524444        -0.10010552
  0.45000000      7112.7715      -0.34176806     -1.0021137        -0.15175454
  0.50000000      7112.9525      -0.39764211     -0.95178307       -0.21558383
  0.55000000      7113.1525      -0.43671904     -0.89223414       -0.28924476
```

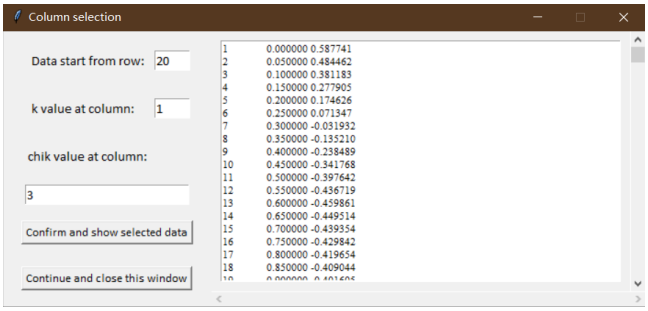
✧ In wtEXAFS data import window, the line number will be displayed at the left of the data display box. And it would look like this:



✧ The user can specify in the input box the **row** where the data starts and the **column** where k, chi(k) resides. For example:

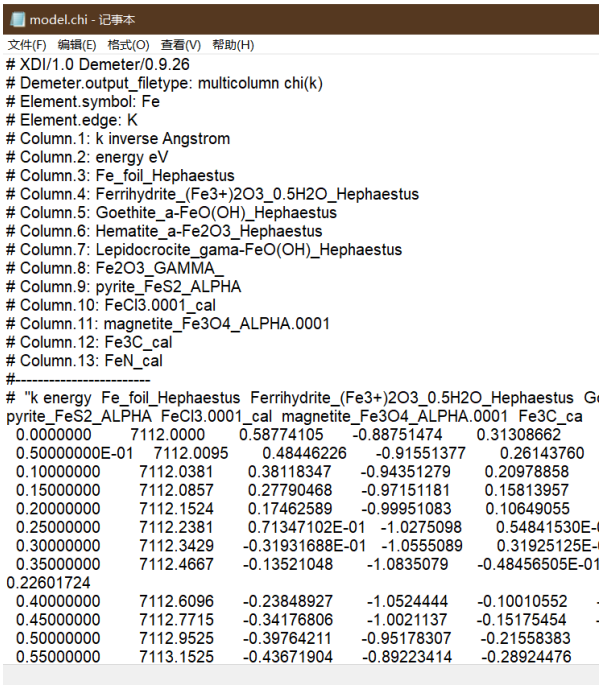


✧ Then click **"Confirm and show selected data"**, the box will refresh:

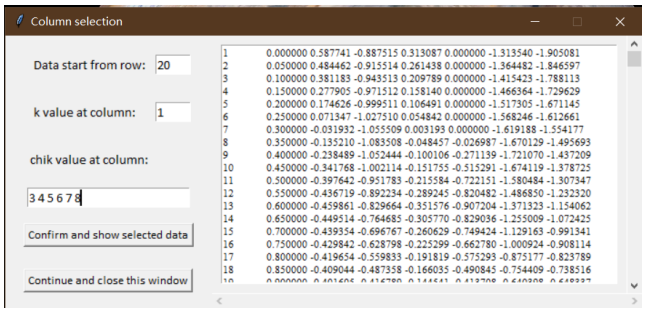


✧ Then click **"Continue and close this window"**. The Column selection window will be closed and back to the main window.

- Type B -- Multiple column mode:
  - **Only** open the *.chi file containing at least two columns, one column is k, the other columns are different chi(k):



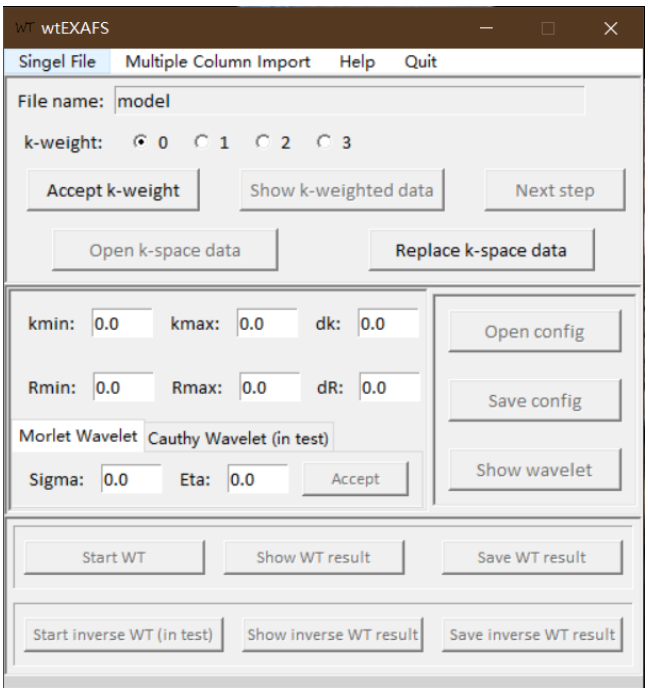
  - In this mode, the user can specify in the input box the row where the data starts and the column where k, chi(k) resides. For the chi(k) column, enter **SPACE** to separate different columns:



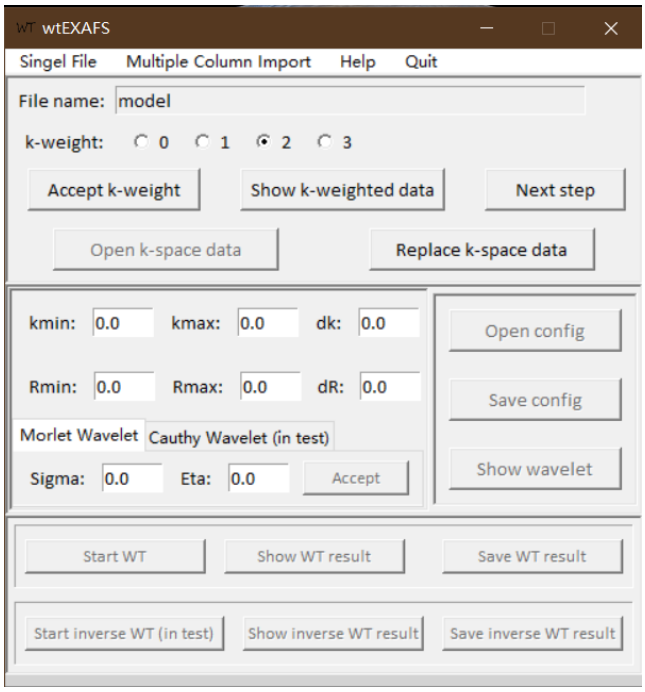
  - Other operations are the same as Single file mode.

1.2 k-weight selection

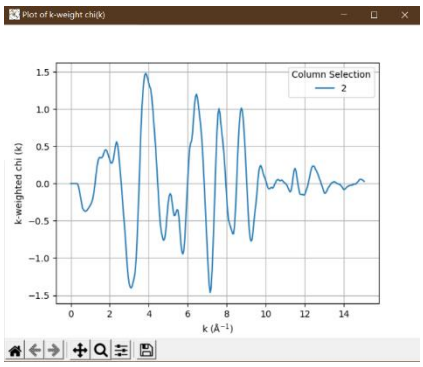
- Once **"Continue and close this window"** button was clicked, The Column selection window will be closed and back to the main window. Now, the filename will be displayed and **"k-weight"** selection and **"Accept k-weight"** button will be available:

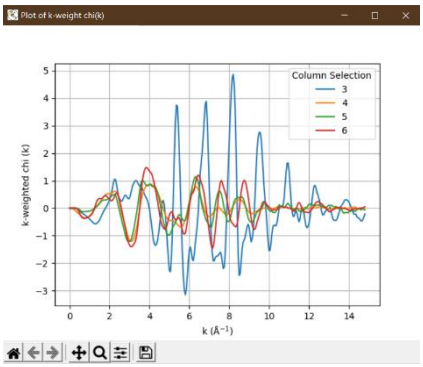


- Choose **"k-weight"**: if the imported data is k-weighted (e.g., k^3chi(k)), select k-weight to 0. If the imported data is not k-weighted, choose k-weight from 1, 2, and 3. And then, click **"Accept k-weight":**

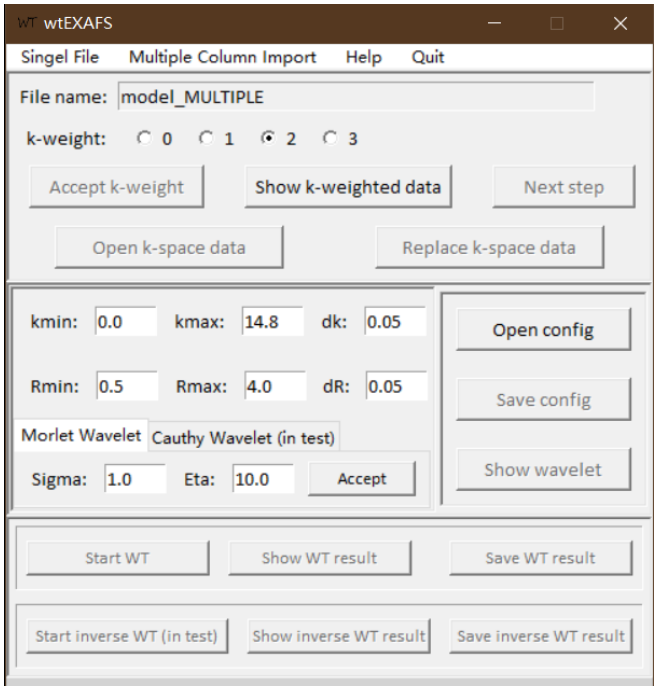


- Now, the **"Show k-weighted data"** and **"Next step"** buttons will be available. That is ok to show the data:





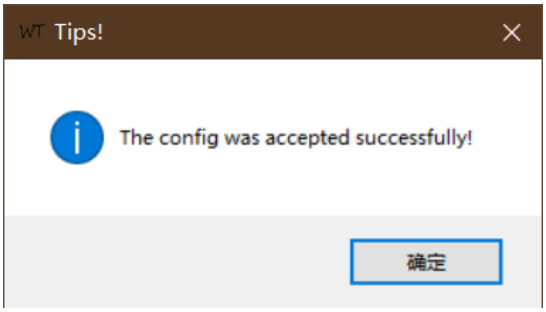
➢ Then click **"Next step"** and typing in parameters is available now:

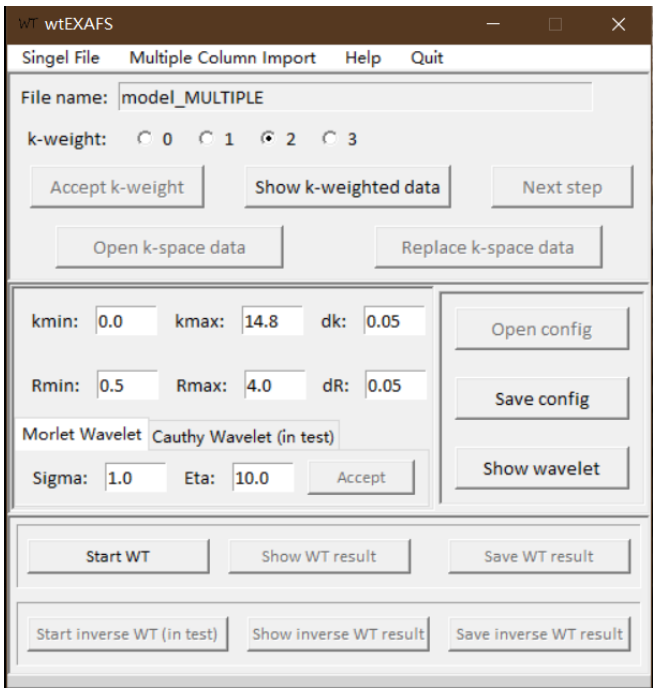


1.3 Custom wavelet transformation parameters

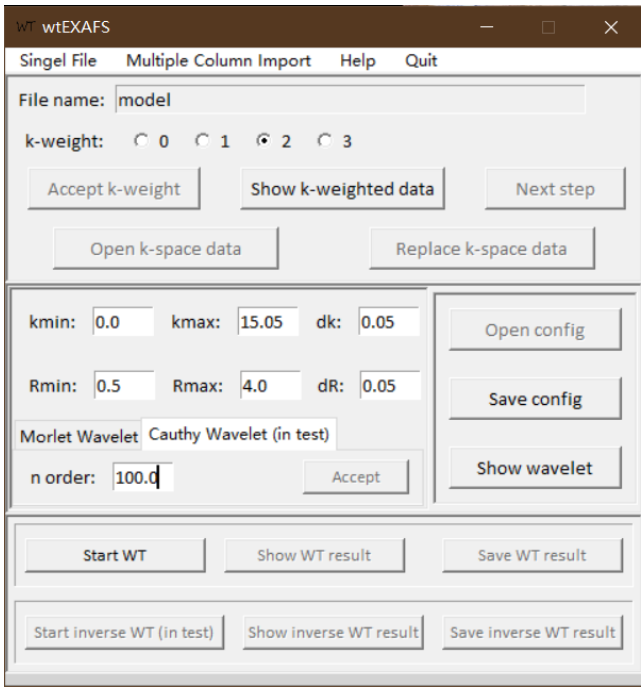
➢ Enter **kmin/kmax/dk**, **Rmin/Rmax/dR** in the input box.

➢ Enter **Sigma/Eta** in the **Morlet Wavelet** page and then **"Accept"** it. Once **"Accept"**, a message box will popup:

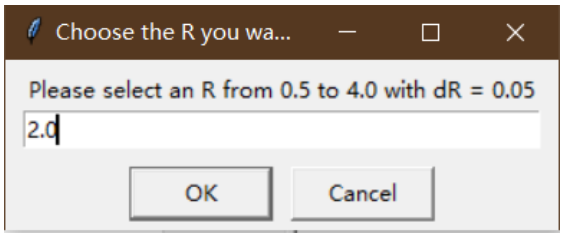


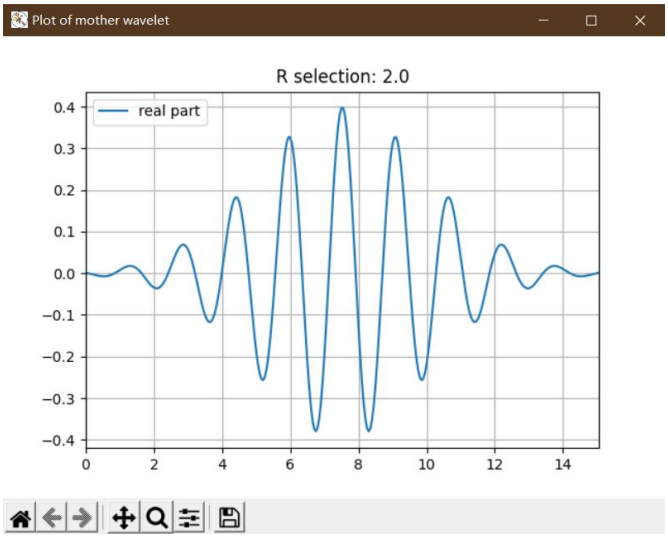


- Or Enter **norder** in the **Cauchy Wavelet** input box and then **"Accept"** it



- The **"Save config"** button will be available, the user can click it to save what they typed in.
- And the **"Show wavelet"** will be available. The user can enter different R to show different daughter wavelets from **Rmin** to **Rmax** with **dR**:



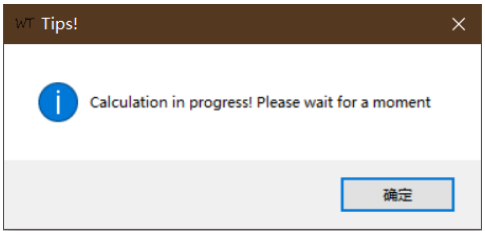


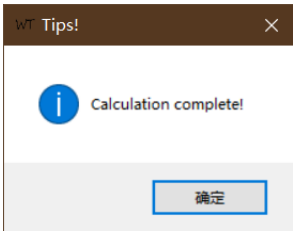
➢ **NOTICE:**

- ✓ **kmin** and **kmax** must be within the data range
- ✓ **Rmin** and **Rmax** must be > 0
- ✓ **Sigma** and **Eta** must be > 0
- ✓ **norder** must be > 1
- ✓ if not sure, the default value is ok
- ✓ If the input **dk** does not match the imported data, interpolation will be automatically performed

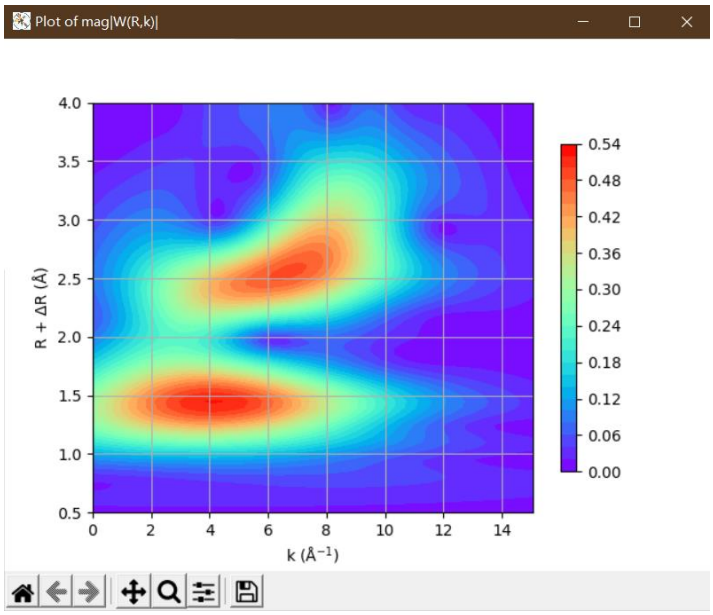
1.4 Start wavelet transformation

➢ Now, **"Start WT"** button will be available, click it to start calculation (usually takes 3 to 5s), and two message boxes will popup:





- After that, **"Show WT result"** will be available, click it:



- And **"Save WT result"** will be available, click it. An output file will be created as a TXT file, with internal structure as follows (**on left: Single file mode; on right: Multiple column mode, coef_3 is the wavelet coefficient for data from column 3 in the original data file**):

wt_model.txt - 记事本

文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)

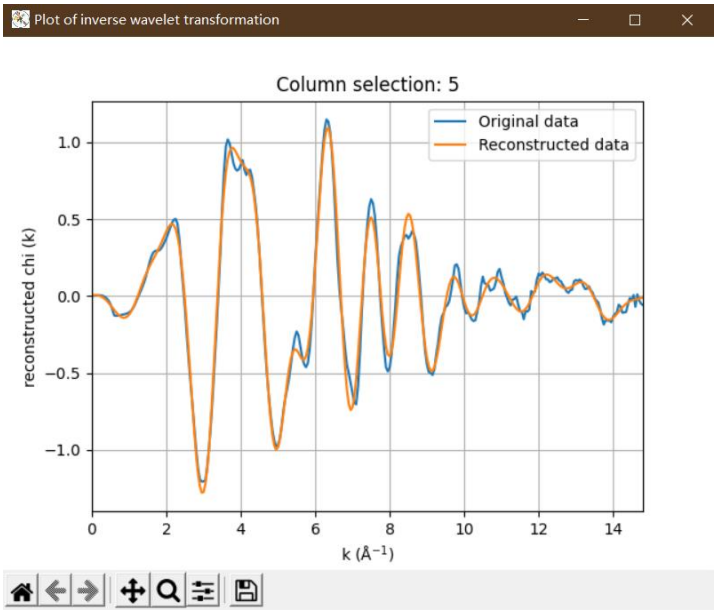
```
-8.000000 0.500000 0.012605
-7.950000 0.500000 0.011638
-7.900000 0.500000 0.010870
-7.850000 0.500000 0.010491
-7.800000 0.500000 0.010483
-7.750000 0.500000 0.010720
-7.700000 0.500000 0.011091
-7.650000 0.500000 0.011481
-7.600000 0.500000 0.011773
-7.550000 0.500000 0.011863
k_value R_value wavelet_coef
-7.400000 0.500000 0.010832
-7.350000 0.500000 0.010284
-7.300000 0.500000 0.009715
-7.250000 0.500000 0.009142
-7.200000 0.500000 0.008598
-7.150000 0.500000 0.008144
-7.100000 0.500000 0.007847
-7.050000 0.500000 0.007711
-7.000000 0.500000 0.007717
-6.950000 0.500000 0.007932
-6.900000 0.500000 0.008475
-6.850000 0.500000 0.009448
-6.800000 0.500000 0.010836
-6.750000 0.500000 0.012484
-6.700000 0.500000 0.014208
-6.650000 0.500000 0.015796
-6.600000 0.500000 0.017066
-6.550000 0.500000 0.017943
-6.500000 0.500000 0.018345
-6.450000 0.500000 0.018250
-6.400000 0.500000 0.017632
```

wt_model_MULTIPLE.txt - 记事本

文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)

```
-8.000000 0.500000 0.090303 0.010383 0.003708 0.014085
-7.950000 0.500000 0.091110 0.010422 0.004116 0.013644
-7.900000 0.500000 0.091861 0.010463 0.004870 0.012785
-7.850000 0.500000 0.092552 0.010507 0.005792 0.011796
-7.800000 0.500000 0.093201 0.010547 0.006696 0.011010
-7.750000 0.500000 0.093825 0.010579 0.007393 0.010623
-7.700000 0.500000 0.094429 0.010597 0.007781 0.010616
-7.650000 0.500000 0.095007 0.010600 0.007788 0.010860
-7.600000 0.500000 0.095533 0.010593 0.007482 0.011240
-7.550000 0.500000 0.096017 0.010580 0.006884 0.011639
-7.500000 0.500000 0.096587 0.010562 0.006050 0.011937
k_value R_value  coef_3  coef_4  coef_5  coef_6
-7.350000 0.500000 0.101728 0.010532 0.003606 0.011490
-7.300000 0.500000 0.105766 0.010550 0.003205 0.010968
-7.250000 0.500000 0.111247 0.010596 0.003085 0.010406
-7.200000 0.500000 0.117799 0.010693 0.003323 0.009823
-7.150000 0.500000 0.124638 0.010851 0.003841 0.009237
-7.100000 0.500000 0.130588 0.011076 0.004480 0.008681
-7.050000 0.500000 0.134382 0.011375 0.005183 0.008217
-7.000000 0.500000 0.135105 0.011742 0.005952 0.007915
-6.950000 0.500000 0.133013 0.012173 0.006738 0.007779
-6.900000 0.500000 0.129583 0.012663 0.007481 0.007784
-6.850000 0.500000 0.126166 0.013180 0.008258 0.008001
-6.800000 0.500000 0.123459 0.013696 0.009090 0.008551
-6.750000 0.500000 0.121513 0.014190 0.009889 0.009541
-6.700000 0.500000 0.119929 0.014624 0.010604 0.010955
-6.650000 0.500000 0.118419 0.014961 0.011128 0.012636
-6.600000 0.500000 0.117090 0.015174 0.011396 0.014393
-6.550000 0.500000 0.116097 0.015259 0.011410 0.016012
-6.500000 0.500000 0.115425 0.015229 0.011138 0.017306
-6.450000 0.500000 0.114889 0.015100 0.010641 0.018199
-6.400000 0.500000 0.114120 0.014877 0.010040 0.018608
```

- If needed, click **"Start inverse WT"** to reconstruct EXAFS spectra according to wavelet type and WT result. **However, the current algorithm may be a bit of problems, because the way of reconstruction is not the same as the formula of inverse wavelet transformation, and the author doesn't know why it works** :(



2. More details about wtEXAFS (to be continued)

In this section, some details about wtWXAFS will be shown.

2.1 A list of files generated during the program running

As the program runs, the following files in the **resources** folder will be created:

- **col_selection.txt**

  A single-column file that records the column selection.

- **energy_coef.txt**

  A single-column file records the value of $\sqrt{2R/\eta}$ (for Morlet wavelet) or $\sqrt{2R/n}$ (Cauchy wavelet). Each value represents a different R.

- **mesh.txt**

  A single-column file records the shape of the wavelet coefficient matrix.

- **temp_iWT.txt**

  A multi-column file records k values and reconstructed chi(k) values.

- **temp_k.txt**

  A multi-column file records k values and original chi(k) values.

- **temp_kW.txt**

  A multi-column file records k values and k-weighted chi(k) values.

- **temp_kWforWT.txt**

  A multi-column file records k values and user-defined k-weighted Chi (k) values (zero fill).

- **temp_MotherWavelet.txt**

  A multi-column file records "wavelet family" with different R and k. The rows are the direction in which R increases, and the columns are the direction in which k increases.

- **temp_paras.txt**

A file records the input parameter.

- **temp_WT.txt**

  A multi-column file records k values, R values, and wavelet coefficients (modulus).

- **temp_WT_c.txt**

  A multi-column file records k values, R values, and wavelet coefficients (complex number).

- **wavelet_fft.txt**

  A multi-column file records R values and Fourier transformed mother wavelet values (modulus).

2.2 Some important formulas

- **Morlet Wavelet**

  The complex Morlet wavelet is shown as:

$$\Psi(k') = \frac{1}{\sqrt{2\pi}\sigma}(e^{i\eta k'} - e^{\left(\frac{-\eta^2\sigma^2}{2}\right)})e^{\left(\frac{k'^2}{2\sigma^2}\right)}$$

  In wtEXAFS, the equation is simplified for $e^{\left(\frac{-\eta^2\sigma^2}{2}\right)}$ is smaller than 10^{-21} if $\eta\sigma > 10$, and can be ignored in most cases:

$$\Psi(k') = \frac{1}{\sqrt{2\pi}\sigma}e^{i\eta k'}e^{\left(\frac{k'^2}{2\sigma^2}\right)}$$

  The parameter σ (**Sigma in wtEXAFS**) is the half-width of the Gaussian envelope, and the parameter η (**Eta in wtEXAFS**) determines the oscillations of the wave.

- **Cauchy Wavelet**

  The complex Cauchy wavelet is shown as:

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

  The Cauchy parameter n controls the resolutions (**norder in wtEXAFS**).

➢ **Continuous wavelet transformation**

The wavelet transformation of the k^n-weighted EXAFS spectrum is given as:

$$W_\chi^\psi(b,a) = \frac{1}{\sqrt{a}}\int_{-\infty}^{+\infty} k'^n \chi(k')\,\bar{\Psi}\left(\frac{k'-b}{a}\right)dk'$$

The parameter b represents the translation of the wavelet in the k-space, and the parameter a is the scaling of the chosen mother wavelet which controls the frequency of the wavelet. And $\bar{\Psi}$ is complex conjugated to the mother wavelet Ψ.

The parameters b and a are related to the k and R space, respectively. b corresponds to values along the k-space with the same dimension (i.e., $b = k$), whereas a is defined here as:

$$a = \frac{\omega_0}{\omega} = \frac{2\pi\omega_0}{2\pi\omega} = \frac{\eta}{2R}(for\ Morlet)\ or = \frac{n}{2R}(for\ Cauchy)$$

where ω_0 is the angler frequency of the mother wavelet and ω is the angler frequency of the daughter wavelet. The angler frequency of the daughter wavelet also shows a relationship with interatomic distance R: $\omega = 2R$.

$W_\chi^\psi(b,a)$ can then be rewritten as:

$$W_\chi^\psi(k,R) = \sqrt{\frac{2R}{2\pi\omega_0}}\int_{-\infty}^{+\infty} k'^n \chi(k')\,\bar{\Psi}\left[\frac{2R(k'-k)}{2\pi\omega_0}\right]dk'$$

where $2\pi\omega_0$ represents η for Morlet wavelet and n for Cauchy wavelet. This formula comes with considerable computational complexity. When implemented digitally, its discrete form is used:

$$W_\chi^\psi[k,R] = C_{energy}\Delta k'[i]\sum_{i=0}^{N-1} chi[i]\,\bar{\Psi}\left[\frac{2R(k'[i]-k)}{2\pi\omega_0}\right]$$

$k'[i]$represents the k-sequence and $chi[i] = k'[i]^n\chi(k'[i])$ represents the chi(k)-sequence obtained from the **temp_kWforWT.txt** data (see **section 2.1**). i is the counts of k-sequence, from 0 to N-1, and N is the length of k-sequence. And $\Delta k'[i]$ denotes the sampling interval of the k-sequence, which in wtEXAFS is the user defined **dk.** C_{energy} denotes the values obtained from **energy_coef.txt** data (see **section 2.1).**

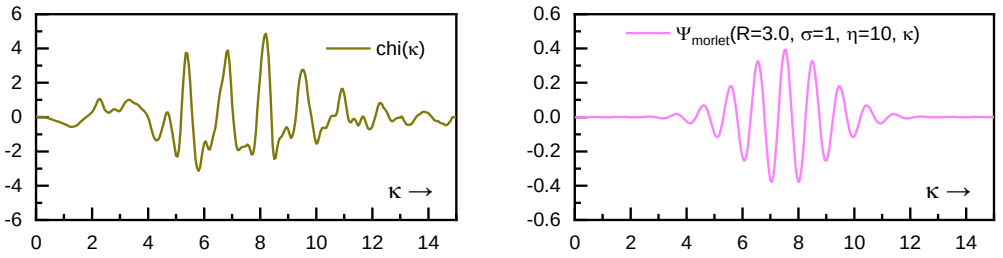
2.3 Algorithm implementation

- **CWT (continuous wavelet transformation)**

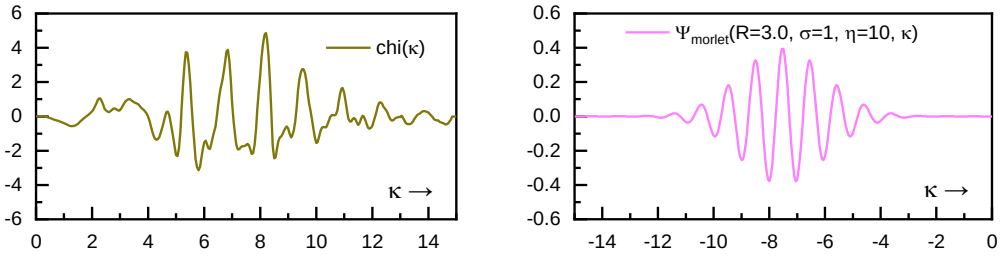
  The definition of wavelet transform suggests that we can implement wavelet transform by convolution. Next, the convolution of an EXAFS signal ($chi([k'[i]])$) and a daughter Morlet wavelet Ψ(R=3, σ=1, η=10, k'[i]) will be introduced as an example:

  - ✧ Express each function in terms of a dummy variable κ.
  - ✧ Reflect one of the functions $\Psi(\kappa) \rightarrow \Psi(-\kappa)$, for Morlet wavelet and Cauchy wavelet, it would not change their shape.
  - ✧ Add a k-offset, which allows $\Psi(k-\kappa)$ to slide along the k-space.
  - ✧ Start k at $-\infty$ and slide it to $+\infty$. Wherever the two functions intersect, find the integral of their product. In other words, at k, compute the area under $chi(\kappa)$ weighted by the daughter wavelet $\Psi(k-\kappa)$.

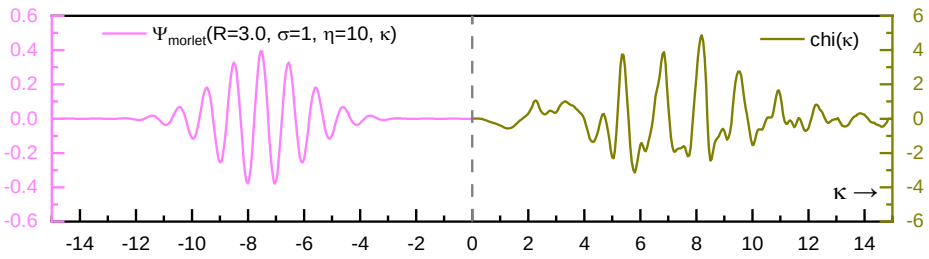
①



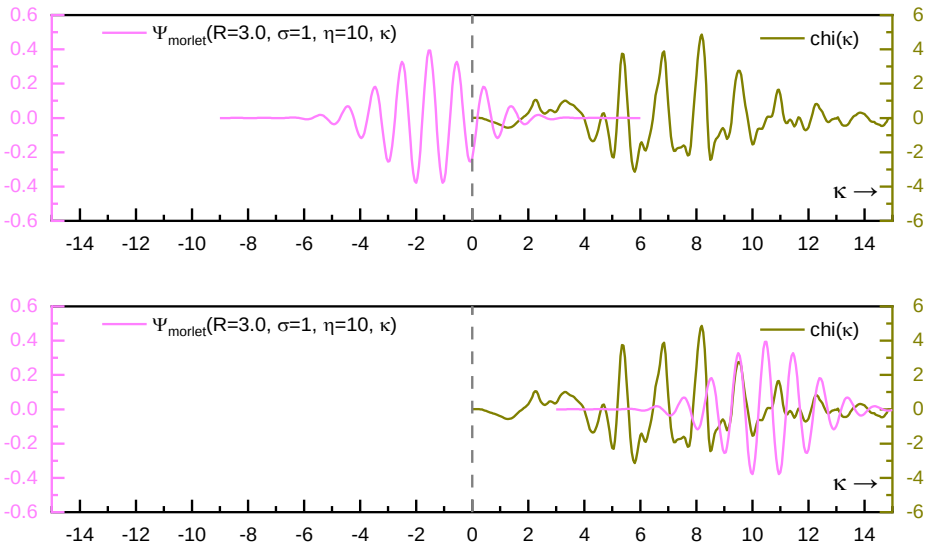
②



③



④



The actual calculation requires multiplying the convolution result by **dk** and C_{energy}, and then the sequence of $W_\chi^\psi[k, R=3]$ can be obtained. To obtain the final wavelet coefficient matrix $W_\chi^\psi[k, R]$, it is also necessary to apply the above operation to the other R. The final matrix $W_\chi^\psi[k, R]$ has $\boldsymbol{X}$ columns ($\boldsymbol{X} = (\boldsymbol{kmax} - \boldsymbol{kmin} + 16 + \boldsymbol{dk})/\boldsymbol{dk}$) and $\boldsymbol{Y}$ rows ($\boldsymbol{Y} = (\boldsymbol{Rmax} - \boldsymbol{Rmin} + \boldsymbol{dR})/\boldsymbol{dR}$).

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