HFAmpl Manual

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Contents

1 Introduction

The quantitative analysis of EXAFS data requires the explicit knowledge of scattering characteristics of X-ray emitted photo-electron. The most popular approach is to apply the phases and amplitudes calculated by FEFF6 or FEFF8 codes [1]. The FEFF approach for the electron scattering calculation is based on building of self-consistent potential for the whole atomic system, which leads to the dependence of scattering characteristics of the details of atomic system geometry, like number of neighbors. Here we present an alternative code for the calculation of scattering phases and amplitudes without self-consistent potential calculation using previously developed formalism by R.V. Vedrinsky and L.A. Bugaev [2–5].

The format of output file is FEFFNNNN.DAT coinciding with Feff [1] format, so that it can be used in different fitting codes: FEFFIT [6], Artemis [7], Larch [8], EDA [9].

The atomistic calculation still require SCF cycles, but they are geometry-independent. The exact Hartree-Fock (HF) exchange potential is used for the calculation of isolated atom wave-functions.

2 Install notes

Unpacked distribution zip-archive directory tree is showed on the Figure 1 as it should look for Windows (left part) and Linux (right part) distributions.

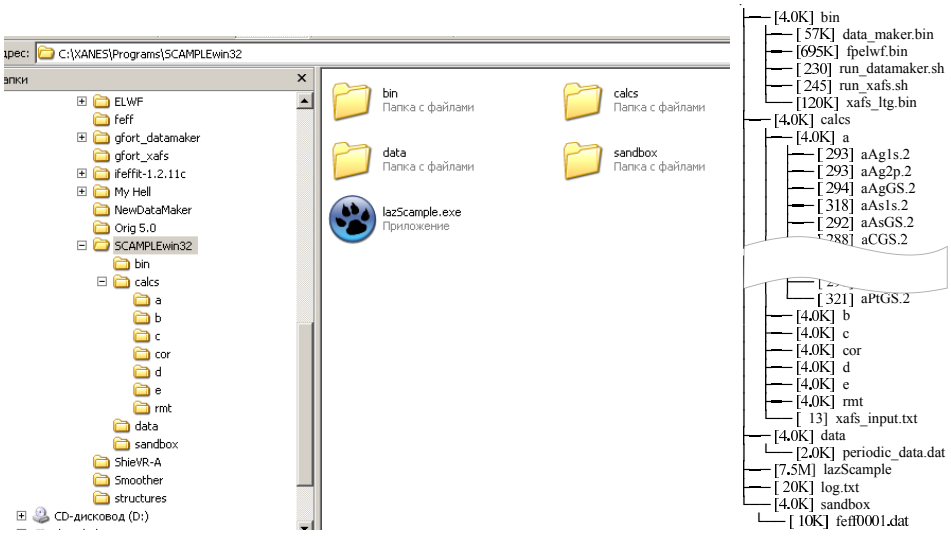

Figure 1: Paths tree on the first start

The meaning of the paths are:

- **bin**: computation codes and corresponding start scripts are placed here. HFAMPL should have permission to execute files in this folder. The computational codes are
  - ELWF – calculator of electron wave function of single atom;
  - XAFS95 – calculation of scattering parameters;
  - DATAMAKER – binding of XAFS95 output in one FEFF [1] path file (feff0001.dat).
- **data**: contains one file with symbols and numbers of atoms in Mendeley's Periodic Table. Needed read permission.
- **sandbox**: Used in the last stage of calculations. All data could be deleted so that directory could be in temp directory (like /tmp in Linux). Needed read and write permissions.
- **calc**: contains subdirectories with input and output files for computational codes. Most important is **a** subdirectory containing input files for first running code, ELWF. Write and read permissions required.

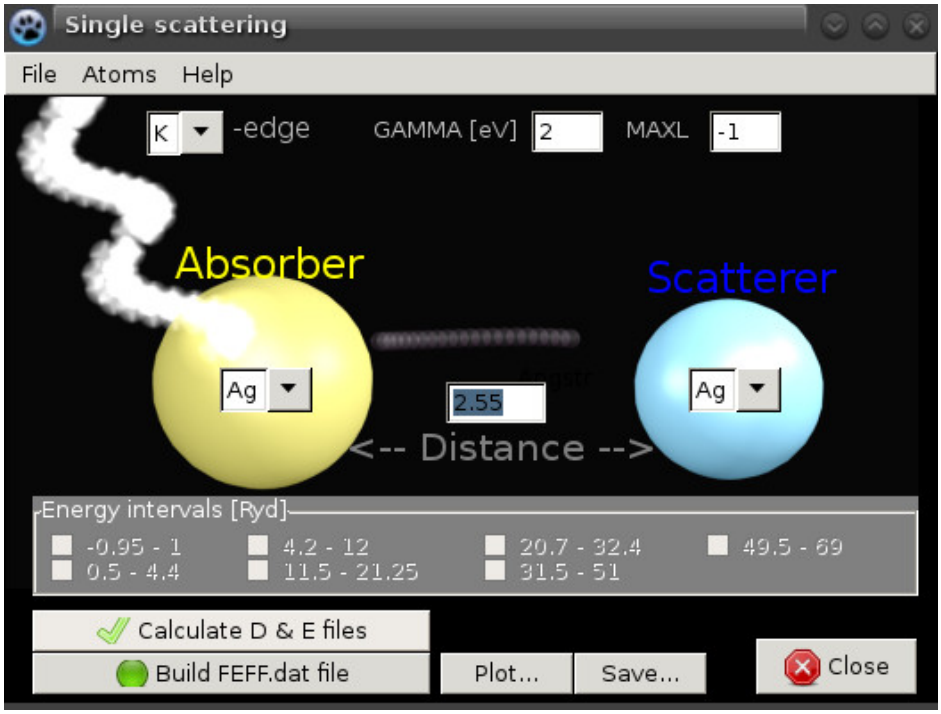

Figure 2: HFAMPL first start. No energy interval available for computation.

3 Usage

The work-flow of the calculations is illustrated on the Figure 3. The three computational steps are performed by three codes: ELWF, XAFS95and DATAMAKER. The first code calculate the properties of isolated atom, using exact HF potential and self-consistent routine. The second code, XAFS95, combines the

3.1 Atom calculations

The software contains pre-calculated atomic presets for ELWF(a-files), so that the changes in the following parameters will not be required. The meanings of the atomic calculation parameters are the following:

- S – number of not empty electron terms (1s, 2s, 2p $\longrightarrow S = 3$). The order of terms is showed on Table 1.
- EN – number of points in energy interval, should be set to 400.
- R – max radius in real space in Ry were excited WF calculated, usually $R = 20 \ldots 25$.

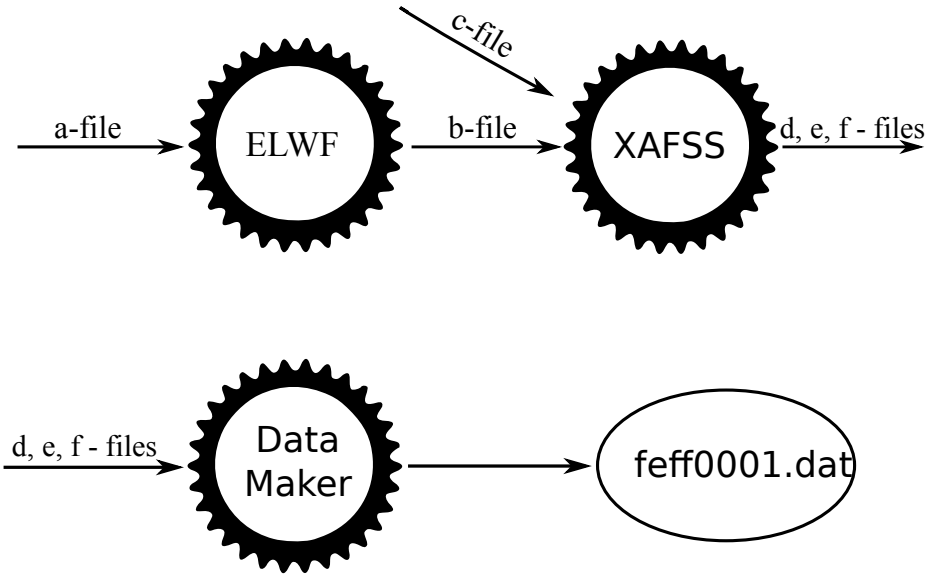

Figure 3: Scheme of HFAMPL calculations.

- H – step in logarithmic energy scale, calculated automatically.
- PEX – type of exchange-correlation function, 1 stands for Hartree-Fock exact exchange.
- RSL – radius of Muffin-Tin sphere used in all further calculations.
- $RCOR$ – radius of stored core electron states.
- ZCH – number of not filled electron terms/shells.
- J – index of changing term, $0 < J \leqslant S$.
- N, L, Q – principal, orbital and occupancy of the electron term. For example $N = 2$, $L = 1$, $Q = 3$ means configuration $2p^3$. Full explanation are given in Table 1.
- $PRIZZ$ – keyword used for treatment of negatively charged atoms, should be 1 one for neutral and positive charged systems.

By default all terms up to S-th are filled with electrons. In order to simulate particular atom one should change several (usually one) last terms by setting appropriate set of parameters J_i, N_i, L_i, Q_i, $i = 1..ZCH$.

Table 1: The order of electron terms used in the code.

Term (filled)	Term number (J)	Principal number (N)	Orbital number (L)	Max occupancy ($Q_{\max}$)
$1s^2$	1	1	0	2
$2s^2$	2	2	0	2
$2p^6$	3	2	1	6
$3s^6$	4	3	0	2
$3p^6$	5	3	1	6
$3d^{10}$	6	3	2	10
$4s^2$	7	4	0	2
$4p^6$	8	4	1	6
$4d^{10}$	9	4	2	10
$5s^2$	10	5	0	2
$5p^6$	11	5	1	6
$4f^{14}$	12	4	3	14
$5d^{10}$	13	5	2	10
$6s^2$	14	6	0	2
$6p^6$	15	6	1	6
$5f^{14}$	16	5	3	14
$6d^{10}$	17	6	2	10
$7s^2$	18	7	0	2

For example for simulation of Oxygen atom in ground state one should change the occupancy of 2p term from default $2p^6$ to actual $2p^4$ by setting $J = 3$, $N = 2$, $L = 1$, $Q = 4$ in the atom wave function form shown on Figure 4.

In order to get atom with core hole which should correspond to the absorbing atom one should change 1s (K-edge) or 2p ($L_{2,3}$-edge) term in the same way.

These are a bit annoying and error-rich parts of the calculation and we are working to make presets for all stable atoms to simplify user experience.

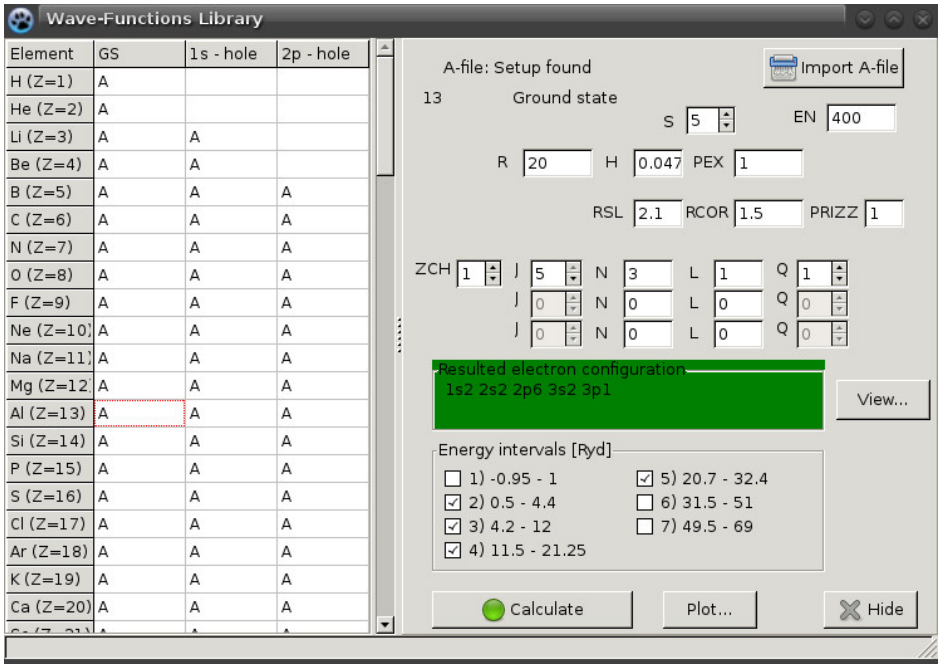

Figure 4: Wave function DB window. Some atom presets available.

The resulting electron configuration could be verified by clicking *View* button. Window showed on Figure 5 should appear. The first data block here demonstrates accounted electron orbitals and their occupancy while the second shows energy levels of these orbitals (Ry).

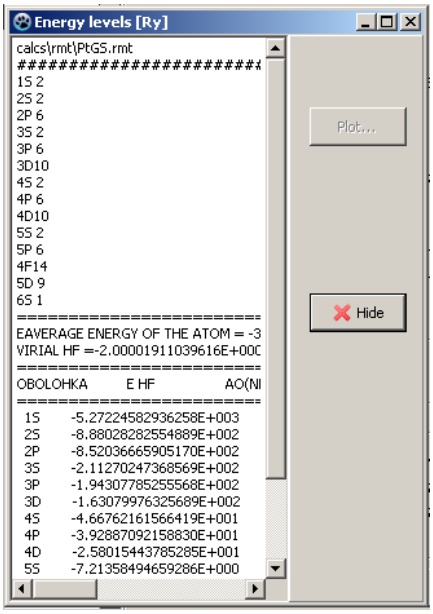

Figure 5: Check electron configuration before proceed.

The next important quantity is $R_{\mathrm{SL}} = R_{\mathrm{MT}}$ radii. It should be chosen at the value of total potential $V_{\mathrm{C}} + V_{\mathrm{XC}}$ = -1.1 Ry. According the Figure 6, R_{SL}=2.2 Bohr for ground state calculation of Platinum atom.

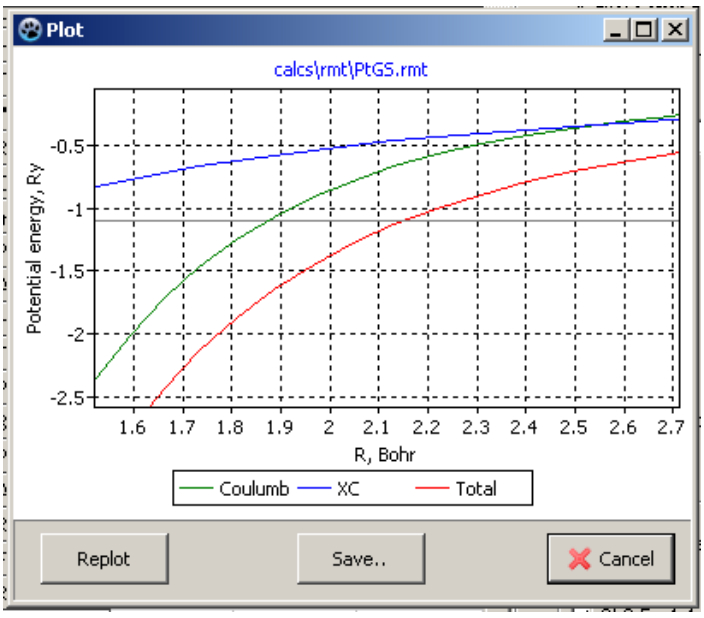

Figure 6: Check value of cutting R_{SL} to be at E_{total}=-1.1 Ry before proceed.

After these preparations all WFs may be computed. Just mark boxes corresponding to the calculated energy intervals and press *Calculate* button. Here ELWF code will be executed several times and B-files should appear in **calc/b** directory.

These calculation should be completed both for absorbing X-ray atom and his neighbors.

3.2 Scattering pair calculations

We are ready to calculate scattering phases for atom pair. As example we will consider Pt-Pt pair, the first Pt is in fully screened core-excited state Pt($1s^1...5d^{10}6s^1$) and the second is in ground state: Pt($1s^2...5d^9 6s^1$).

The types of the absorbing and scattering atoms should be selected from drop-down lists or typed in them. The distance between atom should be typed in the edit area. The usual practice is to recalculate phases if the distance variation of distance exceeds $\sim$0.2 Å.

One of the important step is to check the selected absorption edge in the top left drop-down list. The default edge is K, and L_3-edge could selected.

3.3 Obtaining feff0001.dat file

After all preparations are done, after the clicking of the button "Calcualte D&E files" the scattering properties will be calculated individually for each of the energy interval. The clicking of the button "Build FEFF.dat" will gather all them in the single Feff0001.dat file, readable by common fitting software.

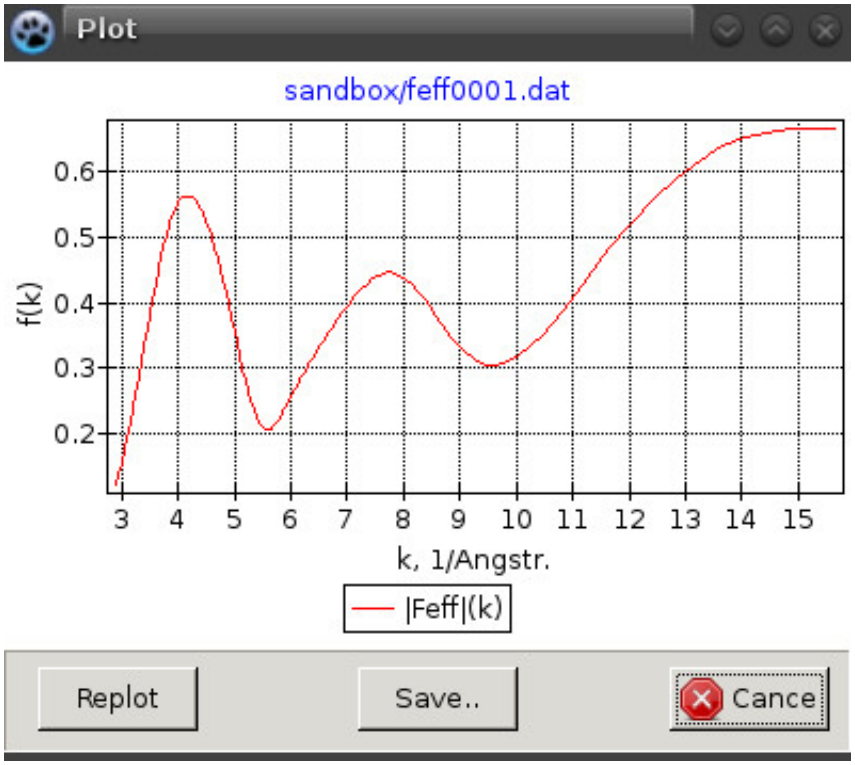

Figure 7: Plot of obtained $|F_{\text{eff}}(k)|$

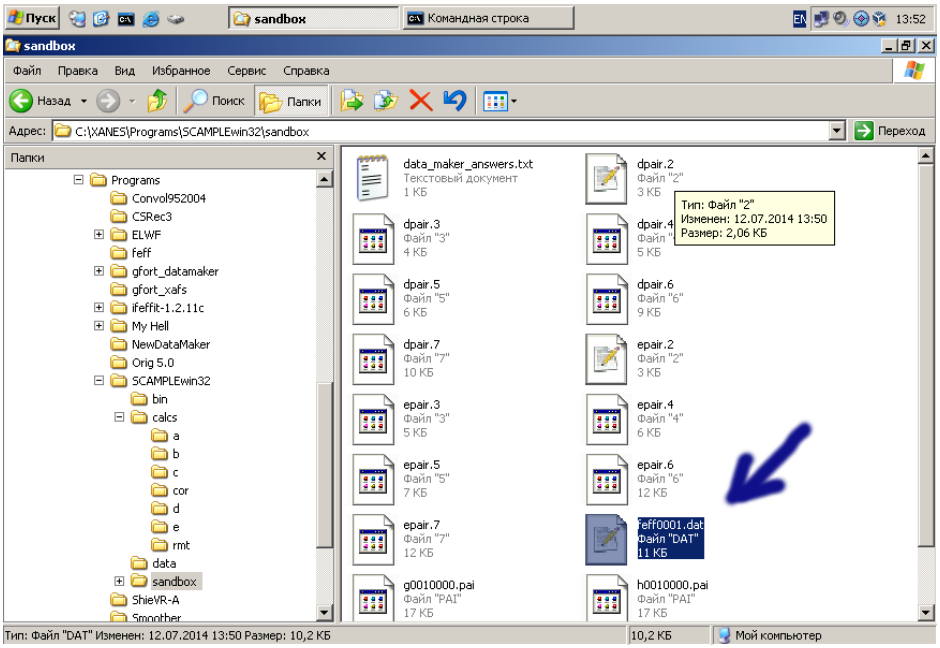

Figure 8: Find feff0001.dat file in **sandbox** directory.

References

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