ESTRA2009
short manual

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ESTRA2009 is a program aimed to treat X-Ray Absorption Spectroscopy data and extract EXAFS structural signal. The ESTRA2009 code derives from the original program package for EXAFS data analysis developed, in the 1980-1990, at the PULS group of Laboratori Nazionali di Frascati (INFN). Many people have contributed to the original package, among them I would like to cite S. Mobilio, F. Boscherini, A. Filipponi. C. Meneghini (meneghini@fis.uniroma3.it) and F. Bardelli (bardelli@esrf.fr) reorganized the original software, revised some of the routines, and packed the different programs in a single one. In order to preserve the portability the ESTRA2009 code is written in F77 and, for the graphic output, includes subroutines writing script to be loaded by Gnuplot program. This allows to compile and run the program on almost any platform, having a F77 compiler and the Gnuplot (www.gnuplot.info) program.

Input to ESTRA2009 are given from command-line interface (DOS-shell in windows) or they can be written in a command file named *estra.inp*. At the startup ESTRA2009 looks for the file: *estra.inp*, if it does not exists the program sequentially asks for input. The input data and commands are saved in the *estra.new* file. After the first run the *estra.new* file can be renamed as *estra.inp* and modified for rapid ESTRA2009 runs.

Output files are all ASCII, in particular the log file (*estra.log*) is written during the run for sake of debugging. Specific output are written after each step and described below. Specific information on data treatment are included in the header of each output files.

NOTE: ESTRA2009 is a beta version, please run carefully and check for the results. Please for notice about problems or bugs to *meneghini@fis.uniroma3.it* .

Here below are briefly described the commands/options for running ESTRA2009.

Firstly ESTRA2009 asks for a title of the run, then ESTRA2009 has 5 main modules:
to convert absorption data (`C`),
to extract $k\chi(k)$ (`E`),
to calculate the k^n weighted Fourier transform $FT(k^n\chi(k))$ `F`,
and to calculate the Fourier filtered signal relative to a given real space region (back Fourier transform) `B`.
These options are invoked by typing `C`, `E`, `F` or `B` in small or capital letters.

A standard EXAFS signal extraction goes trough `C` $\rightarrow$ `E` $\rightarrow$ `F` $\rightarrow$ `B`.

The option `P` after each step causes ESTRA2009 to write the *estra.plt* ASCII file containing scripts to be executed in Gnuplot section using the command: `load 'estra.plt'`

The option `q` ends the program.

Here below the list of ESTRA2009 options:

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***  ESTRA2009 OPTIONS ********
c    Convert              #  C: runs Convert module for raw XAS data conversion.
e     EXAFS               #  E: runs Exafs module for kχ(k) extraction.
f    Fourier              #  F: runs Fourier module for Fourier transform.
b   b-Fourier             #  B: runs back Fourier module for back Fourier transform.
p gnuplot macro           #  P: runs Plot module writing Gnuplo Macro on estra.plt
q Quit
```

Description of ESTRA2009 input cards.

Sample title

`sample_name`	`CARD #0`	Name of the experiment (max 10 characters)

This is the first card, always present in the *Estra.inp* file.

Convert module

`Convert` module allows reading absorption data in multicolumn ASCII format and write absorption vs. Energy two column ASCII file (the maximum number of columns are: xxx). The lines beginning with # are skipped. The following experimental data types can be converted:

- Absorption data (data type **C.1=1**): the file must contains the Energy (eV or keV) and absorption data columns.
- Transmission data (data type **C.1=2**): must contains the Energy (eV or keV), incident intensity I_o and transmitted intensity I_t columns. Absorption are calculated as $\log I_o/I_t$
- Fluorescence single detector data (data type **C.1=3**): must contains the Energy (eV or keV), incident intensity I_o and fluorescence intensity I_f columns. Absorption are calculated as I_f/I_o
- Fluorescence multidetector data (data type **C.1=4**): must contains the Energy (eV or keV), incident intensity I_o and fluorescence intensity I_{f_n} columns. Absorption are calculated as $\sum_n I_f/I_o$
- data from multiple files can be averaged (data type **C.1=5**).

Cards for Convert module, data type 1: absorption data.

File_name.ext	CARD # C.0	
1	CARD # C.1	data type (1)?
C.E C.A	CARD # C.2	data columns (E,Abs)
E.L E.R	CARD # C.3	energy range, if 0 0 the full range is used.

Cards for Convert module, data type 2 (transmission) or 3 (fluorescence single detector) data.

File_name.ext	CARD # C.0	
2 or 3	CARD # C.1	data type (2 or 3)
C.E C.0 C.1	CARD # C.2	Data columns (E,Io,It or If)
E.L E.R	CARD # C.3	energy range, if 0 0 the full range is used.

Cards for Convert module, data type 4 (fluorescence multidetector data) (multidetector) data.

File_name.ext	CARD # C.0	
4	CARD # C.1	data type (4)
C.1 C.0	CARD # C.2	Energy and I_o columns
n	CARD # C.2.4	Number of detectors
D.1,D.2 ... D.n	CARD # C.2.4n	columns for detectors 1...n
E.L E.R	CARD # C.3	energy range, if 0 0 the full range is used.

Cards for CONVERT module dealing with several data files.

File_name.ext	CARD # C.0	
5	CARD # C.1	data type (5)
NF	CARD # C.1.5	Number of files
DT	CARD # C.1b	data type (1-4)
...		
...	CARD # C.DT	cards as for data type 1, 2, 3, 4
...		
File_1	CARD # C.4_1	
...		files to be averaged
File_{NF-1}	CARD # C.4_NF-1	

 # C.0 [C] File name with extension: `File_name.ext`. All the output files will be named `File_name.+++` with `+++` being the appropriate extension.

 # C.1 [I] Data type (DT): 1-absorption (E,$\alpha(E)$), 2-transmission (E,I_o,I_t), 3-Fluorescence single detector (E,I_o,I_f), 4-Fluorescence multi-detector (E,I_o,I_{f_n}), 5-average several data files of 1,2,3,4 type.

 # C.2 [3I] Data columns: 2 columns for DT=1,4; 3 columns for DT=2,3

 # C.3 [2F] Energy range to be used. If E.L $\leq$ 0.0 the full range is used.

 # C.2.4 [I] If DT=4 it is the number of detectors to be used, follow the :

 # C.2.4n [nI] card with the column numbers for the detectors.

 # C.1.5 [I] number of files (NF) to be used if DT=5. Must follow C.1, C.2, C.3 cards accordingly to the data type, and Nf-1 file names to be used.

 # C.4_i [C] NF File names

Dealing with multiple files the abscissa of the NF-1 files are interpolated on the abscissa of the first file.

Output: Absorption data (E, α) are written on a two columns ASCII file named: `File_name.abs`. The header of `File_name.abs` file contains: energy range and number of points.

The `File_name.abs` columns contain:
`1.Energy 2.Absorption`

EXAFS module

EXAFS module allows extract EXAFS structural signal $k\chi(k)$

EPL EPR	CARD # E.1	pre-edge limits
EM1 ETOL	CARD # E.2	Max. energy and tolerance for edge search
NG	CARD # E.3	number of excluded regions (glitches)
$G.L_1$, $G.R_1$		
...	CARD # E.3.1	NG Excluded region limits
$G.L_{NE}$, $G.R_{NG}$		
NS	CARD # E.4	Number of spline intervals
K_1,K_2, ...K_{NS+1}	CARD # E.4.1	NS+1 Spline Knots
D_1, D_2... D_{NS}	CARD # E.4.2	NS Spline degrees
NDE	CARD # E.5	Number of additional discontinuities
EDE_1, ADE_1, WDE_1		
...	CARD # E.5.1	Position, Amplitude, width
EDE_{NDE}, ADE_{NDE}, WDE_{NDE}		
JL JR	CARD # E.6	limits for Jump evaluation
Flg_j Flg_k Wgt	CARD # E.7	constraints for estraction
J	CARD # E.7.1	discontinuity at the edge

If `Exafs` is the first module, as for directly dealing with α(E) data, two cards are required before # E.1:

 # E.0.1 [C] ***FileName****.ext*. In following the same ***FileName*** with different extensions will be used for output files.

 # E.0.2 [2I] column numbers for Energy and Absorption. Energy can be done in eV or in keV.

The other cards are:

 # E.1 [2F]: limits for pre-edge linear fitting $lin(E)$

 # E.2 [2F]: E_o calculation. If EM > 0 the energy maximum is chosen as the maximum of first derivative $d\alpha/dE$. The absolute first derivative maximum E'_M is selected, in the interval between EPR and EM1. The points which derivative is in between E'_M and E'_M*ETOL are selected and the derivative maximum is calculated as the maximum of a second order polynomial spline through the data. If EM < 0 the edge energy is: $E_o = abs(EM)$

 # E.3 [I]: Number of excluded regions (NG) if NG>0 follow NG E.3.1 cards.

 # E.3.1 [2F]: excluded region limits in Energy (eV) or K ($Å^{-1}$) scale. The scale is automatically selected.

 # E.4 [I]: Number of spline intervals.

 # E.4.1 [(NS+1)*F]: Spline knots given in Energy (eV) or K (Å) scale.

 # E.4.2 [NS*I]: Spline degrees.

 # E.5 [I]: number od additional discontinuities NE, for NE> 0 will follow NE E.5.1 cards.

 # E.5.1 [3F]: Additional discontinuities are medelled with arctang functions at EDE_i, in Energy (eV) or K (Å) scale, having amplitude ADE_i (in jump height units) and with WDE_i in eV.

 # E.6 [2F]: limits (in eV or $Å^{-1}$) for JUMP evaluation. JUMP is calculated as the mean value of spline in between JL and JR. Note(version 2011): if JL (or JR) is negative the data will be normalized by fixed jump discontinuity instead of $\mu_o(E)$. The |JL| and |JR| values are used for jump evaluation.

NOTE if E.6 = err R_{cut} ("err" is case sensitive and R_{cut} is a real positive number) data noise is estimated by Fourier filtering the data: the filtered spectrum above R_{cut} is considered as "noise".
The |JL| and |JR| must be given below in a # E.6b card.

 # E.7 [C C F]: extraction constraints: if Flg_j = J the value of spline at E_o is fixed by the next E.7.1 card. The spline is calculated via a least square procedure minimizing the sum:
$\sum_X(\alpha(X) - lin(X) - Poly(X))X^{Wgt}$ If Flg_k = E the abscissa is energy (X=eV), if Flg_k = K the abscissa is wavevector (X=K). The third parameter is Wgt, if absent $Wgt = 0.0$ is used.

 # E.7.1 [F]: fixed background discontinuity at E_o, required if Flg_j = J

Output files:

File_name.pre : The Header contains: pre-edge limits, a and **b** of linear pre-edge spline ($ax+b$), the edge energy E_o used for EXAFS extraction, the White-line energy. The Columns contain:
1: E(eV): Energy in eV;
2: linear pre-edge subtracted absorption spectrum ($\alpha_o(E)$);
3: first derivative $d\alpha_o/dE = \alpha'_o$;
4: second derivative $d^2\alpha_o/dE^2$;
5: Uncertainty estimated for each point calculated as:

$$\epsilon_i = \alpha_o(E_i) - Poly(\Delta E)$$

where $\alpha_o(E_i)$ is the absorption signal measured at E_i and $Poly(\Delta E)$ is a high degree polynomial spline trough the data in the region $E_i - \Delta E < E_i < E_i + \Delta E$

File_name.jmp : the header reports: Limits of excluded regions (eV), parameters used additional discontinuities ...
The columns contain:
1: E(eV): Energy in eV;
2: $(\alpha_o(E) - AD(E))/jump = \alpha_{nor}(E)$ the spectrum, corrected for additional discontinuities, normalized to the jump height;
3: $\alpha_o(E)/jump$ the spectrum, uncorrected for additional discontinuities, normalized to the jump height;
4: $Poly(E)/jump$ polynomial spline through the $\alpha_{nor}(E)$, normalized to the jump height;
5: $(Poly(E) + AD(E))/jump$ atomic background including the additional discontinuities.

File_name.sta : statistical information, the header contains the number of points in the EXAFS region, the variance (σ^2) and standard deviation (σ) of the EXAFS structural signal ($\chi(k)$), the variance ($\sigma^2_{k\chi}$) and standard deviation ($\sigma_{k\chi}$) of the k-weighted EXAFS signal ($k\chi(k)$).
The columns contain:

1: k(Å^{-1});
2: EXAFS signal derivative: $d\chi/dk$;
3: Additional discontinuities background AD(k);
4: Uncertainty estimated for each point calculated as:

$$\epsilon_i = \chi(k_i) - Poly(\Delta k)$$

where $\chi(k_i)$ is the EXAFS structural signal measured at k_i and $Poly(\Delta k)$ is a high degree polynomial spline trough the data in the region $k_i - \Delta k < k_i < k_i + \Delta k$

File_name.exa : EXAFS structural signal. The Header file contains information on extraction: E_o, jump normalized slope at E_o (SLOPE), jump height, White line energy, white line amplitude (jump normalized) maximum K used for extraction.
The columns contain:
1: k(Å^{-1});
2: EXAFS signal $k\chi(k)$;
3: spline knots (k).

FOURIER transform module.

FOURIER module calculate the Fourier transform of $k^n\chi(k)$

FOURIER module cards:

KL KR	CARD # F.1	limits for FT
WT	CARD # F.2	K-Weight for FT
Win	CARD # F.3	Apodization window type: n, g, h
WW	CARD # F.4	Window width
R_{max} dr	CARD # F.5	R max and dR for FT

 # F.1 [2F]: limits for Fourier transform.

 # F.2 [F]: Fourier transform k-weight to calculate the FT of $k^{WT}\chi(k)$.

 # F.3 [C]: Apodization window type: **n**=none, **g**=Gaussian, **h**=Hanning.

 # F.4 [F]: Apodization window width.

 # F.4 [2F]: Maximum R and dR for Fourier transform.

Output file:

File_name.fou : Fourier transform results. The Header file contains the K-window limits, the apodization window type, the apodization window width, the K-weight, the number of points in real (R) and reciprocal (K) space.
The columns contain:
1: R(Å);
2: —FT— of $k^{WT}\chi(k)$: the modulus of k^{WT} weighted fourier transform;
3: *Re* of $FT(k^{WT}\chi(k))$: the real part of k^{WT} weighted fourier transform;
4: *Imm* of $FT(k^{WT}\chi(k))$: the immaginary part of k^{WT} weighted fourier transform;
5: k ($Å^{-1}$) used for the FT;
6: $k^{WT}\chi(k)$ used for the FT;
7: Apodization window used for the FT

Back Fourier transform module.

Back-Fourier module cards:

RL RR	CARD # B.1	limits for BFT
R_o	CARD # B.2	Theoretical R_o for experimental amplitude and phases

 # B.1 [2F]: limits (R) for Back Fourier transform.

 # B.2 [F]: expected distance R_o, used for experimental amplitude and phase signals.

Output file:

File_name.bf : back Fourier transform data. The Header contains: the R limits of the BF, the weight used for direct FT, the theoretical R_{th} used for calculating experimental phase shift, number of points in K space.
The columns contain:
1: k(Å^{-1});
2: $k\chi(k)$;
3: $k^{WT}\chi(k)$;
4: Experimental amplitude A_{exp};
5: Experimental amplitude $A_{exp} * R_{th}^2$;
6: The total phase shift;
7: The total phase shift $\phi_{tot} = 2kR_{th} + \phi_{exp}$;
8: The experimental phase shift ϕ_{exp}.