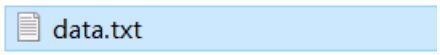
Manual for MorletE

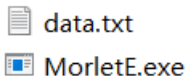
WANG Miao
e-mail: wangmiaow@stu.xjtu.edu.cn
2019.11.05

1. The EXAFS results (e.g., results from Athena) should be put in a “data.txt” file:

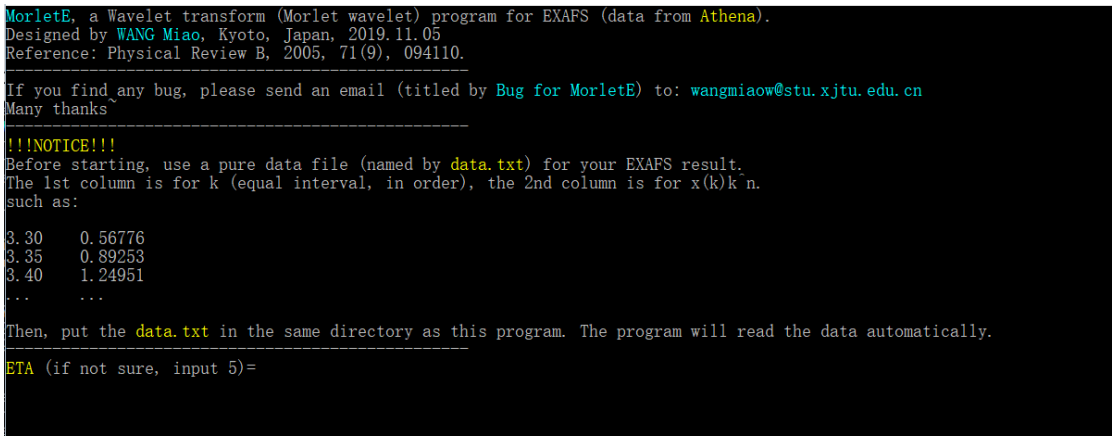


2. Only 2 columns are included in the “data.txt”. The 1st is for k (equal interval, in order), the 2nd is for $\chi(k)k^n$:

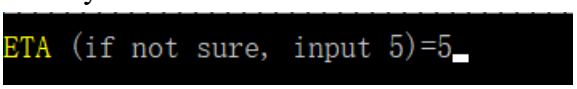
3. Put the “data.txt” in the same directory as this program (MorletE.exe):



4. Double click “MorletE.exe”. It will show like this:



5. Input the parameter ETA (i.e., η, see details at the end). If not sure, input 5 and end with ENTER on the keyboard:



6. Input the parameter SIGMA (i.e., σ, see details at the end). If not sure, input 1 and end with ENTER on the keyboard:

```
ETA (if not sure, input 5)=5
SIGMA (if not sure, input 1)=1
```

7. Input the lower boundary of k (kmin). If not sure, input 3 and end with ENTER on the keyboard:

```
ETA (if not sure, input 5)=5
SIGMA (if not sure, input 1)=1
kmin (if not sure, input 3)=3
```

8. Input the upper boundary of k (kmax). If not sure, input 12 and end with ENTER on the keyboard:

```
ETA (if not sure, input 5)=5
SIGMA (if not sure, input 1)=1
kmin (if not sure, input 3)=3
kmax (if not sure, input 12)=12
```

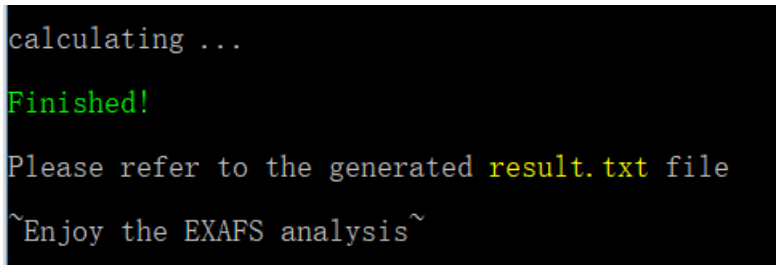
9. Input the lower boundary of R (Rmin). If not sure, input 1 and end with ENTER on the keyboard:

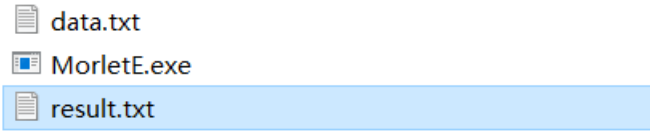
```
ETA (if not sure, input 5)=5
SIGMA (if not sure, input 1)=1
kmin (if not sure, input 3)=3
kmax (if not sure, input 12)=12
Rmin (if not sure, input 1)=1
```

10. Input the upper boundary of R (Rmax). If not sure, input 3 and end with ENTER on the keyboard:

```
ETA (if not sure, input 5)=5
SIGMA (if not sure, input 1)=1
kmin (if not sure, input 3)=3
kmax (if not sure, input 12)=12
Rmin (if not sure, input 1)=1
Rmax (if not sure, input 3)=3
```

11. Then, the program will read the “data.txt” automatically and conduct the wavelet transform. After completing, the results will be saved in a “result.txt” file in the same directory as this program:





12. Open the “result.txt”, the data below include the initial input parameters:

ETA	SIGMA	kmin	kmax	rmin	rmax
5.00	1.00	3.00	12.00	1.00	3.00

---

13. Column “k”, “r”, and “Mag” can be used for the contour map (your target) directly by setting “k” as X axis, “r” as Y axis, and “Mag” as Z axis. “Mag” represents the module of the transformed results, “Real” represents the real part of the transformed results, “Imag” represents the imaginary part of the transformed results:

---

k	r	Mag	Real	Imag
3.000000	1.000000	0.794441	0.346517	0.714886
3.090909	1.000000	0.802836	0.482126	0.641950
3.181818	1.000000	0.810086	0.601703	0.542395
3.272727	1.000000	0.816148	0.699866	0.419864
3.363636	1.000000	0.820986	0.772085	0.279112
3.454545	1.000000	0.824565	0.814912	0.125807
3.545454	1.000000	0.826859	0.826171	-0.033723
3.636363	1.000000	0.827844	0.805086	-0.192779
3.727272	1.000000	0.827503	0.752332	-0.344613

PS: If you use Origin to plot the curves, you’d better to export the plots as a picture (such as .tif) due to the possible poor graphics display in the software window.

Reference: Physical Review B, 2005, 71(9), 094110.

Some important equations.

EXAFS equation:

$$\chi(k) = S_0^2 \sum_{i=1}^{n} \frac{N_i}{R_i^2} \frac{F_i(k,R)}{k} e^{-2R_i/\lambda} e^{-2\sigma_i^2 k^2} \sin(2kR_i + \Psi),$$

Wavelet transform:

$$W_f^{\psi}(a,b) = \frac{1}{\sqrt{a}} \int_{-\infty}^{+\infty} f(t) \psi^* \left(\frac{t-b}{a} \right) dt.$$

Morlet wavelet (the η below is ETA of this program, the σ below is SIGMA of this program):

$$\psi(t) = \frac{1}{\sqrt{2\pi\sigma}} (e^{i\eta t} - e^{-\eta^2\sigma^2/2}) e^{-t^2/2\sigma^2}.$$

The end