





FDMNES
User's Guide

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July 2016

Introduction

The FDMNES program calculates the spectra of different spectroscopies related to the real or virtual absorption of x-ray in material. It gives the absorption cross sections around the ionization edges, that is in the XANES energy range. Calculations can be performed along all the conditions of linear or circular polarization. In the same way, it calculates the structure factors and intensities of anomalous or resonant diffraction spectra (DAFS or RXD). FDMNES also allows the comparison of the simulated spectra to experimental ones with the help of objective criteria.

FDMNES is mainly a fully relativistic DFT-LSDA code. Optionally Hubbard correction (LSDA+U) can be used. It uses two techniques. The first one is based on the Finite Difference Method (FDM) to solve the Schrödinger equation. In that way the shape of the potential is free and in particular avoid the muffin-tin approximation. The second one uses the Green formalism (multiple scattering) on a muffin-tin potential. This approach can be less precise but is faster. The program includes also a multi-electronic extension using the "Time-Dependant DFT" with a local kernel. The program is symmetrized. Symmetry operations are calculated automatically.

The next section contains the information for practical purposes to run the program and in particular the description of the indata files. An introduction to x-ray spectroscopies is available in French.

The FDMNES program can be freely downloaded at the web address:

http://www.neel.cnrs.fr/fdmnes

In case of publication related to the use of the program thanks to cite:

O. Bunau and Y. Joly
Self-consistent aspects of x-ray absorption calculations
J. Phys. : Condens. Matter **21**, 345501 (2009).

The FDMNES program highly benefited from the scientific contribution of Calogero Natoli who has provided a constant and essential help. He is in particular at the origin of all the developments using the multiple scattering theory and the extensions to resonant diffraction and magnetism. Oana Bunau realized the extension towards TD-DFT and participated to the inclusion of self-consistency and Hubbard correction. The program also benefited from the expertise of Delphine Cabaret, Hubert Renevier, Sergio Di Matteo, Christian Brouder, Aline Ramos, Stéphane Grenier and Emilio Lorenzo without whom different advances would have not been realized. Finally, this work has been made greatly easier with the support of Denis Raoux.

From March 2015, Guda, Soldatov *et al*. (Rostov, Russie) make the code far faster by the use of the MUMS library which solves systems of linear equations for sparse matrices. This method is now the default option used when running in the finite difference method mode. When using it thanks to cite also:

Sergey A. Guda, Alexander A. Guda, Mikhail A. Soldatov, Kirill A. Lomachenko , Aram L. Bugaev, Carlo Lamberti, Wojciech Gawelda, Christian Bressler, Grigory Smolentsev, Alexander V. Soldatov, Yves Joly
"*Optimized Finite Difference Method for the Full-Potential XANES Simulations: Application to Molecular Adsorption Geometries in MOFs and Metal-Ligand Intersystem Crossing Transients*"
J. Chem. Theory Comput. **11**, 4512-4521 (2015).

and

P. R. Amestoy, A. Guermouche, J.-Y. L'Excellent and S. Pralet
Hybrid scheduling for the parallel solution of linear systems
Parallel Computing Vol 32 (2), pp 136-156 (2006).

From October 2015, the code also includes the FDMX extension from J. Bourke and Ch. Chantler. When using it, thanks to cite also:

Jay Daniel Bourke, Christopher Thomas Chantler and Yves Joly
"*Extended X-ray Absorption Fine Structure Calculations Using the Finite Difference Method*"
J. Synchrotron Rad. 23, 551-559 (2016).

Running the program

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A- General presentation

I- Computer configuration

FDMNES run on all the computers, under LINUX or Windows. The programming language is Fortran 90. Executables are furnished for Windows and Linux 64 bits for sequential calculations.

Users can also compile the code themselves. The code needs then MUMPS, LAPACK and BLAS libraries. When they are not available, it is possible to use a gaussian solver routine furnished with the other routines

The code can be run on parallel processors if it is linked with the MPI library.

II- The package

Several groups of files can be downloaded: the *fdmnes* program itself and a set of examples of indata files.

- *fdmnes_win64.exe* is the executable for Windows 64 bits,
- *fdmnes_win32.exe* is the executable for Windows 32 bits,
- *fdmnes_linux64* is the executable for linux 64 bits,
- *fdmfile.txt* is an indata file,
- *xsect.dat* and *spacegroup.txt* are data necessary for the program,
- *prog* is a directory containing all the subroutines (*main.f90*, *general.f90*…), and the files included during compilation ("*mpif.h*"…).
- *Sim/in* is a directory containing a set of examples of *fdmnes* indata files.

The list of the modifications done in the code are in the file « FDMNES_Modifications.txt ».

IV- Compilation

The code is more efficient when running with MUMPS library. All the furnished routines, but *mat_solve_gaussian.f90*, *sub_util.f* and *not_mpi.f90*, must then be compiled and linked with the call to this library and the ones whom it depends (SCOTCH, METIS, BLAS, LAPACK…). The files included in this step (*mpif.h*, …) must be set in the same directory (or in a dedicated one).

When this library is not available, one exchanges *mat_solve_MUMPS.f90* by *mat_solve_gaussian.f90*, *sub_util.f* and *not_mpi.f90*, and one compiles and links without call to external library. *sub_util.f* can be replaced by BLAS and LAPACK.

Two examples of « makefile » for linux are provided.

V- Parallelization

Thanks to Keisuke Hatada, Kuniko Hayakawa and Rainer Wilcke, the users having the access to a cluster of computers can, using the MPI library, run the program in parallel mode.

For this purpose, one has to delete the files "*mpif.h*" and "*not_mpi.f*" when compiling and makes the call to the corresponding library.

VI- Running

After compilation, the program can be run following the usual procedure available on your system. The files "*xsect.dat*" and "*spacegroup.txt*" must be set in the same directory than the executable file because they are used in some cases.

As soon as the program is running, it calls the file "*fdmfile.txt*". This file must also be in the same directory than the executable file. It only contains the number of independent calculation to perform, followed the name of the indata file of each of these calculations. For example:

! Indata file for fdmnes
1 → number of indata files
example/cu/cu_inp.txt → name of the indata file

VII- Troubleshooting

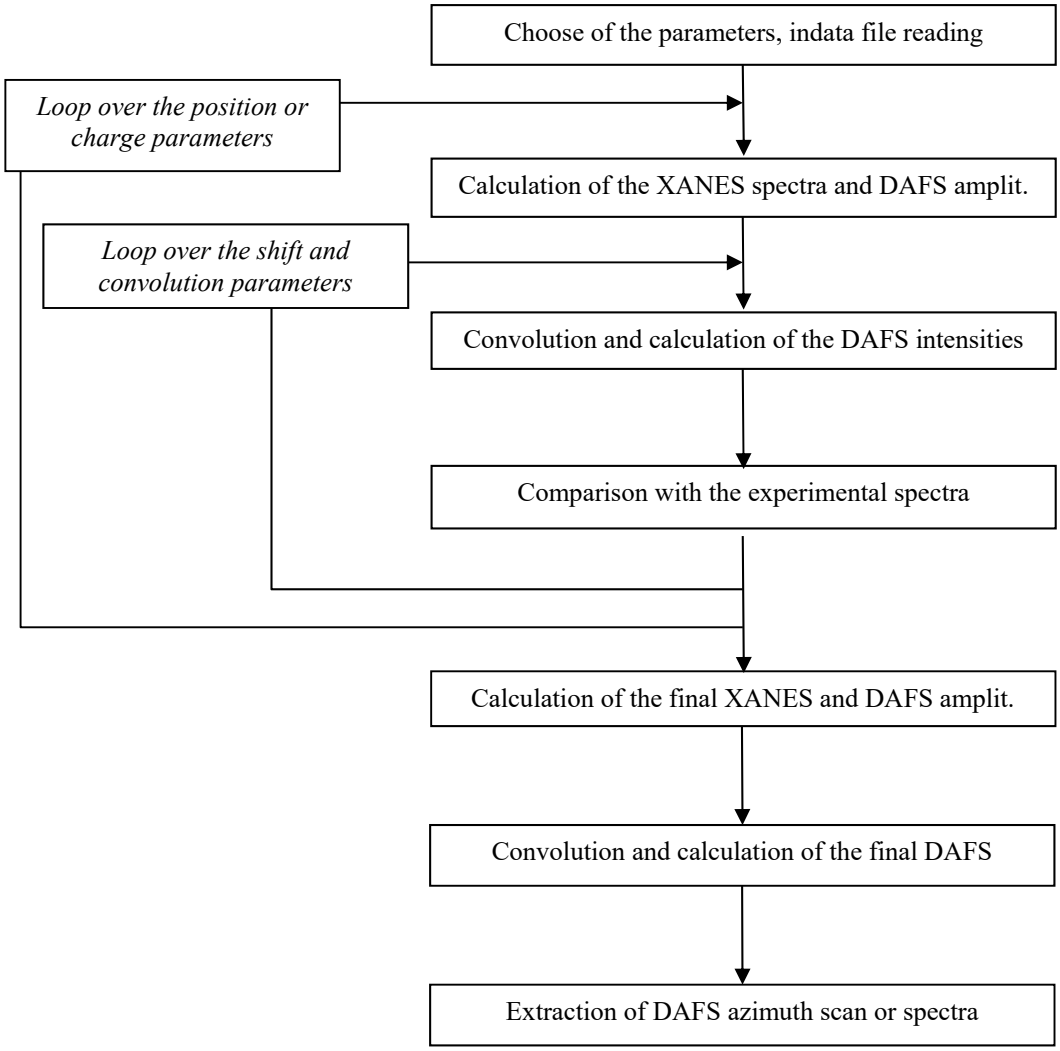
When the program stops without reason, check if an "*fdmnes_error.txt*" file has been created. When created, this file contains a message explaining the trouble. Most often it is due to an error in the indata file. It can also be due to the fact that the indata file is not found. One has to check several points:

1) The called files are in the good directory. The name must contain all the paths.
2) The extensions are correct.
3) Their names are OK (under linux, upper and lower cases must be respected).
4) When using downloaded indata files, some problems of compatibility between systems can occur. It can be better to write again completely these files.

When the program stops without "*fdmnes_error.txt*" file, it can be due to a problem of space memory. Sometimes one gets a message with "stacking fault". In this case try again putting in the indata file the keyword "Memory_save". This keyword can be useful when there are many non-equivalent atoms. An approximation (in fact very good) is then done on the potential calculation. This option saves some memory space.

VIII- Structure of the calculation

The program allows the calculation of spectra from a grid of parameters (position, charge…), to convolute them with other parameters (convolution width, energy shift…), then to compare them to experimental spectra with the help of objective criteria. These different steps can be performed together or separately. The comparison with the experimental spectra is also not mandatory. When used, the parameter fit must be performed with care. In practice many calculations are limited to the step "XANES and DAFS calculation" and "Convolution and calculation of DAFS intensities". These two steps can also be performed together or separately. For a complete calculation one hass the following scheme:



In the output files, the absorption cross section are in Mbarn (1 Mbarn = 10^{-18} cm^2) and summed up over the atoms of same chemical specie in the unit cell or in the cluster. To convert in number of electron one has to multiply by $C = \frac{\hbar\omega_{eV}}{800\pi^2 a_O^2 \alpha R} = 0.004555352 \times \hbar\omega_{eV}$, where R, α et a_0 are respectively the Rydberg constant, the fine structure constant and the Bohr radius in Angstrom, $\hbar\omega_{eV}$ is the photon energy in eV. One has also to divide by the number of atoms if one wants the result per atom. The intensities of the reflexions are in square of number of electron.

The next chapter treats about the principal indata file for the step "XANES and DAFS calculation". Generally this file is sufficient to describe all the necessary data for the calculation because the program calculates its atomic bases and the potential. Nevertheless, the user can prefer use its own atomic bases or uses directly the potential calculated by the band structure program FLAPW WIEN-2k. In both cases, some other files must be furnished. They are described further in the manual. The indata necessary for the steps "Convolution", "comparison with the experimental spectra" and "Extraction of azimuth scan or spectra" can be set in the same indata file, but they are explained separately in the chapter C, D and E.

B- Main indata file

I- General Structure

It contains most of the inputs necessary for the calculation. All the data in input and output are in Angstrom and electron-Volt. Many options are chosen by default. One can modify or add other options using keywords. Text can be in upper or lower case. Blank lines or beginning by "!" are not taken into account. Between number, one must put at least one blank. When getting problem when opening these indata files, one has to check if their name is correct. Moreover some compilers do not like files written under other system (MAC, DOS, LINUX…). In case of difficulties when the program wants to open one of these downloaded files, it can be useful to completely write them again.

The indata file contains several blocks of data, each ones starting with a specific keyword. The end of the indata file is noted by the keyword "*End*". Whatever is after is not red. Here comes an example of indata file:

```
! Fdmnes indata file
! Calculation for the copper K-edge in copper cfc

Filout
 example/cu/cu_out                    → Name of the output files (without extension)

Range
 -10. 0.2 0. 0.5 10. 1. 40.

Radius                                → Cluster radius
 3.0

Crystal                               → crystal structure
   3.610  3.610  3.610  90. 90. 90.   → Unit cell parameters (Å and degrees) : a, b, c, α, β, γ
29  0.0   0.0   0.0                   → Atomic number, position
29  0.5   0.5   0.0
29  0.5   0.0   0.5
29  0.0   0.5   0.5

Convolution                           → to get convoluted spectra

Efermi
-6.

End                                   → end of the indata file
```

Two blocks are necessary for any calculations. The first one starts with the keyword "*Radius*" followed by the value of the radius of the sphere surrounding the area of calculation. The second one is necessary to describe the material structure. When that one comes from the output of the WIEN-2k package, it begins with the keyword "*flapw*". In the other cases, the molecule structure or the elementary unit cell, in case of a 3D structure, is described with the keyword "*molecule*" or "*crystal*", followed by the unit cell parameter and atom positions.

All the keywords related to the convolution or to the fit of the parameters are treated in chapter C and D.

Output file names

By default the output file name is *fdmnes_out*. This name can be modified by the use of the keyword "*filout*" followed by the name we want (without extension). Then one gets several output files with the extensions:

_bav.txt	output file giving details
.txt	contains only the spectra by column
_nrixs.txt	contains only the spectra by column for NRIXS simulations

If a calculation is performed on several non-equivalent crystallographic sites, one gets the extensions:

_i.txt, _j.txt … where i and j are the index of the sites (see keyword *absorber*)

In option or depending on the type of calculation, one can also get the files:

_conv.txt	convoluted spectra scan (keyword *Convolution*).
_scan.txt	dafs versus angles for azimuthal scan (keyword *rxs*).
_sda.txt	state density for the atom number a (keyword *density*).
_atoma.txt	results for one atom at position number 'a' (keyword *allsite*).
_atoma_scan.txt	rxs scan results pour for the atom a (keyword *allsite* and *rxs*).
_tddft.txt	output with the TDDFT option (keyword *tddft*).
_tddft_scan.txt	azimuthal scan in the TDDFT option (keyword *rxs* and *tddft*).
_tddft_conv.txt	convoluted spectra in TDDFT (keyword *Convolution* and *tddft*).

For the analysis of the spherical tensors (keyword *spherical* and *sphere_all*)

_sph_atoma.txt	spherical tensors of the atom a.
_sph_atoma_int.txt	integral of the spherical tensors of the atom a.
_sph_signal_atoma_xan.txt	contribution of each atomic spherical tensor on the average xanes signal.
_sph_signal_atoma_poli.txt	contribution of each atomic spherical tensor on the xanes polarisation number i.
_sph_signal_atoma_rxsi.txt	contribution of each atomic spherical tensor on the rxs reflection number i.
_sph_signal_xtal_xan.txt	contribution of the crystal spherical tensor on the average xanes signal.
_sph_signal_xtal_rxsi.txt	contribution of the crystal spherical tensor on the rxs reflexion number i.
_sph_xtal.txt	spherical tensors of the crystal.
_sph_xtal_int.txt	integral of the spherical tensors of the crystal.
_sph_xtal_rxsi.txt	spherical tensor of the crystal for the rxs reflexion number i.

For the analysis of the cartesian tensors (keyword *cartesian*):

_car_atoma.txt	cartesian tensors of the atom a.
_car_xtal.txt	cartesian tensors for the crystal
_car_xtal_rxsi.txt	cartesian tensors for the crystal for the rxs reflection number i.

II- Basic keywords

1) Output file names

The different output files have names with the same root. The extensions automatically added depending on the chosen option. To define this root use :

Filout
example/cu/cu_out → Name of the output files (without extension)

The files can eventually be in a subdirectory.

2) Radius of the cluster

The final states are calculated inside a sphere, whose radius is defined with the keyword "*radius*" (or "*rayon*"). Only the atoms inside this sphere are considered. By default, the sphere is centered on the absorbing atom.

Radius → Mandatory keyword preceding the radius of the cluster.
3.5 → value in Angstrom of the cluster radius.

For calculations on large energy range (typically used in EXAFS), it can be convenient using a decreasing radius when energy increases. For this purpose, one can set energy ranges with decreasing radius:

Radius
8.3 100 7 250 5 500 4 → 8.3: radius up to 100 eV, 7 radius between 100 and 250 eV…
4 : radius beyond 500 eV

3) Cluster or crystal structure

Under "*crystal*" or "*molecule*" stand all the data describing respectively the unit cell or the molecule. If the calculation is done using the flapw output, this block is useless because the structure is red in one of the flapw output files. Under the keyword, come the mesh parameters (Å) and the angles (degrees). Then come all the atoms (and not only the non-equivalent ones, but when is specified the space group using the keyword "*spgrou*p"). By default and in the absence of the keyword "*absorber*", the absorbing atom chemical specie corresponds to the first atom in the list.

Example 1: cfc copper crystal:

Crystal → Crystal structure
3.610 3.610 3.610 90. 90. 90. → a, b, c, α, β, γ
29 0.0 0.0 0.0 → Atomic number, position
29 0.5 0.5 0.0
29 0.5 0.0 0.5
29 0.0 0.5 0.5

Example 2: FeO_6 octahedron:

molecule

	1.900	*1.900*	*1.900*	*90.*	*90.*	*90.*	→ a, b, c, α, β, γ
26	*0.0*	*0.0*	*0.0*				→ Atomic number, position
8	*1.0*	*0.0*	*0.0*				
8	*-1.0*	*0.0*	*0.0*				
8	*0.0*	*1.0*	*0.0*				
8	*0.0*	*-1.0*	*0.0*				
8	*0.0*	*0.0*	*1.0*				
8	*0.0*	*0.0*	*-1.0*				

The atomic structure can also be given in cylindrical or spherical coordinates. To use cylindrical coordinates, it is sufficient to give only two numbers under "*molecule*". The program will understand they are *a* and *c* and that the positions of the atoms are given by r, ϕ and z. Thus to describe the same octahedron as previously:

molecule

	1.900	*1.900*		→ a, c
26	*0.0*	*0.0*	*0.0*	→ Atomic number, position (r, ϕ and z)
8	*1.0*	*0.0*	*0.0*	
8	*1.0*	*180.0*	*0.0*	
8	*1.0*	*90.0*	*0.0*	
8	*1.0*	*-90.0*	*0.0*	
8	*0.0*	*0.0*	*1.0*	
8	*0.0*	*0.0*	*-1.0*	

To use spherical coordinates, only one number (*a*) must be set after "*molecule*". The position of the atoms is then given by r, θ, ϕ. For the same octahedron:

molecule

	1.900			→ a
26	*0.0*	*0.0*	*0.0*	→ Atomic number, position (r, θ, ϕ)
8	*1.0*	*90.0*	*0.0*	
8	*1.0*	*90.0*	*90.0*	
8	*1.0*	*90.0*	*180.0*	
8	*1.0*	*90.0*	*270.0*	
8	*1.0*	*0.0*	*0.0*	
8	*1.0*	*180.0*	*0.0*	

It is possible, in the non-magnetic case, to specify only the non-equivalent atoms. Then one has to give the space group under the keyword "*Spgroup*". The complete name, as in the international table, must be given. For example, for magnetite, one gets:

Spgroup

Fd-3m:1	→ it is also possible to write 227:1

Crystal
8.3940 8.3940 8.3940 90.0 90.0 90.0

26 .6250 .6250 .6250 ! Fe 16d
26 .0000 .0000 .0000 ! Fe 8a
8 .3800 .3800 .3800 ! O 32e

Note that for the calculation of the symmetry, it is important de define the atom position with a sufficient number of digits (say 10). For instance, for graphite one has to write:

Spgroup
P63mc

Crystal
2.456 2.456 6.696 90. 90. 120. = a, b, c, alpha, beta, gamma
6 0.0 0.0 0.0
6 0.3333333333 0.6666666667 0.0

Putting in the last line for example 0.3333, would create false atoms. Program would stop immediately with an error message.

It is also possible to have an occupancy rate not full for the atoms. Fot this "_t" must be added after keyword "crystal" or "molecule" and a fifth column after the atom position contains this weight :

Crystal_t → (or ***Molecule_t***)
2.456 2.456 6.696 90. 90. 120.
6 0.0 0.0 0.0 0.8 → *weight 80 %*
6 0.25 0.25 0.0 1. → *weight 100%*

During the building of the cluster, when 2 atoms are at the same position, only the one with the highest weight is kept. The final signal is taken with the given weights.

It is possible to use directly the structure given in pdb or cif files. These ones contain all the geometry, the space group… In this case use, one of the following way:

Pdb_file
File_name.pdb

Cif_file
File_name.cif

4) Atomic electronic densities

An electronic configuration is used by default for all the atoms. It is possible to modify it by the use of the keyword "*atom*". Moreover under "*crystal*" or "*molecule*" one must not anymore put the atomic number, by the atom type number. For example in case of a FeO_6 octahedron with the Fe $3d^6 4s^2$ and O $2s^2 2p^4$ configuration:

Atom → keyword preceding the atomic electronic densities
26 2 3 2 6. 4 0 2. → atomic number of the chemical specie of type 1, number
8 2 2 0 2. 2 1 4. of valence orbital and (n,l,pop) of each of these orbitals

molecule

	1.900	*1.900*	*1.900*	*90.*	*90.*	*90.*	→ a, b, c, α, β, γ
1	*0.0*	*0.0*	*0.0*				→ Atom type, position
2	*1.0*	*0.0*	*0.0*				
2	*-1.0*	*0.0*	*0.0*				
2	*0.0*	*1.0*	*0.0*				
2	*0.0*	*-1.0*	*0.0*				
2	*0.0*	*0.0*	*1.0*				
2	*0.0*	*0.0*	*-1.0*				

Important remark: contrary to what one can think, the formal charges attributed to the atoms in the ionic compounds are far from the true charge. Thus one has to perform exchange of charge between atoms with care and in a moderate way. A good technique is, for example for 3 d elements, the good number of "d" electron, following the formal charge, but keeping the neutral atom, putting electrons in the large radius 4s or 4p orbitals.

Another possibility permits to keep the atomic number in front of each atom in the list after *Crystal* or *Molecule* and to give the electronic configuration only for some of them. For this use the keyword:

Atom_conf
3 1 2 4 2 3 2 5. 4 1 1. → nbr of atom with the configuration then index of these atoms,
1 3 2 3 2 6. 4 1 0. Then number of orbital and configuration of them

Crystal
4. 4. 4. 90 90 90
26 0. 0. 0.
26 0.5 0. 0.
26 0. 0.5 0.
26 0. 0. 0.5
26 0.5 0.5 0.5

In the example above the atoms 1, 2 and 4 of the list under « *Crystal* » have the configuration $3d^5 4p^1$. The atom 3 has the configuration $3d^6$. The remaining atoms have the default configuration.

5) Absorbing atoms

All the atoms present in the structure participate to the absorption or scattering. By default, the calculated spectra correspond to the sum of the scattering produced by all the atoms of the same atomic number than the first one in the list under "*crystal*" or "*molecule*".

When one wants to select some of the absorbing atoms, one has to use the keyword "*absorber*". For example, if one wants that the absorbing atom is the n^{th} of the list and only this one (under "*crystal*" or "*molecule*"), put:

Absorber
3 → absorbing atom number (here the 3rd in the list).

If this example goes with the FeO_6 structure defined just above, the result in the output file would correspond to a calculation of an oxygen atom summed over the 6 atoms because they are equivalent by symmetry. If one wants the result from a unique site, use the keyword "*symsite*" or "*allsite*" (see further on).

If there are non-equivalent sites, one has to perform independent calculations. For this, one must specify each atom number under "*absorber*". The name of each of the corresponding output file get the suffix "*_n*" where n it the atom number.

Filout
copper_out

Absorber
1 5 → atom numbers whom results will in output file copper_out_1 and copper_out_5

The summation over these different sites and the eventual energy shifts is to be performed during a following step.

Another possibility is to define the atomic number of the absorbing atoms. This is done with the keyword:

Z_absorber
26 → all the atoms with Z = 26 are absorbing atoms

6) Energy range

The energy range E that one defines in the indata is the energy of the photoelectron relative to the Fermi level. The kinetic energy, Ec, of the photoelectrons when they leave the cluster must be positive. Ec is related to the input energy by:

$$Ec = E - W - Vm,$$

where W is the work function and Vm the average potential (equivalent to the muffin-tin ground) in the cluster.

In the case of a calculation using the *flapw* the coulombian part of the average potential Vm is zero. So Vm is greater than zero. Thus the work function is not anymore subtracted and the input energy is defined relatively to the vacuum.

By default the energy range is -5 to 60 eV by 0.5 eV step. One can change the range, the step or even have a variable step using:

Range → keyword for the energy range
1. 0.5 60. → E_{min}, step, E_{max}

Other example with variable step:

Range
1. 0.1 10. 0.5 20. 1. 60.00 → E min, step, E intermediate, step …

To get a continuously increasing step (k step constant) put:

Rangel
1. 0.1 200. → E min, step at the Fermi level, E max

By default, the output energy range is relatively to the Fermi level. If one wants that the output energy is the photon energy put the keyword:

Energpho

7) Multiple scattering mode

If one wants to calculate in the multiple scattering mode use the keyword:

Green

Then the potential is automatically a muffin-tin one. The mode is faster than the finite difference method, so one has to use it first.

8) Threshold type

By default the threshold is the K one. For other threshold put the keyword:

Edge → keyword preceding the threshold type
L1 → threshold (K, L1, L2, L3, M1 …)

It is possible in a single run to calculate 2 edges with the same initial (n,l), that is the edges L2 and L3 or M2 and M3 or M4 and M5 … For this write:

Edge → keyword preceding the threshold type
L23 → threshold L2 and L3, or M23, M45, N23, N45.

9) Multipolar expansion

By default only the transition electric dipolar component (E1E1) is calculated. This is modified by the keywords:

Quadrupole → quadrupolar calculation (E1E2 and E2E2)
Octupole → octupolar calculation (E1E3 and E3E3)
Dipmag → magnetic dipole calculation (E1M1) and (M1M1)
E1E2 → calculation of E1E2
E1E3 → calculation of E1E3
E2E2 → calculation of E2E2
E3E3 → calculation of E3E3
E1M1 → calculation of E1M1
M1M1 → calculation of M1M1

No_E1E1 → No calculation of the dipolar-dipolar component (E1E1)
No_E2E2 → No calculation of the quadrupolar-quadrupolar component
No_E1E2 → No calculation of the dipolar-quadrupolar component
No_E1E3 → No calculation of the dipolar-octupolar component
Dip_rel → To take into account the spin-orbit transition term in E1E1

10) Polarization and dichroism

By default the calculation is performed along 1, 2 or 3 orthogonal polarizations in the dipole mode (and up to six in quadrupolar) depending of the symmetry, and only the average corresponding to a powder is given. To get the spectra for the different polarization, use:

Polarize

To get linear or circular dichroism, one must specifies polarization and wave vector (in quadrupolar) orientations. These vectors must then be given in the non-orthogonal, but normalized crystal basis:

Polarize
1.0 1.0 0.0
1.0 -1.0 0.0
0.0 0.0 1.0

For a quadrupolar calculation, one has to specify the wave vector after the polarization:

Polarize
1.0 1.0 0.0 0.0 0.0 1.0
1.0 -1.0 0.0 0.0 0.0 1.0
0.0 0.0 1.0 0.0 0.0 0.0

Each line contains the polarization vector, the wave vector. If the wave vector is zero this polarization is calculated in the dipolar approximation.

It is possible to perform an average on different polarizations adding a new number at the end of the line is the corresponding weight. If at least two weights are non zero, in the output, there will be a new column with the weighted average of the different polarization.

Polarize
1.0 1.0 0.0 0.0 0.0 1.0 1.
1.0 -1.0 0.0 0.0 0.0 1.0 1.
0.0 0.0 1.0 0.0 0.0 0.0 0.

If one wants to have a circular polarization, one just has to put this one to zero followed by the value of the wave vector:

Polarize
0.0 0.0 0.0 0.0 0.0 1.0

In the output one will have the calculation in right polarization, then the left polarization, then the difference. In this example, the calculation corresponds to the polarization x+iy and x-iy.

II-10) Doping

It is possible, more specifically for crystal to calculate the absorption of a doping element set in substitution in place of another one. For this one uses the keyword « Doping », followed by the atomic number of the doping element and the index of the atom to substitute in the list under « *Crystal* »:

Doping
27 1 → substitution by Cobalt of the atom in the first site.

The doping atom is supposed to be at low concentration, thus the clust built around it is the same than the one given by the crystal. Symmetries are kept.

III- Non resonant X-ray inelastics cattering (NRIXS)

The non-resonant inelastic scattering (NRIXS or X-Raman) is very close to XANES. The first order term is equivalent to the dipolar approximation in XANES. One can obtain a more precise simulation, depending on the momentum transfer q, using the keyword:

NRIXS
12. 1. 18 → q first value, step , last q value

The corresponding output file will have the extension "_nrixs".

If one wants the results resolved in ℓ, the Bessel quantum number associated to the expansion of $exp(i\boldsymbol{q}.\boldsymbol{r})$ in the transition operator, write:

All_nrixs

By default the maximum value of ℓ is 3. To change it, write :

Lmax_nrixs
4 → ℓ maximum value.

IV- Anomalous or resonant diffraction

1) Reflections and polarization

In case of anomalous (or resonant) diffraction (DAFS, DANES, RXS, RXD) calculation, put the keyword "*RXS*" (or "*DAFS*") followed by the index of the beams to calculate. The orientation of the polarization and wave vector can be described by different way. When working in σ–σ, σ–π, π–π or π–s, or in circular polarization, put the number 1, 2, 3, 4 or 5 for the polarization respectively σ, π, circular right, circular left or linear along a general direction, in input then in output.

RXS
0 0 2 *1 2 45.* → reflection indexes, σ, π, azimuth
0 0 2 *1 1 45.* → reflection indexes, σ, σ, azimuth

When the polarization is linear but not σ or π, but with an angle α such that α = 0° when it is σ and 90° when it is π, one must write:

RXS
0 0 2 *1 0. 5 10. 45.* → reflection indexes, σ, angle, rectilinear, angle, azimuth
0 0 2 *1 0. 5 -10 45.*

Note that in this case, one must specify both incoming and outgoing polarization angles, even when one of them is σ, π or circular. When it is circular, the angle is not taken into account.

Let's take $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$, the unit cell vectors, $\boldsymbol{i_a} = \boldsymbol{a}/|\boldsymbol{a}|$, $\boldsymbol{i_c} = \boldsymbol{c}/|\boldsymbol{c}|$, and $\boldsymbol{Q}$ the normalized diffraction vector. We define the azimuthal angle, φ, using the base $(\boldsymbol{I},\boldsymbol{J},\boldsymbol{Q})$ such that:

$$\boldsymbol{I} = \boldsymbol{Q} \times \boldsymbol{i_c} \times \boldsymbol{Q}/|\boldsymbol{i_c} \times \boldsymbol{Q}|, \qquad \boldsymbol{J} = \boldsymbol{Q} \times \boldsymbol{I}$$

When $\boldsymbol{Q}$ is along $\boldsymbol{c}$, $\boldsymbol{i_c}$ is substituted by $\boldsymbol{i_a}$. One then gets, versus the Bragg angle θ_B the incoming and outgoing wave vectors:

$$\vec{k}_i = \cos\theta_B \cos\varphi\vec{I} - \cos\theta_B \sin\varphi\vec{J} - \sin\theta_B\vec{Q},$$
$$\vec{k}_s = \cos\theta_B \cos\varphi\vec{I} - \cos\theta_B \sin\varphi\vec{J} + \sin\theta_B\vec{Q}.$$

For the σ and π polarizations, one gets:

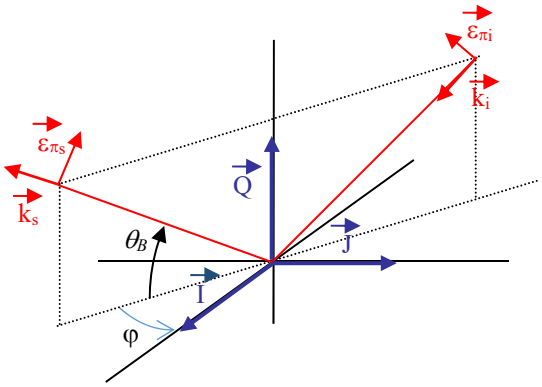
$$\vec{\varepsilon}_\sigma = \sin\varphi\vec{I} + \cos\varphi\vec{J}$$
$$\vec{\varepsilon}_{\pi i} = \vec{k}_i \times \vec{\varepsilon}_\sigma = \sin\theta_B \cos\varphi\vec{I} - \sin\theta_B \sin\varphi\vec{J} + \cos\theta_B\vec{Q}$$
$$\vec{\varepsilon}_{\pi s} = \vec{k}_s \times \vec{\varepsilon}_\sigma = -\sin\theta_B \cos\varphi\vec{I} + \sin\theta_B \sin\varphi\vec{J} + \cos\theta_B\vec{Q}$$

By this way, φ increases when the sample is rotated trigonometrically. For example with an orthogonal unit cell: reflexion (h,0,0), $(\boldsymbol{I},\boldsymbol{J},\boldsymbol{Q}) = (\boldsymbol{i_c}, -\boldsymbol{i_b}, \boldsymbol{i_a})$

1 1 0. → corresponds to σ-σ with polarization along $-\boldsymbol{i_b}$.
1 1 90. → corresponds to σ-σ with polarization along $\boldsymbol{i_c}$.

reflexion (0,0,ℓ), $(\boldsymbol{I},\boldsymbol{J},\boldsymbol{Q}) = (\boldsymbol{i_a}, \boldsymbol{i_b}, \boldsymbol{i_c})$

1 1 0. → corresponds to σ-σ with polarization along $\boldsymbol{i_b}$.
1 1 90. → corresponds to σ-σ with polarization along $\boldsymbol{i_a}$.



If one does not put the angle, this implies that one performs a φ scan and all the amplitudes are calculated for all the angles by 2° step. There is then a supplementary output files with the extension "_scan.txt".

It is also possible to perform a 360° scan by 2° step for the tilinear incoming or outgoing polarizations. For this, one has to write 10 in place of the σ–π notification:

RXS
0 0 2 *10 1 45.* → incoming polarization is scanned
0 0 2 *2 10 45.* → outgoing polarization is scanned

The first value (angle = 0°) corresponds to the σ polarization. 90° corresponds to π polarization.

It is possible to write the exact polarization directions. This can be useful for peculiar uses as in photoemission. In case of linear polarization write:

RXS
0 0 0 → Reflection index
0. 0. 1. 0. 1. 0 → ε_i, k_i
0. 0. 1. 0.7071 0.7071 0. → ε_s, k_s

For circular polarization, it is complex:

RXS
0 0 0 → reflection index
0.7071 0.7071 0. 0. 0. 0. 1. 0. → ε_i, k_i (ε_{xr} ε_{xi} ε_{yr} ε_{yi} ε_{zr} ε_{zi} k_{ix} k_{iy} k_{iz})
0.7071 -0.7071 0. 0. 0. 0. 1. 0. → ε_s, k_s

When one does not want phase term between atoms, for example to simulate photoemission, just write 0 0 0 as reflection index.

Note that it is possible to choose any other origin for the azimuth, just using another vector than $\boldsymbol{i_c}$ to define the basis vector $\boldsymbol{I}$ and $\boldsymbol{J}$. For this just write:

Zero_azim
0. 1. 1. → vector in the direct crystal base

It is now possible to calculate the self-absorption corresponding to the incoming and outgoing photon polarizations. For this put the keyword:

In some cases, as in biology, one has a very large number of diffracted beams. It is then simpler to specify the beams to calculate using experimental files. In this case one must give the corresponding file names containing the experimental spectra, the orientation matrix giving the incoming polarization versus the unit cell and for each file the rotation angle. One thus has to write:

RXS_exp

11.231547 3.519121 -71.823997 → matrix
12.573563 -170.027649 -6.364535
-86.558281 -5.978752 -11.279972
0. → angle for the first file
MoFe/Refl_R5to2_1.txt → name of the first file
10. → angle for the second file
MoFe/Refl_R5to2_2.txt → name of the second file …

Each experimental file contains some number of spectra in column along the format :

-1 16 28 -1 20 18 → (h,k,l) for each reflections (integer)
Energy D[-1,16,28] D[-1,20,18] → one line of comment
7080 -3.19 -7.96 → Energy, intensity for each reflections
7100 9.75 16.65

One must have at least one space between each number, but no tabulation or coma between the numbers. The number of digit or space between the numbers is free.

Self_abs

Then one gets in the output files, after each reflection two new columns containing the linear absorption coefficients, the unit being the μm^{-1}. They contain after the convolution also the absorption coming from the other atoms and the other edges. That is that the absorption before the edge is not zero. The new data allows the correction due to the self-absorption in order to compare with experimental spectra. The corrected spectra are, after convolution in columns following the non-corrected spectra. Their names begin with "Ic".

One can make a more sophisticated correction taking into account the birefringence. For this put the keyword:

Full_self_abs

It is then necessary to calculate all the reflections along the 4 polarizations $\sigma\sigma$, $\sigma\pi$, $\pi\sigma$ and $\pi\pi$ and in this order:

RXS
2 0 0 1 1 0.
2 0 0 1 2 0.
2 0 0 2 1 0.
2 0 0 2 2 0.

In first approximation, this correction is equivalent to *Self_abs*. It allows the taking into account of the rotation of the polarization when the electromagnetic wave propagates into the media.

Note that from this, it is possible to calculate circular polarizations reflection intensity for any value of the Stokes parameters. This part is performed in the "convolution" step. See thus the corresponding paragraph.

By default the scan step is 2°. To modify it, use:

Step_azim
0.5 → step indegres of the azimuthal scan

2) Non resonant magnetic scattering

The non-resonant magnetic scattering is taken into account for the RXS. This term can be decreased, or put to zero, using a multiplicative factor:

No_res_mag
0.8 → factor

An additional factor can be applied to the contribution from the orbital moment. This factor corresponds to L/2S (and not L/S):

No_res_mom
-0.3 → factor for the orbital moment

By default, this factor is calculated using the Hund rules and multiplied by 0.2.

V- Potential, magnetism and calculation technique

1) Relativistic calculation

To perform a relativistic calculation, put the keyword:

Relativism

2) Spin polarized calculation

If one wants to make a spin polarized calculation put the keyword:

Magnetism

By default this calculation is done neglecting the spin-orbit coupling. If one wants to take into account this last put the keyword:

Spinorbite

The keyword "*magnetism*" is thus useless. If the polarized potential comes from LAPW, "*spinorbite*" or "*magnetisme*" must be before "*flapw*".

With the spin-orbit interaction, the calculation is automatically relativistic. To get a non-relativistic calculation put:

Nonrelat

When the calculation does not use the flapw output, the use of the keyword "*atom*" is necessary to specify the electronic configuration, different for the spin up and spin down parts. The orbital occupancy must be given for each spin in doubling the corresponding columns.

Example of metal fcc nickel:

Magnetism

Atom
28 2 3 2 5. 4. 4 0 0.5 0.5

Crystal
3.52387 3.52387 3.52387 90. 90. 90.
1 0.0 0.0 0.0
1 0.5 0.5 0.0
1 0.5 0.0 0.5
1 0.0 0.5 0.5

The configuration is $3d^9 4s^1$ with 5 electrons 3d up and 4 electrons 3d down, 0.5 electron 4s up and 0.5 electron 4s down.

In case of an antiferromagnetic structure, one must put a minus sign in front of the atom type number to specify the atom with the reverse spin. For example in V_2O_3 monoclinic:

Atom
23 3 3 2 2. 0. 4 0 1. 1. 4 1 0.5 0.5
8 2 2 0 1. 1. 2 1 2. 2.

Crystal
7.255 5.002 5.548 90.0 96.75 90.0 / a, b, c, alfa, beta, gamma
1 0.34380 0.00080 0.29910 V8
1 0.65620 0.99920 0.70090 V6
1 0.84380 0.99920 0.29910 V3
1 0.15620 0.00080 0.70090 V7
-1 0.84380 0.50080 0.79910 V4
-1 0.15620 0.49920 0.20090 V5
-1 0.34380 0.49920 0.79910 V2
-1 0.65620 0.50080 0.20090 V1

2 0.40700 0.84500 0.65200 O 1 8f
2 0.09300 0.84500 0.34800 O 2 8f
2 0.59300 0.15500 0.34800 O 3 8f
2 0.90700 0.15500 0.65200 O 4 8f
2 0.90700 0.34500 0.15200 O 5 8f
2 0.59300 0.34500 0.84800 O 6 8f
2 0.09300 0.65500 0.84800 O 7 8f
2 0.40700 0.65500 0.15200 O 8 8f
2 0.25000 0.19100 0.00000 O 1 4e
2 0.75000 0.80900 0.00000 O 2 4e
2 0.75000 0.69100 0.50000 O 3 4e
2 0.25000 0.30900 0.50000 O 4 4e

3) Spin axis

By default the spin axe is along the *c* axis but in the trigonal unit mesh where it is along the *c* axis of the associated hexagonal unit mesh. This axis can be orientated along any (but uniform) direction:

Axe_spin
-0.08909 0. -0.15025 → in unit mesh

Another way to specify this axis is using the Euler angles. The orthogonal basis to do that is such that z is along c, but for trigonal system where z is along the hexagonal axis, x is along b x c and y is along z x x. One then has to write:

Ang_spin
45. 90. 0. → rotation around z, then around y, then around x. In this case spin axis is along (1,1,0) in the internal basis

Note that it is possible to define non collinear spin using atomic local basis. In this case one has to define the Euler local angles after the keyword crystal or molecule, in the line just before the corresponding atoms. See "non-spherical atom". Example:

```
Crystal
 7.7400   7.7400   3.8400  90.   90.   90.
45. 90.                                  ! spin axis along (1 1 0)
 1  0.0    0.0     0.0
 2  0.25   0.25    0.5
135. 90.                                 ! spin axis along (-1 1 0)
 1  0.5    0.0     0.0
 2  0.75   0.25    0.5
315. 90.                                 ! spin axis along (1 -1 0)
 1  0.0    0.5     0.0
 2  0.25   0.75    0.5
225. 90.                                 ! spin axis along (-1 -1 0)
 1  0.5    0.5     0.0
 2  0.75   0.75    0.5
```

4) Self-consistent calculations

By default a calculation cycle is performed over the occupied states to determine the Fermi energy. The XANES calculation corresponds to the cycle 2, but this one is done with the initial potential. To avoid this Fermi (non SCF) energy determination, use the keyword :

No_Fermi

To perform a self-consistent calculation, use the keyword:

SCF

The calculation is then really self-consistent. The potential is calculated again at each cycle. The final XANES calculation uses this SCF potential. By default the convolution uses the calculated Fermi energy as cutting energy.

When using SCF calculation, the cluster radius for the SCF is the same than the one for the XANES. For a single evaluation in one cycle of the Fermi energy the radius is equal to the minimum between the XANES cluster radius and 3.5 A. In both cases, this radius can be change using the keyword :

R_self
3. → Value of the radius for the SCF and/or Fermi energy evaluation.

With SCF calculation, the maximum number of cycle is fixed to 30. To modify this number use the keyword:

N_self
20

The electronic density of the cycle n+1 is interpolated between the electronic density of the two previous cycles. The initial weight of the cycle is 0.1. This weight decreases or increases according to the quality of the convergence between 4 and 0.25 times the initial value. To change this initial weight use:

P_self
0.05 → Initial weight.

The convergence is considered as realized when the variation of the total energy is less than N_a x ΔE_{conv}, where N_a is the number of atom and ΔE_{conv} a criteria fixed at 0.1 eV. To modify ΔE_{conv} put:

Delta_E_conv
2. → Value of ΔE_{conv}.

It can happend, that when the weight increase up to 2 or 4 times the p_self, value, the calculation become very unstable (it can be seen on the orbital occupancy). On can then limit this increse by the parameter p_self_max:

P_self_max
0.05 → value of the maximum weight. When used, the best is to put it equal to p_self.

The SCF calculation is done with a non-excited cluster. The excited potential of the absorbing atom is taken into account only in the K and L_1 edges in the XANES final calculation by difference. If one wants to perform a SCF calculation with an excited cluster, use the keyword:

SCF_exc

If one wants perform a simulation with SCF in excited state but without any screening, that is with a cluster charged +1, with SCF_EXC one has to use keyword "*Screening*" with the value 0 (see this keyword).

For a magnetic calculation, by default the spin polarization is kept fixed in amplitude. The total number of spin up and spin down electron is fixed along the self-consistent (for an anti-ferro, for the total on the atoms, the number of majoritarian spin and minoritarian spin electron are kept fixed). To have it free (equivalent to version before 7th of June 2012), use the keyword:

SCF_mag_free

5) Hubbard correction

To include a Hubbard correction, use the keyword:

Hubbard
5. → value in eV of the Hubbard parameter (U-J).

This correction is applied to the "localized valence orbitals" of the chemical specie first in the list under "*crystal*" or "*molecule*" or under "*atom*" if used. Most often, it is convenient to perform also a self-consistent calculation. To apply different Hubbard corrections on different

atoms, just put several numbers in the same line, following the order of the chemical species. Note that in principal this correction can be applied only on insulating compounds.

6) TDDFT calculations

TDDFT calculations can be performed using the keyword:

TDDFT

Then a first mono-electronic (LSDA) calculation is performed, followed by the TDDFT cycle. Then a correction is performed making a mixing between the edges. This can be useful for the L_{23} edges of the transition *3d* elements. Calculations use a local Kernel with its Coulomb and exchange-correlation parts. To have only the Coulomb part, use the keyword:

RPA

7) Energie zero

From June 2016, the zero energy has been modified. It is now set at the Fermi level. To get the previous version origin use the keyword :

Old_zero

VI- Sophisticated keywords

1) Use of atomic electronic densities coming from external files

When using electronic densities coming from external files, these ones must be specified with the keyword "*atom*". One eventually has to specify one atom more because the absorbing atom is a special chemical specie different of the non-excited atoms. Its files must also contain the electron initial orbital before excitation (for instance the 1s one for a K edge). For the format of these files see chapter F. In the case there are two atoms:

Atom → keyword preceding the atomic electronic densities
Fe*_exc.txt* → name of the file containing the excited atom
Fe*.txt* → name of the file containing the type 1 atom
Oxygen*.txt* → name of the file containing the type 2 atom

One can also put one or several atoms calculated internally among the exterior files:

Atom
Fe*_exc.txt* → name of the file containing the excited atom
Fe*.txt* → name of the file containing the type 1 atom
8 2 2 0 2. 2 1 4. → type 2 atom calculated internally

Once defined the atoms types, the molecule or mesh description uses the atom type number and not the atomic number. For example, for the cfc copper crystal:

Atom
c:\users\joly\dirac\cu\trdrslcu.e01 → excited copper file
c:\users\joly\dirac\cu\trdrslcu.001 → standard copper file

Crystal → Crystal structure
3.610 3.610 3.610 90. 90. 90. → a, b, c, α, β, γ
1 0.0 0.0 0.0 → Type number, position
1 0.5 0.5 0.0
1 0.5 0.0 0.5
1 0.0 0.5 0.5

The first index is now the atom type number (but the excited one) in the list under "atom".

2) Uses of atomic electronic densities of Clementi and Roetti

By default the program calculate the atomic basis using a Hartree-Fock-Dirac procedure. If you prefer the Clementi and Roetti basis use the keyword:

Clementi

Note that the Clementi basis exists only for Z < 55. When using this basis, the self-consistent calculations are not anymore possible as well as the automatic evaluation of the Fermi level (The program takes automatically the option « No_Fermi »).

3) Non spherical atomic electronic densities

When calculating using the finite difference method, it is possible to define non spherical atomic electronic densities. This is done under the keyword "crystal" or "molecule". For each non spherical atom one performs an expansion in spherical harmonics of these non-spherical orbitals. In practice, on the line "atom type, position", one adds an integer giving the number of non-spherical orbitals, then next lines the expansion in (l,m) of each of these orbitals with at the end the number of electron it contains. Optionally a rotation of the local atomic basis can be performed using the Euler angles (see keyword "*spin_axis*", for the Euler angle definition). In this case, the Euler angles must be given in the line in front of the atom. Example:

molecule

1.9 1.9 1.9 90. 90. 90.	→ a, b, c, α, β, γ
0. 45. 0.	→ 45° rotation around the Oy axis
1 .0 .0 .0 1	→ there is one non spherical orbital
0. 0. 0. 0. 0. 0. 1. 0. 0. 1.	→ (l,m) in the natural order, here (l=2,m=0) has 1 *2*
1.0 0.0 0.0	electron
2 -1.0 0.0 0.0	
2 0.0 1.0 0.0.	
2 0.0 -1.0 0.0	

4) Orbital dilatation

It is possible to modify the valence orbitals defined above dilating or contracting them. This can be very useful for ionic material, for instance oxygen 2^-, where the atomic bases are calculated for neutral atoms. For this purpose introduce the "*dilatorb*" then for each orbital one wants to dilate, the atomic type (number in the list "*atom*"), the valence orbital number and the expansion coefficient:

Dilatorb

3 1 0.3
3 2 0.3

5) Screening

By default, the screening is one electron on the first non-full valence orbital of the absorber. If one wants to modify this value or the number of the orbital, use the keyword "*Screening*" followed by the quantum numbers of the valence orbital and the value in number of electron (better inferior to 1 !) of the screening. In this case the cluster is not anymore necessary neutral.

Screening

3 2 0.2 → n, l, and screening on the valence orbital

One can omit the orbital quantum number. In this case the code, by default will choose the first non-full valence orbital and one just write:

Screening

0.2 → Screening on the valence orbital

6) Mesh or molecule charge

The unit mesh must be neutral. A molecule is also often neutral. A test is performed in the program to verify this neutrality. If one wants to omit it, put:

Chlibre

7) Exchange-correlation potential

By default the calculations are done using the real Hedin, Lundqvist and Von Barth potential. If one wants to use the Xalpha potential, one must introduce the keyword *Xalpha* followed by the value of the corresponding parameter:

Xalpha
0.3333 → value of the Xalpha parameter

Remark : the value of the Xalpha parameter the closest to the other models is 2/3.
In the case of using the exchange-correlation potential coming from *flapw*, if one wants to keep this potential independent of the energy put the keyword "*xalpha*" with any value beneath. The potential will not be Xalpha but the one calculated by *flapw*.

If one prefers to use the Perdew and Wang's potential, put the keyword:

Perdew

This potential will be used with the parametrization of Moruzzi, Janak and Williams but keeping the energy dependency proposed by Hedin and Lundqvist.

8) Reference of the photoelectron wave vector

By default the reference of the electronic wave vector (and so of the kinetic energy outside the sphere of calculation and the muffin-tin ground in case of muffin-tin calculation) is taken as the average of the potential between the absorbing atom and the first crown when calculating in green and at the outer sphere frontier in FDM. It is possible to impose this ground potential at the Fermi energy. The dependence versus the kinetic photoelectron energy is then added automatically to this term. Put then the keyword:

V0imp
-11.5 → value of the ground potential at the Fermi energy.

9) Maximum potential

For a calculation performed on a molecule, the potential increases when going away from the atoms. When this molecule is not in the gaz phase, but in solution or in any relatively dense surrounding, this incease is artificial. In case of calculation under the finite difference mode, this reach to faulse bounded states very thin in energy. It can be usefull to give a maximum value to this potential to avois this phenomena with the use of the keyword "*Vmax*", followed by the value of this potential :

Vmax
-6.

10) Complex energy

It is possible to use a complex energy when working in the multiple scattering mode (green). For this, one has to specify the imaginary part (positive) of this energy in a table versus the photoelectron energy, under the keyword "*Eimag*":

Eimag
0. 0.5
10. 0.7
30. 3.
50. 5.
100. 6.

When a uniform broadening is sufficient, it is not necessary to specify the photoelectron energy:

Eimag
0.1 → value of the uniform width (eV)

The use of a small width (0.1 eV) is sometimes useful for the calculations at low kinetic energy of the photoelectron because the localized level (3d or 4f) can be too thin in energy to be correctly evaluated. It is even truer for photoemission calculation (see keyword "*photoemission*"). If this broadening is small it has no effect on the forthcoming convolution to take into account the widths of the hole and final states.

11) Radius of the cluster for the superposition of the potential

The potential inside the sphere of calculation with a radius R_s set under the keyword "*radius*", is calculated by superposition. To avoid frontier problems, the atoms taken into account for the superposition are all the atoms inside the calculation sphere plus an outer shell. By default this outer shell is 2.5 Å thick, giving thus a new sphere with a R_s + 2.5 radius. If one wants a bigger radius (useful for the oxides) put the keyword:

Rpotmax
15. → radius of the cluster for superposition in Angstrom

12) ℓ+1 approximation for the selection rule

If one wants to make the ℓ +1 approximation where only the transition Δ ℓ = +1 is authorized (so one neglects Δ ℓ = -1, for example for the threshold L_2 and L_3, the transitions are only toward the *d* states), put the keyword:

lplus1

In the same way if you want only the ℓ -1 states put:

lminus1

13) Rydberg series

One can add an outer sphere having a -1/r potential to analyze Rydberg series. In this case put the keyword "*Rydberg*":

Rydberg

14) Cluster origin

By default, the cluster origin is set on the absorbing atom. If one wants that this origin is not changed from the indata file put the keyword:

Noncentre

If one wants to impose a specific center put:

Center
0 0.25 1 → coordinates in mesh parameter unit of the center

The center can be automatically chosen at the center of the cluster when writing nothing after the keyword center:

Center

The center can be chosen at the center of the cluster considering only the chemical specie of the absorbing atoms with the keyword:

Center_abs

15) Cut of the potential

To get a cut of the potential in the output, along a line or a plan put:

Trace

0 1. 0. 0. 0. 0. 0. → l,a,b,c,p,q,r

l = 1, cut along a line with vector (a,b,c) crossing the point (p,q,r) in unit mesh parameter
l = 2, cut along the plane ax + by + cz = p
l = 3, gives all the points

16) Density of state

To get the partial projection of the density of states and their integral for any harmonics on the absorbing atom, put the keyword:

Density

Then one gets a new output file with the extension *_sd0.txt*. It contains, in column, first the integral of the total atomic electron density, then the density and its integral of each (ℓ,m) followed by the sum over m, that is the density and its integral for each ℓ. For magnetic calculation, the expansion is split between the "up" and "down" components. By default, real harmonics are used because they are directly the familiar p_x, p_y, p_z, d_{xy}, d_{xz}… states. The correspondence is the following:

(0,0)	(1,-1)	(1,0)	(1,1)	(2,-2)	(2,-1)	(2,-0)	(2,1)	(2,2)
s	p_y	p_z	p_x	d_{xy}	d_{yz}	d_{z^2}	d_{xz}	$d_{x^2-y^2}$

It can be interesting, for example to get the orbital magnetic moment, to prefer output with the usual complex spherical harmonics. For this, use the keyword:

Density_comp

General remark on the values one gets: Usually for a transition metal, at the end of the *d* band, the integral must be close to 10 (because there are 10 *d* electrons!). At the end of the rather unlocalized *s* and *p* bands, the integrals rarely reach 2 or 6, because the electrons are counted only inside the atomic sphere of radius R_{mstd} (see in the bav file for its value). These orbitals having a rather big radius they are not all inside such atomic sphere. Calculation being performed in the continuum one also has to recall that *n* is not anymore a "good" quantum number. Consequently the integral continue to increase indefinitely with energy. At the end of a *d* (or *f*) band, rather localized, one nevertheless reaches more or less at 10 (or 14). In this case one can find the Fermi level energy just looking the energy where the integral reach the supposed number of electron in the corresponding level of the atom. Sometimes the integral never reach 10 (or 14) or goes far higher. One of the reasons can be that the starting energy is too high, one thus loses the beginning of the band, and another reason can be the energy grid is not sufficiently thin. One has, in this case to take a path smaller (down to 0.01 eV or even less for 4*f* elements). In order to avoid such a thin grid, it is also possible de broaden a bit these localized states using the keyword "*Eimag*" (this works only in "Green" mode).

To get the projection on all the atoms in the cluster (or unit cell) put the keyword "*Density_all*" in place of "*Density*". Then one gets *n* new output files with the extensions *_sdi.txt*, "*i*" being the atom number:

Density_all

17) Spherical tensors

To get the spherical tensors (in number of electron) put the keyword:

Spherical

One gets new files with the extension *_sph_atom1.txt* and *_sph_xtal.txt* for the atom and crystal. If one uses such file as indata for the convolution process one gets the f' and f'' of each tensor component of the atom. Another file *_sph_int_atom1.txt* contains the integral of the spherical tensors.

To get the contributions of the tensor components on each polarization and reflections, put in place of "*spherical*" the keyword:

Sphere_all

Then one gets a series of output files with the extensions *_sph_signal_xan.txt*, *_sph_signal_pol1.txt, _sph_signal_rxs1.txt* for the contributions on each polarization and reflections. The number after *pol* or *rxs* is the number of the polarization or reflection.

18) Cartesian tensors

To get the atomic cartesian tensors put the keyword:

Cartesian

One gets a new output file with the extension _car.txt. Then, one can use other keywords making that from this output file will be calculated f' and f '' for any tensor component. For this purpose put the keyword "*fprim*" in the indata file.

19) Calculation area boundary

By default in FDM, the meshing is performed in a sphere extending up to the last atom inside the sphere of radius given under "radius" plus the atomic radius (by default 0.65 A) plus one inter-point distance (0.2 A by default). In order to use a bigger sphere put

Overad
1.2 → distance over the last atom + its radius to take into account.

20) Displacement of the absorbing atom

To move the absorbing atom in reference to its position given under "*molecule*" or "*crystal*" put:

Dpos

0.2 0.0 0.0 → displacement vector in Angstrom

21) Getting back the tensor components from a previous calculation

It is possible to get back the tensor component from a previous calculation (it is in the *fdmnes_out_bav.txt* type file) and to compute other polarizations putting the key word "*Extract*" followed by the corresponding name:

Extract
c:\users\joly\xanout\calcul_prec_bav.txt

In case of calculations for different absorber position whose number is the number of output files, one has to extract the tensors from these n files if there are n nonequivalent absorbing atoms. This is automatic. If the calculation is to be performed on only one or some of the non-equivalent atom sites, this must be specified by the keyword "*absorber*" followed by the keyword "*extractpos*" to select in the bav file the corresponding atom:

Absorber
4 8

Extractpos
2 3 → in the bav file, the prototypical atoms 2 and 3 are chosen. Their tensors are used respectively by the atoms 4 and 8 in the list in the indata file.

It is possible to make rotations of the local repair. It can be useful when using tensor calculated in a different base. It is possible de make 1, 2 or 3 rotations around the axes 0z, then Ox, then Oy. Each rotation defines a new local base, starting point of the next rotation. For this write:

Rotsup
30. 0. 45. → 30° rotation around Oz, 0° around Ox then 45° around Oy.

For the same purpose on can apply symmetry operation on the extracted tensors. They are codified as explained in the manual with the "*symsite*" keyword. They must be given in the same order than the extracted files. These codes are given after the keyword *extractsym*:

Absorber
4 8

Extractsym
1 25 → *code 1 for identity, 25 for inversion.*

22) Energy shift of the spectra

If one has gotten a reference for the initial orbital, it is possible to give it under the keyword "*Epsii*". This will produce a shift of the output spectra equal to the difference between this energy and the energy calculated in the program. It is safer to perform this operation with the shift parameters during the convolution step.

Epsii
6253.1 → positive value in eV.

23) Expansion in path

In the multiple scattering mode it is possible to avoid the matrix inversion, but to make an expansion in path. One has to give the number of way:

Chemin
3 → number of path

24) Spectra by atom

If one wants to get the signal coming from each atom one has to add the keyword:

Allsite

One then gets, at most of the usual output files, new output files of the type atom1.txt, atom2.txt, etc… The suffixes _atom1, _atom2 correspond to the number of the atom.

25) Use of densities and potential coming from FLAPW

If the potential is imported from a FLAPW calculation, one has to introduce the keyword "*flapw*" in place of "*atom*". The keyword "*crystal*" or "*molecule*" becomes also unnecessary. Then must stand the names of the 5 FLAPW output files in case of spin un-polarized calculation and the 7 files in case of spin polarized calculation:

Flapw → names of the output FLAPW files
tio2.struct structure and symmetry
tio2.vcoul coulombian potential
tio2.r2v exchange-correlation potential
tio2.clmsum electronic density
tio2.ti1s initial wave function

In case of polarized calculation the keyword "*magnetism*" must be before the keyword "*flapw*":

Magnetism

Flapw
tio2.struct structure and symmetry
tio2.vcoul coulombian potential
tio2.r2v exchange-correlation potential spin up and spin down
tio2.clmsum total electronic density
tio2.clmup valence electron electronic density, spin up
tio2.clmdn valence electron electronic density, spin down
tio2.ti1s initial wave function

The last file contains the wave function of the initial core orbital. If one is ok with the initial wave function calculated internally, one can avoid it. One must in this case substitute the keyword "*flapw*" by "*flapw_psi*".

If one wants to have an energy dependent exchange-correlation potential, one must add the keyword "*Hedin*".

By default, the absorbing atom is the first one in the "*struct*" file list. If one wants that it is the n^{th}, put the keyword:

absorber
n

For the actual version of wien2k and magnetic calculations, the exchange-correlation potential for spin up and spin down is given in two different files. In this case one must use the keyword:

Flapw_n
tio2.struct
tio2.vcoul
tio2_up.r2v exchange-correlation spin up
tio2_dn.r2v exchange-correlation spin down
tio2.clmsum
tio2.clmup
tio2.clmdn
tio2.ti1s

when not using the wien2k core state use :

Flapw_n_p
tio2.struct
tio2.vcoul
tio2_up.r2v
tio2_dn.r2v
tio2.clmsum
tio2.clmup
tio2.clmdn

Note also that sometimes, it is necessary to increase the value of number of point in the radial mesh. In this case the value to put is given in an error message. It is possible using the keyword nrato.

Nrato
950 → new value given in the error message

26) Jump in the indata file

It is possible to jump over a part of the information written in the indata file with the keywords "*Jump*" and "*Endjump*". All what is between them is not red. For example:

Jump

Quadrupole
Spinorbite

Endjump → the keywords "*Quadrupole*" and "*Spinorbite*" are not considered.

27) Comment

It is possible to introduce a line of comment which will be copied in the output files. For this purpose write:

Comment
Iron K-edge in magnetite → line of comment

28) Atomic spectra

To get in last column the atomic absorption spectra (without the neighbour atoms), put the keyword:

Xan_atom

29) Different absorbing atoms calculated in one run

The electronic structure is calculated in all the cluster of calculation and thus in all atoms in it. Consequently, it is in principal possible to get the absorption spectra of all the atoms in only one run. In principal, the absorbing atom is nevertheless "excited", thus becomes intrinsically different and one calculation must be performed for each absorbing atom. When neglecting this difference, it is possible to get all the absorption spectra of the all the atoms, equivalent and non-equivalent by symmetry operation, of the same chemical specie in only one run using the keyword:

One_run

For the L_{23} and M_{45} edges, the default calculation is such that the absorbing atom is not excited, thus the result in *one run* is in principal good. With "*One_run*" all the absorbing atoms are calculated, one thus must take care that they are all in the sphere of calculation. The use of keyword "*Center*" or "*Center_abs*" is sometimes helpful is this context.

VI- Technical keyword

Here stand the technical keywords necessary for specific tests and optimization of the code, for expert users.

1) Details on the calculations

To get details on the calculations done in every routine, put the keyword:

Check
3 3 3 3 1 1 1 2 1 1
1 1 2

Up to 30 numbers can be given. The correspondence between the number and the routine is given by :

1 : Lecture	2 : Atom / Dirac	3 : Symsite	4 : Init-run
5 : Agregat	6 : Polarization	7 : Atom_selec	8: Etafin
9 : Reseau	10 : Potato	11 : Orbval	12 : Pot0
13 : Potentiel	14: Enrgseuil	15 : Ylm	16 : Potex
17 :	18 : Sphere	19 : Mat / MSM	20 : Tenseur
21 : Coabs	22 : Tddft – sphere	23 : Tddft – Kernel	24 : Tddft - Chi_0
25 : Tddft – Chi	26 : Hubbard	27 : SCF	28: State
30 : Convolution			

Values can go from 0 to 4 giving more and more for each routine. By default, there is 1 for all the routines. One can also write:

check_all → equivalent to icheck = 3 for all the subroutines
no_check → equivalent to icheck = 0 for all the subroutines
check_conv → équivalent to icheck = 3 for the convolution
check_pot → equivalent to icheck = 3 for all the subroutines concerning the potential
check_mat → equivalent to icheck = 3 for the matrices MSM or FDM
check_sph → equivalent to icheck = 3 for the subroutine "sphere"
check_coabs → equivalent to icheck = 3 for the subroutine "coabs"

2) Symmetry

The point symmetry is calculated automatically. Anyway the expert users can impose it by the keyword:

Sym
2/m → Schoenflies coefficient or international table of crystallography coefficient. Be careful that these symmetries are possible only for the mesh axis defined in the indata.

3) Tensor basis

By default the atomic tensors given in the output files are expressed in the orthonormal basis R_1 where z is the crystal *c* axis (but for the trigonal structure where z is the c axis of the associated hexagonal mesh), *x* is along $b \times c$ and *y* along $z \times x$. Nevertheless it is possible to express it in the basis where it is in fact calculated, the so-called basis R_2. From R_1, another rotation is performed for magnetic calculation when the spin axis is not along z. Then a another ±45° rotation is sometimes performed when a 2 fold axis or a symmetry plane is found along a diagonal. For this purpose put the keyword

Base_spin

4) Calculation basis

By default the connection to the continuum is performed in real base (neuman, bessel). To use a complex base (bessel, hankel) put:

Basecomp

5) Equivalent atoms

The program automatically calculates the total signal resulting from the equivalent atoms by symmetry. It is nevertheless possible, for the expert *fdmnes* user, to impose the symmetry relation between the atoms and thus to impose this summation. One must then use the keyword "*symsite*". Following this keyword, stands the number of non-equivalent atoms (or number of group of atoms), then for each of them, the number of equivalent atoms followed the list of the relative symmetry to the first atom of the list and the atomic position in mesh unit. The symmetry are codified by number going from 1 to 64, see the list given bellow.

Symsite

```
 3                ! Number of non-equivalent atoms (or group of atoms)
 4                ! Number of equivalent atoms, group 1
  1  0.2500  0.2500  0.2500
 24  0.7500  0.7500  0.2500
 23  0.7500  0.2500  0.7500
 22  0.2500  0.7500  0.7500
 4                ! Number of equivalent atoms, group 2
  1  0.0000   0.0000   0.0000
 22  0.0000   0.5000   0.5000
 23  0.5000   0.0000   0.5000
 24  0.5000   0.5000   0.0000
 4                ! Number of equivalent atoms, group 3
  1  0.5000   0.5000   0.5000
 23  0.0000   0.5000   0.0000
 22  0.5000   0.0000   0.0000
 24  0.0000   0.0000   0.5000
```

The negative indexes correspond to the same symmetry plus time reversal (in case of magnetism).

Symmetry code:

1: identity

2: rot 2π/3 around (1,1,1)
3: rot 4π/3 around (1,1,1)
4: rot 2π/3 around (1,-1,1)
5: rot 4π/3 around (1,-1,1)
6: rot 2π/3 around (-1,1,1)
7: rot 4π/3 around (-1,1,1)
8: rot 2π/3 around (1,1,-1)
9: rot 4π/3 around (1,1,-1)

10: rot 2π/2 around (1,1,0)
11: rot 2π/2 around (-1,1,0)
12: rot 2π/2 around (1,0,1)
13: rot 2π/2 around (-1,0,1)
14: rot 2π/2 around (0,1,1)
15: rot 2π/2 around (0,-1,1)

16: rot 2π/4 around 0x
17: rot 2π/4 around 0y
18: rot 2π/4 around 0z
19: rot -2π/4 around 0x
20: rot -2π/4 around 0y
21: rot -2π/4 around 0z

22: rot 2π/2 around 0x
23: rot 2π/2 around 0y
24: rot 2π/2 around 0z

25: inversion

26: rot 2π/4 around 0x and inversion
27: rot 2π/4 around 0y and inversion
28: rot 2π/4 around 0z and inversion
29: rot -2π/4 around 0x and inversion
30: rot -2π/4 around 0y and inversion
31: rot -2π/4 around 0z and inversion
32: rot 2π/3 around (1,1,1) and inversion
33: rot 4π/3 around (1,1,1) and inversion
34: rot 2π/3 around (1,-1,1) and inversion
35: rot 4π/3 around (1,-1,1) and inversion
36: rot 2π/3 around (-1,1,1) and inversion
37: rot 4π/3 around (-1,1,1) and inversion
38: rot 2π/3 around (1,1,-1) and inversion
39: rot 4π/3 around (1,1,-1) and inversion
40: plane perpendicular with 0x
41: plane perpendicular with 0y
42: plane perpendicular with 0z

43: diagonal plane y = z containing Ox
44: diagonal plane x = z containing Oy
45: diagonal plane x = y containing Oz
46: diagonal plane y = -z containing Ox
47: diagonal plane x = -z containing Oy
48: diagonal plane x = -y containing Oz

49: rot 2π/3 around 0z
50: rot 4π/3 around 0z
51: rot 2π/6 around 0z
52: rot 10π/6 around 0z
53: rot 2π/3 around 0z, negative axe
54: rot 4π/3 around 0z, negative axe
55: rot 2π/6 around 0z, negative axe
56: rot 10π/6 around 0z, negative axe

57: plane at 30° containing 0z
58: rot 2π/2 around axe at 30° perp. 0z
59: plane at 60° containing 0z
60: rot 2π/2 around axe at 60° perp. 0z
61: plane at 120° containing 0z
62: rot 2π/2 around axe at 120° perp. 0z
63: plane at 150° containing 0z
64: rot 2π/2 around axe at 150° perp. 0z

6) Bounded states

If one wants to make positive the kinetic energy for the calculation of bounded states (beneath the average potential), put the keyword "*etatlie*" followed by the kinetic energy in eV:

Etatlie
0.05 0.5

The first value is for the atomic scattering, the second one only used in FDM is for the cluster scattering. Default values are respectively 0.2 and 1 eV.

7) Inversion of the matrix in the multiple scattering mode

By default one inverts the matrix $(\kappa^{-1}+i + G)$ where κ corresponds to the neuman-bessel normalization. To avoid eventual convergence problems (not seen yet), one can prefer to calculate $(1 + G\tau)^{-1}\tau$. For this use the keyword:

Normaltau

8) Muffin-tin potential

If one wants to use the muffin-tin approximation in FDM put the keyword:

muffintin

9) Non excited absorbing atom

At the K, L1, M1 edges the absorbing atoms is calculated excited that is with a hole in the core level and an extra electron in the first non-occupied valence state. To perform a calculation with a non-excited absorbing atom, that is with an absorbing atom without a hole in its core level and without screening put:

Nonexc

At the other edges, the absorbing atom is not excited. To make it excited put the keyword:

Excited

10) Modification of the grid of point parameters

By default the finite difference calculation is performed at order 4 with an inter point distance equal to 0.25 Å, the radius of the spherically symmetric area is around 0.65 Å (less for the light elements). To modify them write:

Rmt → to modify the muffin-tin radius
0.65

Iord → To modify the order of the Taylor expansion.
2

Adimp → to modify the interpoint distance
0.20

It is possible to use inter-point distance, δ, decreasing with energy. This can be useful in EXAFS, because at high photoelectron kinetic energy, lower δ are necessary to get the same precision. For this, write :

Adimp
0.24 100. 0.20 250. 0.16 400. 0.12 500. 0.08

→ δ = 0.24 up to 100 eV, δ = 0.2 between 100 and 250 eV,… δ = 0.08 beyond 500 eV

Remark: when using different cluster radius, the energy values where δ change, can be the same than for the radius (see « Radius » keyword).

11) Expansion in spherical harmonics

An expansion in spherical harmonics is performed in the atoms both in the multiple scattering mode and in the finite difference mode, but with a smaller radius. The maximum value of ℓ is obtained from the formula $kr = \sqrt{\ell_{\max}(\ell_{\max}+1)}$, where k is the photo electron wave vector and r the muffin-tin radius (Rmtg in the bav file). By default, to this value one adds 1. To fix a value of ℓ_{max} independent of energy just write:

Lmax → The ℓ_{max} value is fixed at 3
3

If one wants to keep the energy dependent formula but adding 1, 2 or more to this formula, put a negative sign in from of 1 :

Lmax → The ℓ_{max} value is now given by the formula plus 2.
-2

When the energy is increasing, ℓ_{max} increases. By default the maximum value of ℓ_{max} is set at 2 for Z = 1, at 3 for Z = 2 then at 4 for Z ≤ 18, then at 5 for Z ≤ 36, then at 6 for Z ≤ 54, then at 7 for Z ≤ 86 and 8 for Z over. To avoid this limitation put the keyword:

Lmaxfree

When working using the finite difference mode, the connection to the outer sphere also needs an expansion in spherical waves. This one uses the same formula that for the atom but r is now the radius of the outer sphere. To modify this ℓ_{max} one proceeds exactly in the same way with positive value to fix an energy independent value, and negative value to keep the formula but adding to the formula. By default the additional value is 5. The key word is now *lmaxso* :

Lmaxso
20

12) Muffin-tin radius

By default the muffin-tin radius is calculated to have a jump of potential the smallest as possible and closed between the atoms. One can modify it by the use of 3 different keywords.

If one wants that this radius is calculated using the Norman procedure introduce the keyword:

Norman

If one wants than the muffin-tin radius is the half value of the interatomic distance, introduce the keyword:

Raydem

By default there is a 10% overlap between the spheres. If one wants modify this put the keyword "*overlap*" followed by the value of the overlap:

Overlap
0.15 → 15% overlap

If one wants that the muffin-tin radius be determined by the value it gets when the atomic potential is equal to the interstitial potential, put the keyword *rmtv0*, followed by the value of this potential (takes place the one define by the keyword *v0imp*):

Rmtv0
-12.

If one wants to impose the radius for each chemical species put *Rmtg* followed by the radius in Angstrom for each of them.

Rmtg
0.65
1.1

13) Continuity of the potential at the muffin-tin radius

To limit potential jump between the interstitial area and the muffin-tin sphere, a linear interpolation on the potential is performed in the last 10% of the radius. For this put:

Supermuf

14) Atomic charge

The program gives in the output file the atomic charge integrated up to the muffin-tin radius. If one wants to get this value for a different radius put:

Rchimp → corresponding keyword
1.2 → radius value for each type of atom
0.7

15) Line length

Lines are red over a specific length. When reading files containing a large number of columns (for example calculation of more than 100 RXS spectra), the default line length (3020 characters) can be not sufficient. To modify this put:

Length_line
4000 → maximum number of character in one line

16) Resolution in initial state

The outputs are resolved in initial states only for magnetic calculation. For a non-magnetic calculation, it is possible to get anyway the output resolved be initial state using the keyword:

Core_resolved

It is then possible in the step convolution to select one of these states.

17) Memory save

For low symmetrical material, it can be useful to save some memory space. This makes an approximation (but a good one) on the potential calculation. For this use the following keyword:

Memory_save

C- Convolution

I- Introduction

The f*dmnes* program allows performing:

1) the convolution by a lorentzian of absorption spectra eliminating the occupied states. For the anomalous diffraction, it makes the integration over energy of the unoccupied states then calculates the intensity of the diffracted peaks.

2) a weighted summation over different outputs of the *fdmnes* program. This summation can include a relative shift between the spectra.

This step of the calculation can be done together with the previous one, just adding the corresponding keywords. It can also be done independently, writing another input file contains only the keywords related to the convolution. Here comes an example:

Calculation → To give the file name resulting from the previous step.
g_rs43.txt → name of the file

Conv_out → To give the file name of the convoluted spectra
g_rs43_conv.txt → name of the file

Convolution → keyword to specify an "arctangent" shape for the broadening"

Efermi → keyword to specify the Fermi energy (E_F) relative to the calculation
-5.5

II- Keywords for the convolution

1) File names

The indata files for the convolution step are the output files of the previous step whose names are defined under "*filout*". When the convolution is performed together with the main calculation, it is not necessary to specify again this name. In the other cases one has to introduce it or them with the keyword "*Calculation*":

Calculation → To give the file names resulting from the previous step.
g_rs43.txt → name of the file

Another example with 2 indata files and with different shifts:

Calculation → To give the file names resulting from the previous step.
Fe_rs64_01.txt → name of the file 1
1.0 0.2 → weight, shift
Fe_rs64_02.txt → name of the file 2
1.0 -0.2 → weight, shift

The weight is applied on the XANES and the anomalous scattered amplitudes. For the RXS calculations, the output files, before convolution contain in second line the Thomson factors plus the anomalous part of the non-resonant atoms. The weighting applied on these terms is the weight divided by the sum over the files of the different weights. In this way is taken into account the average configuration for substitutions of atoms of different chemical specie on the same sites, but when it is the resonant atom, one has not an occupancy rate equal to one. In this last case one also has to use the keyword "Thomson".

The name of the convolution output file is by default the input file name with the added suffix "*_conv.txt*". Anyway it is possible to impose another name with the keyword:

Conv_out
Fe_rs64_sum_conv.txt → name of the convoluted spectra file

To specify a working directory put the keyword directory followed by the directory name with at the end the separator (/ or \):

Directory
C:/Documents and Settings/joly/Mes documents/xanes/xanout/v2o3/

2) Fermi level

The states beneath the Fermi level are occupied. Thus the cross section is set to zero, before convolution. By default, when in the previous step the *No_Fermi* keyword was used, this level is set to -5 eV. Nevertheless most often, this value must be specified with the keyword:

Efermi → keyword to specify the Fermi energy (E_F) relative to the calculation
-5.5

The Fermi level is applied before the energy shift because in principle it is used to simulate the core level shift. Anyway it is possible to apply it after the shift adding the keyword:

Dec

It is also possible to have different values of the Fermi level for the different files. This is written in third column after each file name:

Calculation → To give the file names resulting from the previous step.
Fe_rs64_01.txt → name of the file 1
1.0 0.2 -5. → weight, shift, Fermi level
Fe_rs64_02.txt → name of the file 2
1.0 -0.2 -5.9 → weight, shift, Fermi level

The Fermi energy written under "*Efermi*" when specified, is then not considered.

3) Convolution width

The convolution to apply depends on the core level width (Γ_{Hole}) and the final state width. Γ_{Hole} is automatically determined. Nevertheless, it is possible to modify it with the keyword:

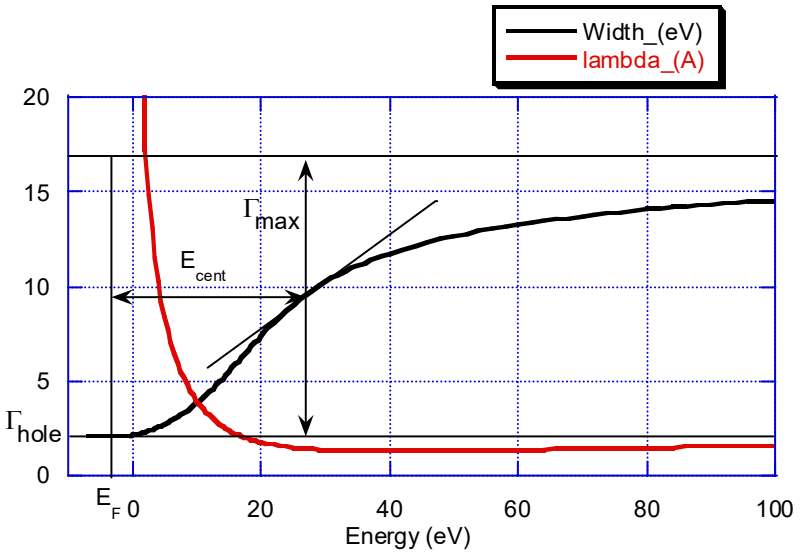
Gamma_hole
2.05 → Core level width (Γ_{Hole}) in eV.

To have different values of Γ_{Hole} for a double edge like L_{23}, just put 2 numbers.

There are different ways to calculate the energy dependent broadening. The first one uses an arctangent formula:

$$\Gamma = \Gamma_{Hole} + \Gamma_m \left(\frac{1}{2} + \frac{1}{\pi} \arctan\left(\frac{\pi}{3} \frac{\Gamma_m}{E_{L\arg}} \left(e - \frac{1}{e^2} \right) \right) \right)$$

with: $e = \dfrac{E - E_F}{E_{cent}}$ where Γ_m, E_{cent} and E_{larg} are respectively the maximum width (at high energy) of the final state, the center and the width of the arctangent function. The depth at the center of the arctangent is Γ_m/E_{larg}. A typical curve is given bellow:



Such a convolution is introduced with the keyword:

Convolution

Default values for E_{larg} , E_{cent} and Γ_m are respectively: 30, 30 and 15 eV. It is possible to modify them with the keywords:

Ecent
30. → E_{cent}

Elarg
30. → E_{larg}

Gamma_max
20. → Γ_m

In the convolution, along the integration it is the width of the running energy which is taken. It is possible to use the width of the final state energy corresponding to the energy of the elastic photon. One then makes the integration with a constant width. This procedure improves the agreement with experiment especially in the pre-edge range where the other procedure increases the background. To impose nevertheless a variable width along the integration in XANES uses the keyword :

Gamma_var

It is also possible to use the Seah-Dench formula for the calculation of the broadening. In this case one gets:

$$\Gamma = \frac{A\Gamma_m E_p}{\Gamma_m + AE_p} + \Gamma_{Hole}, \qquad \lambda = \frac{1}{A\sqrt{E_p}} + \frac{\sqrt{E_p}}{\Gamma_m}, \qquad \text{with:} \quad E_p = E - E_F.$$

This is performed with the keyword:

Seah
1. 20. → A,Γ_m

One can also use a simple table with the keyword "*table*":

Table
0.0 1. → Energy ($E-E_F$) and broadening $\Gamma(E-E_F)$
10.0 1.5
20.0 2.
30.0 3.5
100.0 5.

When the keyword "*Efermi*" is used without the keywords "*Convolution*" or "*Seah*", the width of the convolution is constant and equal to the width of the core hole. In all cases, the curve shape is written in the talkative “bav” file when the convolution is done in the same run than the main calculation. When convolution is done alone, to get this curve write the keyword:

Check_conv

To simulate the experimental resolution, it is also possible to convolute by a Gaussian. This convolution is performed after the lorentzian. For this write:

Gaussian → keyword
1. 0.05 → width of the gaussian

This same convolution can be used as a first approximation to simulate the thermal vibration effects. This is valid only in the extended part of the spectra. In this case one applies the rule “kr = constant” and the convolution width becomes proportional to the energy. The

parameter to write is the relative vibration amplitude in relation to the interatomic distance. This is done, writing a second number under "*Gaussian*":

Gaussian → keyword
1. → width of the Gaussian, relative amplitude of the vibration

4) Starting energy

To get output spectra starting at a lower energy put:

Estart
-8. → Value of the starting energy (eV)

5) Photoemission

With the keyword "*photoemission*", it is the photoemission spectrum which is calculated. In such calculation the cutting is simply above the Fermi level and not beneath it as in xanes. The convolution broadening is the independent of energy and is fixed by default to the hole width. This with can nevertheless been modified by the use of the keyword "*Gamma_hole*". Note that would have interest having previously performed a calculation in "green" mode with a minimum energy width (keyword "*eimag*") at least 0.1 eV, all this within an energy range convenient for photoemission:

Photoemission

6) Damping due to multi-electronic effects

In a simple approach, the multi-electronic phenomena can be seen as a simple damping in the absorption cross section and in the anomalous scattering amplitude in diffraction. This damping not taken into account, by default, can be introduced using the keyword "*S0_2*". It is typically around 0.8.

S0_2
0.8 → value of the damping

When setting S0_2 = 0, in diffraction, one keeps only the non-resonant term.

7) Selection of the transition from a peculiar initial state

The fdmnes output files, before convolution, contain the spectra by transition from all initial states when the calculations are magnetic and by threshold in the other case. It is possible to perform the convolution for only one of this component (avoiding thus their summation) with the keyword "*Selec_core*". One has then to write below the number of the selected initial state:

Selec_core

1 → Number of the selected initial state. For a K edge resolved in spin, this correspond to the $1s_{1/2}$, that is to a pure spin down state, the number 2 corresponds to spin up.

III- Keywords specific for resonant diffraction

1) Azimuthal scan

If there is an azimuthal scan in anomalous diffraction, one has also to give the corresponding indata file names (type *_scan.txt*) and the new output file. This is set after the keyword "*scan_file*":

Scan_file
Fe_rs64_01_scan.txt → name of the indata dafs file 1
Fe_rs64_02_scan.txt → name of the indata dafs file 2

Scan_conv
Fe_rs64_scan_conv.txt → name of the new output file with the convoluted scan

When the convolution file is included in the "main" calculation file, it is not necessary to specify the scan file names because they are known by the code. In this case, if one wants to convolute also these files just uses the "*Scan*" keyword:

Scan

2) Thomson

Thomson term is calculated by default. It is possible to modify it using the following keywords.

To eliminate the Thomson factor f_0 (as for a forbidden beam) put:

Forbidden

It can be useful to impose specific value for each RXS reflections for the non-resonant (Thomson) structure factors and the resonant one of the other atoms. That is : $\sum_a p_a\left(f_{0a} + f'_a + if''_a\right)e^{i\vec{Q}.\vec{R}_a}$, with f'$_a$ and f ''$_a$ considered only for the other chemical species and where p_a is the site *a* occupancy rate. This is the case for example for occupancy rate non equal to one. These complex terms taken as a constant in all the energy range can be introduced through the keyword:

Thomson
1.1670478E+02 1.0583769E+02 1.1477827E+02 -8.2670689E+01

In the second line stand these terms, here for 2 reflections. They replace the values calculated by the program and placed in the second line of the output file.

3) Getting f' and f"

To get in the output file, the f' and f" values, put the keyword:

Fprime

In the output file for each reflection, there are three columns, f', f" then intensity. The intensity is for the mesh, f' and f" are for one atom of the mesh. f' contains also f_0. To get only f', put also the keyword "*forbidden*".

It is also possible to get the atomic (but in the solid) f' and f" values without RXS simulations. For this the best is to run the main simulation with the keyword "*spherical*". In a second step one convolute with the keyword fprime the corresponding output file "…_sph_atom1.txt"

To get the isolated atomic f' and f":

Fprime_atom

The values of the atomic f' and f" are then in the talkative "bav" file, eventually created at this time when the convolution is done in an independent job.

4) Getting other polarization conditions

When the main calculation is performed for any reflection for the 4 polarization situations σσ, σπ, πσ and ππ, it is possible in the "convolution step" to calculate the intensities of the spectra for the incoming polarizations circulars right and left. For this add the keyword:

Circular

It is also possible to get the intensity corresponding to any Stokes parameters (S1= +/-1 sigma and pi, S2 diagonal S3 = +1(-1) circular right (left)) or with or without analyzer, this one with any angle. For example without analyzer one writes:

Stokes
0 0 1 → S1, S2, S3
0 0 -1
0 0.31 0.95
0 0.31 -0.95

Stokes
0 0 1 30. 50. → S1, S2, S3, rotation and Bragg analyzer angles

If the Bragg angle analyzer is not specify, it is supposed perfect, that is 45°:

Stokes
0 0 1 30 → S1, S2, S3, rotation analyzer angle (0 = σ, 90 = π)

It is possible then to specify column name in the output file to make simplest the column identification, writing:

Stokes_name
no_name → default name
no_name
+00+31+95 → name appearing in the first line, in the corresponding column
+00+31-95

5) Corrections

It is possible to make a double absorption correction, corresponding to a measurement done at the maximum of the « rocking curve » and thus not integrated over it. For this write the keyword:

Double_cor

This correction is effective only with *self_abs* or *Full_self_abs* in the main calculation step. One gets then in the output file after convolution a new column with 'Id' which contains the intensity doubly corrected.

Another correction is possible to take into account a dead layer, that is a disordered layer at the surface, not participating to the diffraction, but damping the signal in the incoming and in the outgoing. This is done with the keyword:

Dead_layer
150 → thickness in Angstrom of the dead layer.

This correction is also done during the convolution part of the calculation.

D- Parameter optimization

It is possible to compare the calculated spectra to the experimental ones with the help of metric distances and R factor. The metric distances to compare the individual theoretical ($f_{th}^{(i)}$) and experimental ($f_{\exp}^{(i)}$) spectra are given by:

$$D_1^{(i)} = \tfrac{1}{2}\int \left| \tfrac{1}{c_{th}^i} f_{th}^{(i)}(e) - \tfrac{1}{c_{\exp}^i} f_{\exp}^{(i)}(e) \right| de ,$$

$$D_2^{(i)} = \tfrac{1}{2}\int \left| \tfrac{1}{C_{th}^i} F_{th}^{(i)}(e) - \tfrac{1}{C_{\exp}^i} F_{\exp}^{(i)}(e) \right| de ,$$

with each time the normalization factors: $c = \int_{E_{\min}}^{E_{\max}} f(e)de$

The *F* are the integrals of *f*. The R factor is a conventional one (see E. Zanazzi and F. Jona, Surf. Sci. 62, 61 (1977)) given by:

$$R_X^{(i)} = \tfrac{13}{6} \frac{\sum_e \left| c_i f_{th}^{(i)}(e) - f_{\exp}^{(i)}(e) \right|^2}{\sum_e \left| f_{\exp}^{(i)}(e) \right|^2}, \quad \text{with } c_i \text{ such that: } \frac{\partial R_X^{(i)}}{\partial c_i} = 0$$

Then for n different spectra, one gets the total metric distance or R factor by:

$$D_{1,2} = \sum_{i=1,n} p_i D_{1,2}^{(i)} \qquad \text{and} \qquad R_X = \tfrac{6}{13}\left(\tfrac{3}{2n} + \tfrac{2}{3}\right) \sum_{i=1,n} p_i R_X^{(i)}$$

where p_i is the relative weight for the spectra $''i''$ given by $p_i = \frac{E_{\max}^{(i)} - E_{\min}^{(i)}}{\sum_{j=1,n} E_{\max}^{(j)} - E_{\min}^{(j)}}$

It is possible to vary some parameters in order to optimize the agreement between calculation and experiment. Then results are given for a multi-dimensional grid of parameters. The values of the metric distances are given in a special output file. By default for a complete calculation, the file name is the fdmnes conventional output file name with the suffix *_fit.txt*. For a calculation starting calculating the convoluted spectra, the default output file name is *fdmfit_out.txt*. This name can be modified using a specific keyword.

To do this task different keyword must be added in the main indata file:

Experiment → Keyword preceding the file names containing the experimental
Nom_exp spectra.

Gen_shift → Minimum and maximum energy shift between calculation and
7108 7114 21 experiment and number of value to test

Metric_out → Keyword preceding the output file name containing the metric
File_name_fit.txt distances

Parameter → Keyword preceding any group of correlated parameters
Par_Gamma_max → Keyword to specify the convolution broadening Γ_m as a parameter

15. 25. 5 → First and last values and number of values

Parameter

Par_Posx

-0.05 0.05 3

Par_Posy

-0.05 0.05 3

In the previous example the parameters *Posx* and *Posy* of the atom 1 are completely correlated. Thus the atom is displaced along the diagonal.

The parameters can be fitted are:

For the convolution:

Par_ecent → Central energy for the arctangent
Par_elarg → Energy width for the arctangent
Par_efermi → Fermi energy
Par_gamma_hole → Hole width
Par_gamma_max → Maximum width for the final states
Par_gauss → Gaussian width (or resolution)
Par_shift → Energy shift
Par_aseah → First parameter of the Seah-Dench formula

For the spectra calculation:

Par_a → Contraction or expansion of the mesh parameter a in %
Par_b → Contraction or expansion of the mesh parameter b in %
Par_c → Contraction or expansion of the mesh parameter c in %
Par_abc → General contraction or expansion in %
Par_anga → Value of the unit mesh angle α
Par_angb → Value of the unit mesh angle β
Par_angc → Value of the unit mesh angle γ
Par_poporb → Orbital occupancy
Par_posx → Atom position along x
Par_posy → Atom position along y
Par_posz → Atom position along z
Par_occup → occupancy of the atom
Par_dposx → shift of the atom position along x from the original position
Par_dposy → shift of the atom position along y from the original position
Par_dposz → shift of the atom position along z from the original position
Par_theta → position along θ for an atom in spherical coordinate
Par_phi → position along ϕ for an atom in spherical or cylindrical coordinate

Under each parameter must be written the first and last values of the parameter followed by the number of value. For the parameters *Par_posx*, *Par_posy*, *Par_posz*, *Par_theta*, *Par_phi* The number of the atom must also be specified. Under the parameter *Par_poporb*, *Par_occup* must be also set the number of the orbital found in the order given under the keyword *atom*. For example, to specify an exchange of charge between two atoms (titanium and oxygen), one has to write:

Atom

22 3 2 2. → 3d titanium orbital with 2 electrons for the initial occupancy
8 2 1 4. → 2p oxygen orbital with 4 electrons for the initial occupancy

Parameter
Par_poporb
2. 0. 3 1 → The first orbital under *atom* is the 3d titanium.
Par_poporb
4. 6. 3 2 → The second orbital under *atom* is the 4p oxygen.

By default the metric distances are calculated in all the energy range is the intersection between the experimental and calculated spectra. It is possible to cut the lower or and the higher energy part of the spectra by the use of the keyword:

Emin
-10. → Minimum energy for all the spectra

Emax
100. → Maximum energy for all the spectra

It is possible to have different values for the different spectra:

Emin
-10. -5. -20. -20. → Minimum energy for each spectra

Emax
45. 100. 100. 100. → Maximum energy for each spectra

If the energy of the experimental spectra is in keV and not in eV, put the keyword:

Kev

When there are several spectra to compare simultaneously, for the calculation they must be in the same output file. One then must give the number of the column contains the calculated spectra and associate it at the corresponding experimental file. This is done adding a line after each experimental file contains the number of the column. If there are 2 numbers, the first one is the number of the column in the experimental file, the second one being the number of the column in the calculated file. When there is no number, this means than in both experimental and calculated file, the spectra are in the second column, the first one being the energy. Example:

Experiment → keyword
Nom_exp_1.txt → Name of the file containing the first experimental spectra
2 → Number of the column in the calculated file containing the corresponding spectra
Nom_exp_2.txt → Name of the file containing the second experimental spectra
3 → Number of the column in the calculated file containing the corresponding spectra
Nom_exp_2.txt → Name of the file containing the third experimental spectra
4 3 → Numbers of the column in the experimental file *Nom_exp_2.txt*, followed by the number of the column in the calculated file

By default, three confidence factors are used. A fourth one “Rxg” can also been calculated. It is equivalent to Rx but with a unique normalization factor between experiment and calculation. When there is a single spectra, Rxg is equivalent to Rx. To get this confidence factor put the keyword:

Rxg

E- Extraction of DAFS scans and spectra

When realizing a DAFS simulation with azimuth dependence (scan), the output scan file after convolution contains the intensity of all the reflections at all energies and all azimuth angles. Often, it is useful to extract from this big file some spectra at specific azimuth angle or some scan at specific energy. It is what is done in this part with the following indata file:

!Indata file for FDMNES, Selection part

Selec_inp → keyword for the input file name (output of the convolution part)
xanout/fe3o4/2008_bland/cc_1221_1221_orig_1m10_scan_conv.txt

Selec_out → keyword for the output file name
xanout/test/fe3o4_scan_selec_conv.txt

Energy → keyword for the selected energy for the scan
4. → value of the energy for the scan in eV.

Reflection → keyword for the selected reflections
2 5 6 9 → number of the selected reflections

End

The azimuth scan is extracted at the energy (in eV) given after keyword "*Energy*".
It is also possible to extract spectra at a given azimuth angle. For this, no keyword "*Energy*" but the keyword "*Azimuth*" and next line the value of the selected azimuth:

Azimuth
30. → Value of the azimuth

It is possible to have several reflections in the output file at one energy (or one azimuth). It is also possible to have several energies but only one reflection for the scan or several azimuth angles but one reflection for the spectra.

Energy
4 7.5 → selected energy for the scan

Reflection
2 → reflection number 2 selected

or:

Reflection
2 → reflection number 2 selected

Azimuth
30. 60. 90. → Azimuth selected

Without the keyword « *Reflection* », all reflections are given when there is only one energy or one azimuth asked.

F – Unit cell multiplication

FDMNES contains a tool to build the list of atoms of a unit cell superstructure from the atom list of a simple unit cell. This can be used as the starting list corresponding to a unit cell corresponding to a decrease in symmetry or to specific magnetic order.

Example:

Filout → Output file where is given the list of atom of the superstructure unit cell
xanout/test_stand/mult_out

Mult_cell → Multiplication factor along a, b and c
2 2 1 → Here one buids a (2a, 2b, c) unit cell

Atomic_nu → Atomic number corresponding to the atom type under « *Unit_cell* »
26 38 33

Unit_cell → to introduce the original unit cell
3.92430 3.92430 12.36440 90. 90. 90. → a, b, c, α, β, γ
1 0.50000 0.00000 0.25000 → list of all the atoms of the unit cell
1 0.00000 0.50000 0.25000
1 0.50000 0.00000 0.75000
1 0.00000 0.50000 0.75000
2 0.00000 0.00000 0.00000
2 0.50000 0.50000 0.50000
3 0.00000 0.00000 0.36000
3 0.00000 0.00000 0.64000
3 0.50000 0.50000 0.86000
3 0.50000 0.50000 0.14000

End

The original unit cell is introduced with the keyword « *Unit_cell* » under which are given the unit cell parameters, and the list and the list of all the atoms in it. In first column is set the atomic number, but if using the optional keyword « *Atomic_nu* ». In this case, first column contains the atom type number and the correspondence between atom type number and atomic number is given under « *Atomic_nu* » .

G - FDMX User's guide

FDMX is an extension from J. Bourke and C. Chantler, University of Melbourne, Australia. When using it, thanks to cite:

J. D. Bourke, C. T. Chantler, Phys. Rev. Lett. **104**, 206601 (2010).

FDMX is an enhanced approach to calculating both XANES and XAFS spectra using the finite difference method and the core routines of FDMNES. The easiest way to use FDMX is to simply include the keyword ***fdmx*** in your regular input file, and the code will automatically optimize computational parameters to ensure accuracy over a wide energy range. FDMX will process the spectrum to include thermal effects and electron/hole lifetimes, and add background absorption from more loosely bound electrons. The code is currently designed for use with K-edge calculations only, however most functionality will also work with other edges (note keywords for hole widths and background absorption). Additional (optional) controls for FDMX are possible with specific keywords.

As calculations using FDMX may take several hours, particularly for structures with few or no axes of symmetry, it is strongly recommended that you compile and run the code using the MUMPS libraries.

fdmx

Activates FDMX computation and optimization of parameters with respect to energy, allowing for accurate EXAFS spectra, and triggers the processing routine at the end of the calculation. When this keyword is used, *the Radius keyword is no longer required.*

fdmx_proc

Use to activate a post-processing routine from FDMX, implementing thermal, inelastic scattering, background, and other effects without explicitly calculating the absorption spectra. This requires an existing output file with absorption cross sections from a previous calculation.

Efermi
4.0 ! Val

Similar to the keyword for ***convolution*** in FDMNES, this will suppress transitions below the nominated Fermi level, expressed in eV. Some absorption will still be possible below this level due to the hole width and IMFP effects, and background absorption from other edges. **Use of this keyword is strongly recommended.**

Radius
8.3 100. 7. 250. 5. 400. 4. ! *Val, En, Val ...*

Allows the user to specify how the cluster radius changes with energy. By default when using fdmx procedure, the radius is set (as above) to 8.3 Å for energies up to 100 eV, then 7 Å for energies up to 250 eV, then 5 Å etcetera. Using a high or constant radius at high energies may

result in very long calculations, while low radii will cause XANES and XAFS structure to be missing.

adimp
0.24 0. 100. 0.20 250. 0.16 400. 0.12 500. 0.08 ! *Val, En, Val ...*

Allows the user to specify how the inter-point distance (grid density) changes with energy. By default, the inter-point distance is set (as above) to 0.25 Å for energies up to 0 eV, then 0.22 Å for energies up to 10 eV, then 0.18 Å etcetera. Using a high or constant inter-point distance at high energies may produce inaccurate results, while low values will lead to long calculations.

Gamma_hole
2.3 ! *Val*

By default, FDMX will include a core-hole relaxation based on K-shell tabulations from Scofield and Kostroun (Z=21-50) and "B" (Z=51-100)? Alternatively one may provide an explicit core-hole lifetime (in eV) with the keyword ***Gamma_hole*** or suppress this effect by using the keyword:

nohole

It is required that you use either ***Gamma_hole*** or ***nohole*** for calculations involving edges other than K.

IMFPin
imfpdatafile.txt ! *Filename*

By default, FDMX will include photoelectron lifetime broadening based on the electron inelastic mean free path (IMFP) of the absorbing material. For elements the IMFP values are tabulated from optical data model calculations, while for compounds they are estimated using the TPP-2M equation. Users may instead include their own IMFP values with the ***IMFPin*** keyword followed by a filename that contains IMFPs in the format:

En Val

where *En* is in eV and *Val* is in Å. Alternatively, IMFPs can be calculated directly from optical energy loss data (i.e. optical ELFs), which may be obtained from band structure packages such as WIEN2k (in WIEN2k this data is obtainable using the *optic* routines and is output to a file named *case.eloss*). To use ELF data to compute the IMFP, use the keyword:

ELFin
elfdatafile.txt

where the data is formatted the same as for an IMFP input file, excepting that the values are unitless. The use of ***ELFin*** will overwrite other IMFP values up to the maximum energy of the ELF provided (or 120 eV, whichever is lower), after which default IMFP values will be used. By default, the IMFP is calculated from the ELF using a Lindhard (fast) representation of the

dielectric function. However, it is recommended that you use an additional keyword for a Mermin representation:

Mermin
1 ! Val

The number following the ***Mermin*** keyword specifies an iteration value, with 0 corresponding to a Lindhard representation, 1 to a standard Mermin representation (recommended), and higher values to successive iterations of a self-consistent Mermin model. This calculation may take some hours, and iteration values higher than 3 will not normally be useful for XAFS. For more information see Bourke & Chantler, *J. Phys. Chem. Lett.* **6** 314 (2015).

Use of the ***ELFin*** keyword will generate an additional output file with the extension _ELF.txt containing the energy- and momentum-dependent ELF of the system. Use of ***Mermin*** without ***ELFin*** will produce no effect.

noIMFP

Use to omit the effects of photoelectron lifetime, and hence represent an infinite IMFP.

Tmeas
298 ! Val

Use to define the temperature, in Kelvin, at which the absorption is being calculated. This value will affect the Debye-Waller Factor, and is set to 0 by default.

TDebye
345 ! Val

Use to define a Debye temperature (in Kelvin). This is strongly recommended for compound structures.

DWfactor
0.13 ! Val

Use to define an effective Debye-Waller factor (in Å). By default, this will otherwise be calculated based on the dominant oscillators contributing to the high energy XAFS spectrum.

noDW

Use to omit thermal effects – effectively a zero Debye-Waller factor.

noBG

By default, FDMX will include background absorption from more loosely bound electrons (i.e. L, M edges etc). Use this keyword to omit such contributions. Note that the background absorption currently only works properly for K-edge calculations, and therefore for other edges this keyword is required.

For comparison with experimental data, it is useful to define an extra function to address the edge jump discrepancy (triangle effect). This function comes in two flavours, and is implemented by the following relation:

$$\mu_0(E) \rightarrow \mu_0(E)(1 + f(E))$$

where μ_0 is the atomic (or atom-like) background absorption.

Victoreen
0.8 0.4 ! Val A, Val B

Adds a background function from the Victoreen Equation with *A* and *B* parameters following:

$$f(E) = A\left(\frac{E_0^3}{E^3}\right) + B\left(\frac{E_0^4}{E^4}\right)$$

This applies to all energies above the absorption edge E_0. A+B provides the relative edge jump correction, while A/B controls the rate of decay.

Expntl
0.1 100. ! Val A, Val B

Adds a background function of an exponential form with *A* and *B* parameters following:

$$f(E) = Ae^{-\frac{(E-E_0)}{B}}$$

This applies to all energies above the absorption edge E_0. A provides the relative edge jump correction, while *B* controls the rate of decay.

cm2g

Output results in units of cm^2/g instead of Mbarn.

H - 2D Diffraction

FDMNES can simulate 2D – resonant diffraction experiments. The corresponding output are (*h,k,l*) peaks with non-integer indexes. Surface is supposed perpendicular to the (a,b) plane, thus eventually, the unit cell must be especially written in this way. Note that c is not necessarily perpendicular to the surface.

The surface to simulate must contain a film of a specific thickness. The resonant atoms are only in this film. To understand that FDMNES work in 2D diffraction, the indata file must contains the keyword "*Film*".

Optionally, the film can be set on a substrate and covered by a cap layer. Then the 3 elements of the system participate to the scattering.

Film

Keyword stating that we simulate 2D diffraction by a film.

Film_thickness

75

Thickness of the film with its value in Angström. Periodicity along c is applied up to this value, with eventually a non-integer number of unit cell. Without this keyword, the thickness is set to contain all the atoms along c, without periodicity.

Film_roughness

4.

Film roughness with its value in Angström. erfc(z) function is applied. Note that when there is a cap layer, the same roughness is also applied to the bottom side of the cap.

The substrate can be added with the corresponding keywords:

Bulk ! Structure of the substrate
8.1724 8.1724 4.0862 90. 90. 90. = a, b, c, alpha, beta, gamma
47 0.0 0.0 0.0 ! Z, x, y, z
47 0.5 0.5 0.0
47 0.5 0.0 0.5
47 0.0 0.5 0.5

The interlayer distance between the topmost substrate layer and the bottom film layer is set equal to the sum of the corresponding atom radii. This can be change with the following keyword:

Film_shift

0. *0. 3.5* ! x, y, z

The 2 first values are x and y shifts in reduced unit, 3rd value is the shift along c in Angström.

Film_shift

1. *0. 3.5 45.* ! x, y, z, angle

A fourth number can be added. It is the angle between the *a* film axis and the *a* bulk axis. Can be useful for epitaxial growth when the a film corresponds to the (a,b) diagonal of the bulk

By default, the bottom atom in the film is the one defined with the lowest z position under the keyword “Crystal”. This can be changed defining a new zero, in reduced unit. The atoms between z = 0 and this value are just shifted by +1.

Film_zero
0.249 → The bottom atom will be the next one with z > 0.249. Then the stacking is as usual.

To have to top most substrate layer at a difference inter-layer distance than the bulk layers use the keyword:

Bulk_layer
0.9 → Multiplicative term on the bulk interatomic distance.

In the same way the cap layer is added with:

Cap_layer
2.8837228875 2.8837228875 7.0636496 90. 90. 120.
79 0. 0. 0. 1. *! last value is the occupancy*
79 0.6666666667 0.3333333333 0.3333333333 1.
79 0.3333333333 0.6666666667 0.6666666667 1.

Cap_thickness
17.1

Cap_roughness
17.1

A Debye disorder in Angstroem can be given by:

Cap_disorder
2.0

By default the distance between film and cap is the sum of the atom radii. This can be changed with:

Cap_shift
3.0

The wanted (h, k, l) can be written in the indata file as usual.
It is also possible to get scan along the rod by the way:

DAFS
0 0 0.04 0.04 8.16 1 1 0. ! h, k, l_{min}, l_{step}, l_{max}, sigma, sigma, azimuth
0 0 8.18 0.002 8.24 1 1 0.
0 0 8.28 0.04 10.00 1 1 0.

There is thus a scan along the rod from l_{min} of to l_{max}.
Note that *h* and *k* can be used as non-integer when the (*a,b*) film periodicity is rational (and not equal) to the bulk periodicity.

It can be interesting in the convolution part of the calculation to get not only the spectra but also the scan along the rod at specific energies. To get the corresponding new file (with extension "_tr"), write:

Transpose_file
15. 17.
The new file is in fact just a transpose of the standard output file, taken in the example at the energies 15 and 17 eV.

By default the (*h,k,l*) indexes correspond to the bulk. It can correspond to the film indexes with keyword:

hkl_film

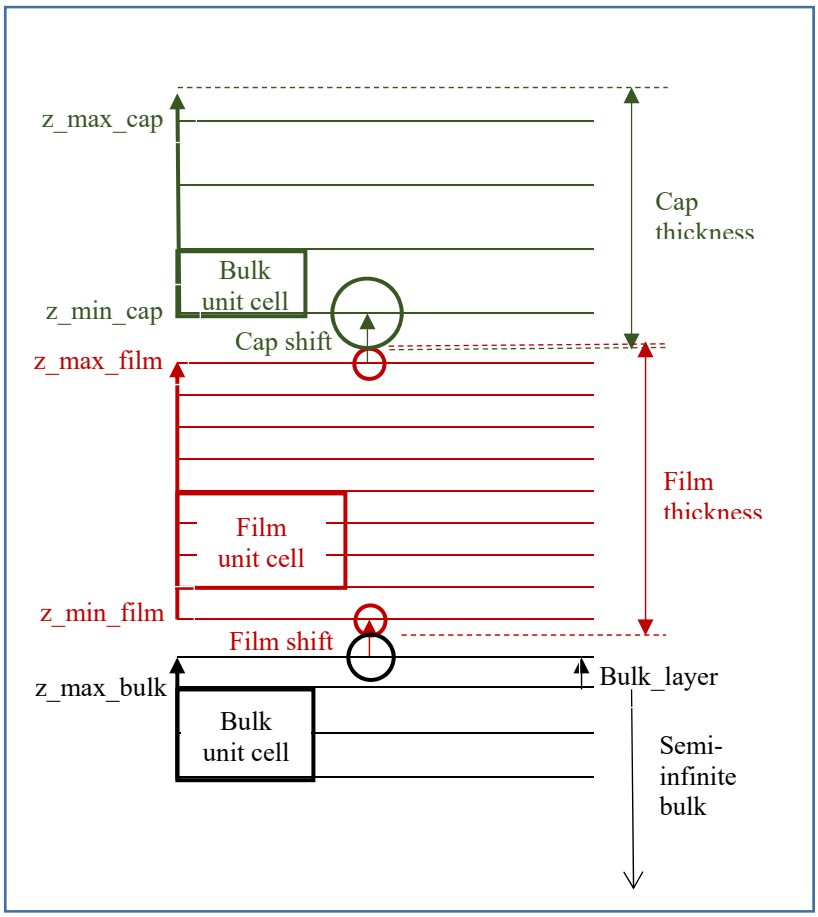


Fig. Film with cap and semi-infinite bulk
Default : cap and film shift = sum of atomic radii
Cap and Film thickness used = z_max – z_min + ½ (top inter layer + bottom inter layer)

Liste des mots clefs de *fdmnes*

Absorber	16, 38, 40	Dec	51
Adimp	46	Delta_E_conv	29
All_nrixs	21	Dilatorb	32
Allsite	39	Dip_rel	19
Ang_spin	27	Dipmag	18
Atom	15, 26, 31, 59	Directory	50
Atom_conf	16	Doping	20
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