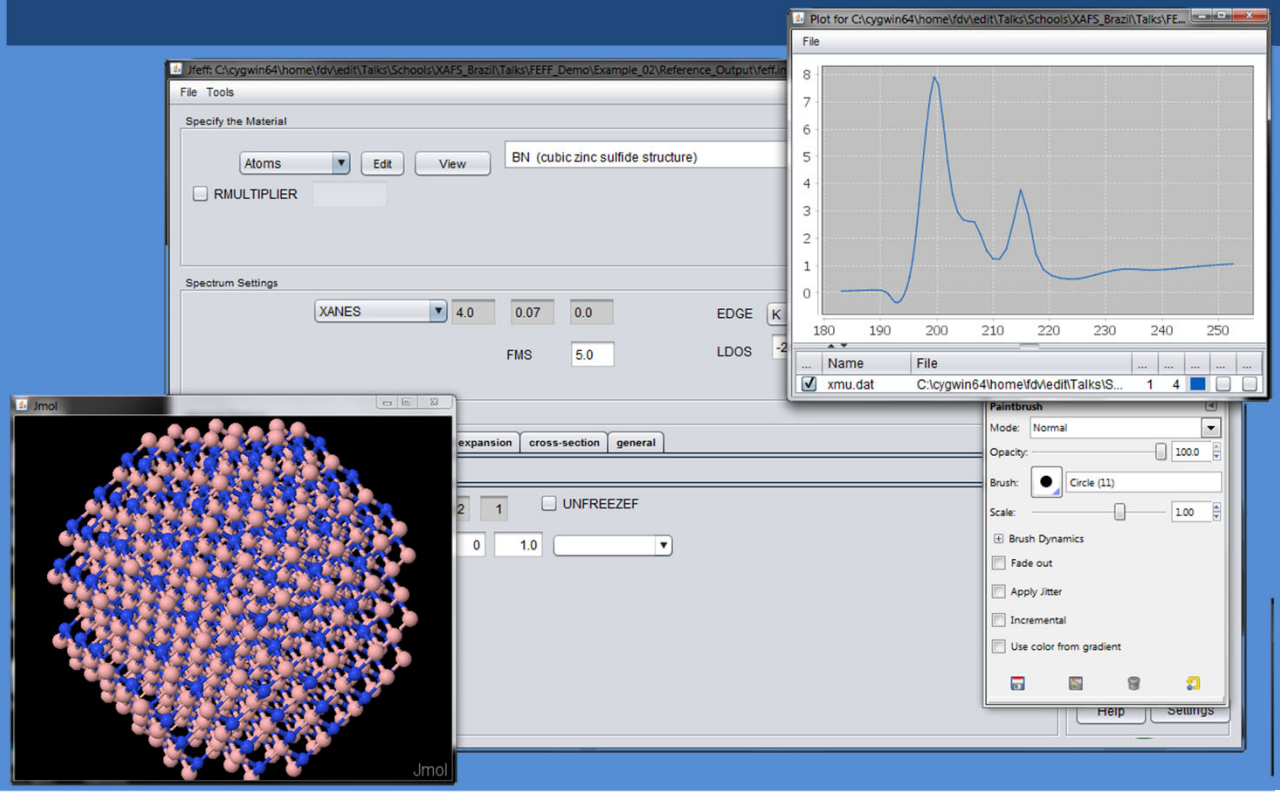
Los Alamos Computational Condensed Matter Summer School June 23, 2026

Hands-on Xray Spectroscopy with FEFF10

J. J. Rehr, J. J. Kas, and F. D. Vila

University of Washington and SLAC



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TIMES

Outline

- Installation of FEFF10 and JFEFF10
- Intro to JFEFF10 - the FEFF10 GUI
- Structure of FEFF10 code (aka FEFF) and main code modules
- FEFF input with or without JFEFF
  - Common input settings
  - Potentials
  - Structure
  - Where to get feff.inp and other input data
- Output files and print options
- Practical considerations
- Advanced topics
- Hands-on exercises

FEFF Demo: Getting the code and GUI

Getting and installing FEFF10 and JFEFF10

Website: times-software.github.io/feff10

Please register before downloading

1. feff10 users guide

2. jfeff GUI and executables for your system OSX,Win,or Linux

3. jfeff-feff10_installation_instructions

JAVA: Check installation instructions for version for your system
JAVA is needed for the JFEFF GUI

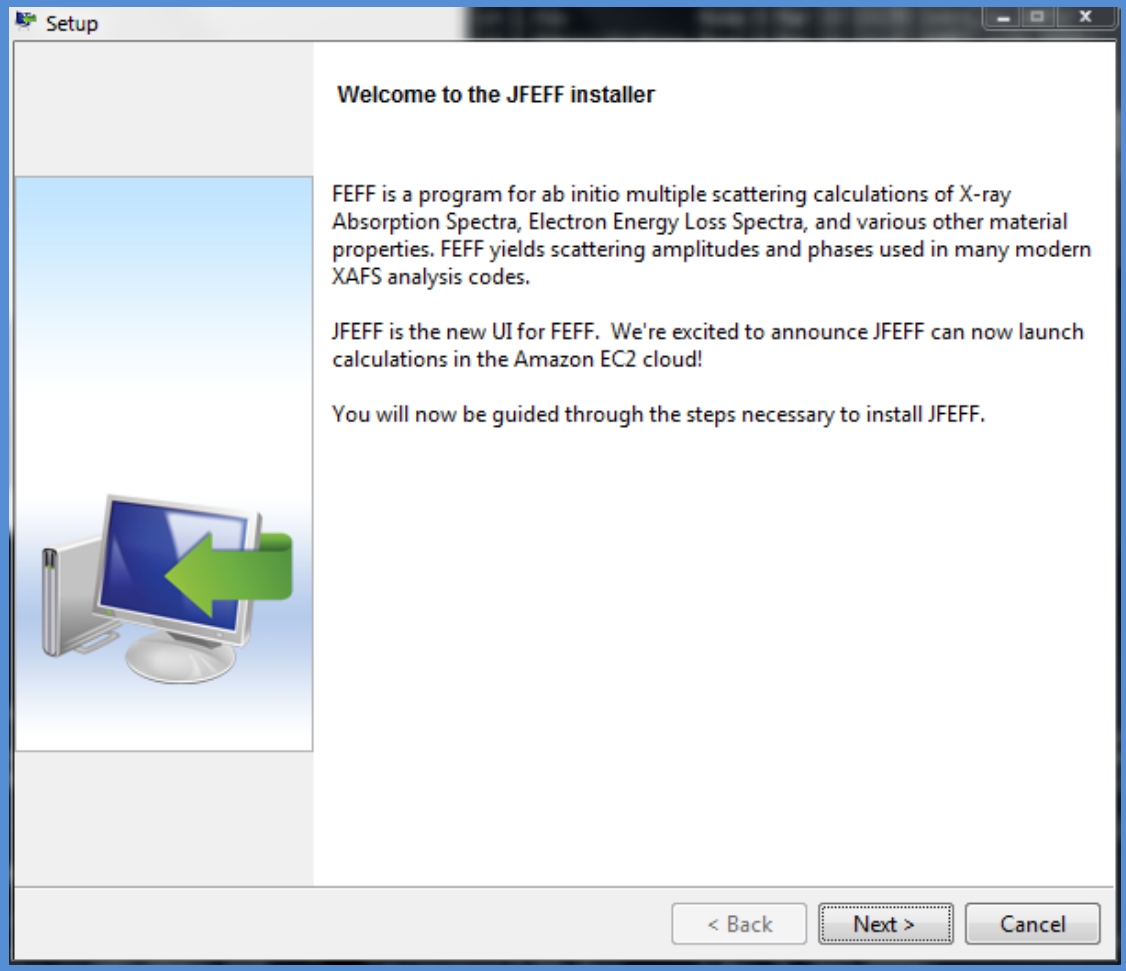
Installation

Easy:

Run installer

Follow instructions carefully

Find feff10 user guide

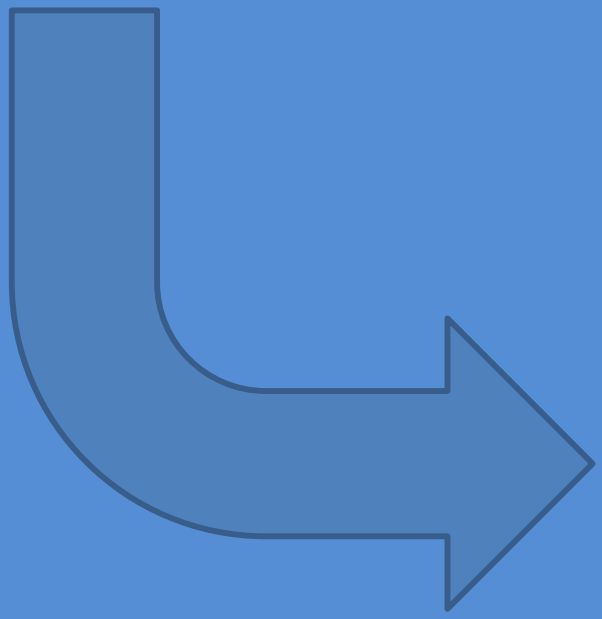


Examples:

jfeff_examples or feff10_examples

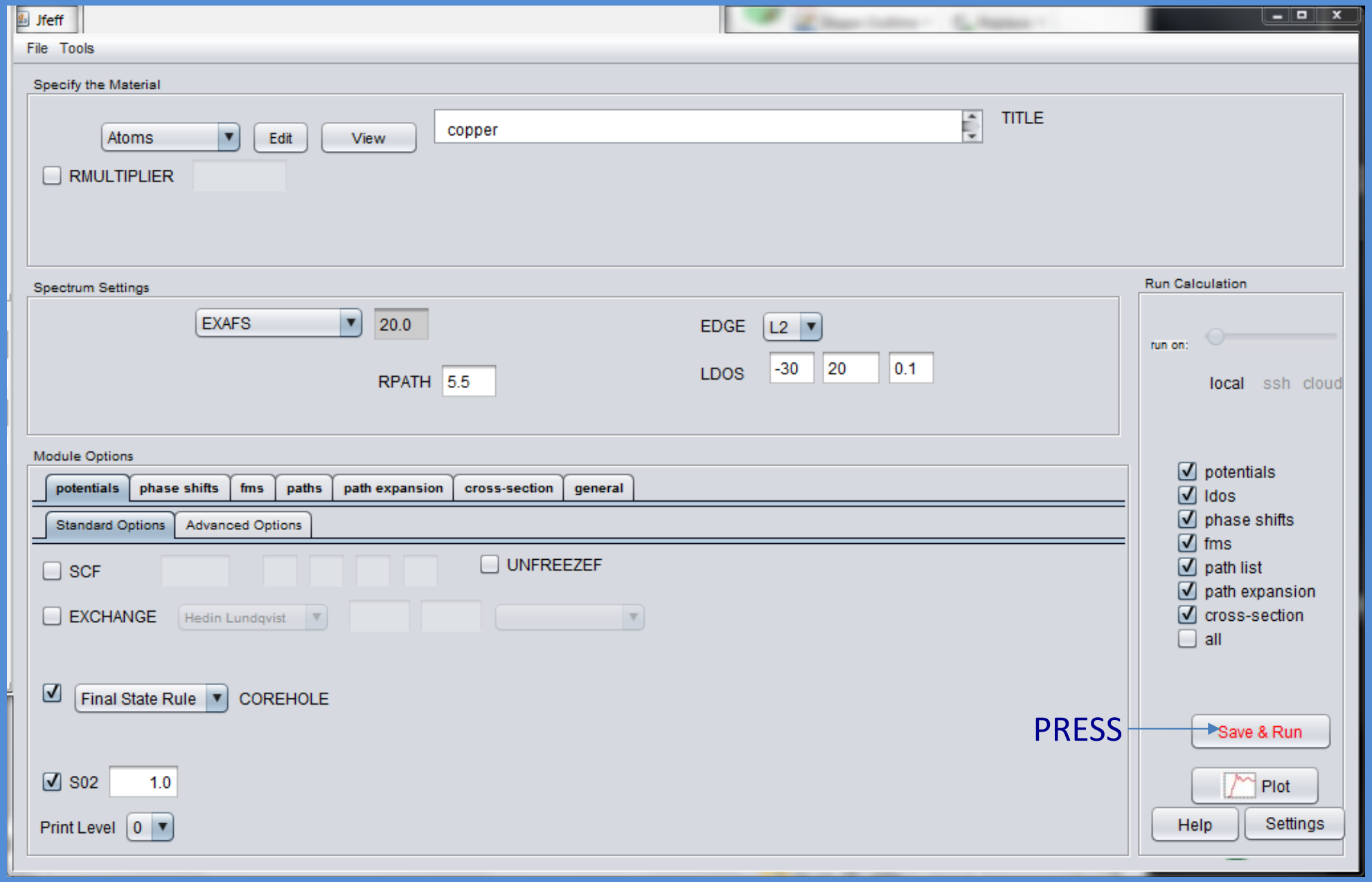
Usually located in your home directory

Installation



Installation

JFEFF GUI: Quick start with preloaded Cu input file

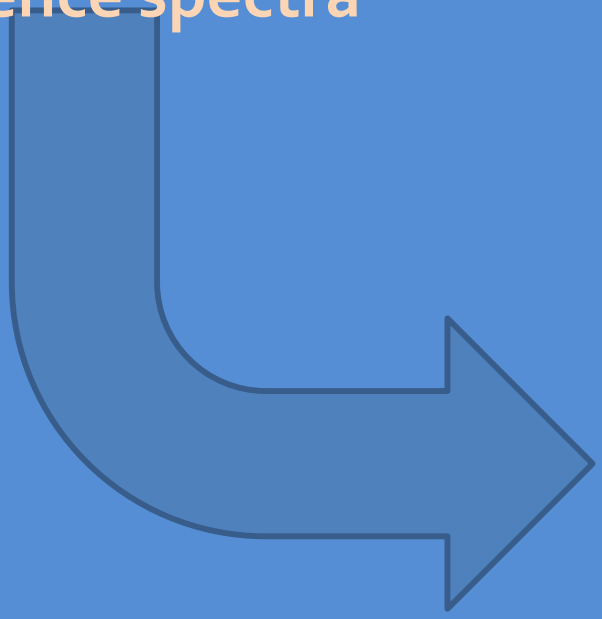


JFEFF GUI: Quick start

Run quick tests 1: Preloaded Cu and
2: $GeCl_4$ in feff10_examples

Verify that the code is working and runs to completion

Plot output xmu.dat and compare with reference spectra



Example_01

Recap of Real-space Multiple-Scattering Formalism

$$H_i = -\frac{1}{2}\nabla^2 + v_i$$
$$t_i = v_i + v_i G_0 t_i$$
$$G_c = G_0 + G_0 t_c G_0$$

$$\mu(\omega) \propto \mathrm{Im} \sum_i \left\langle i \left| d^\dagger G(\omega + E_i) d \right| i \right\rangle \theta_\Gamma(\omega + E_i + E_{Fermi})$$

EXAFS

$$G = G_c + G_c \sum_{i \neq c} t_i G_c + G_c \sum_{i \neq c} \sum_{j \neq c} t_i G_0 t_j G_c + \cdots$$

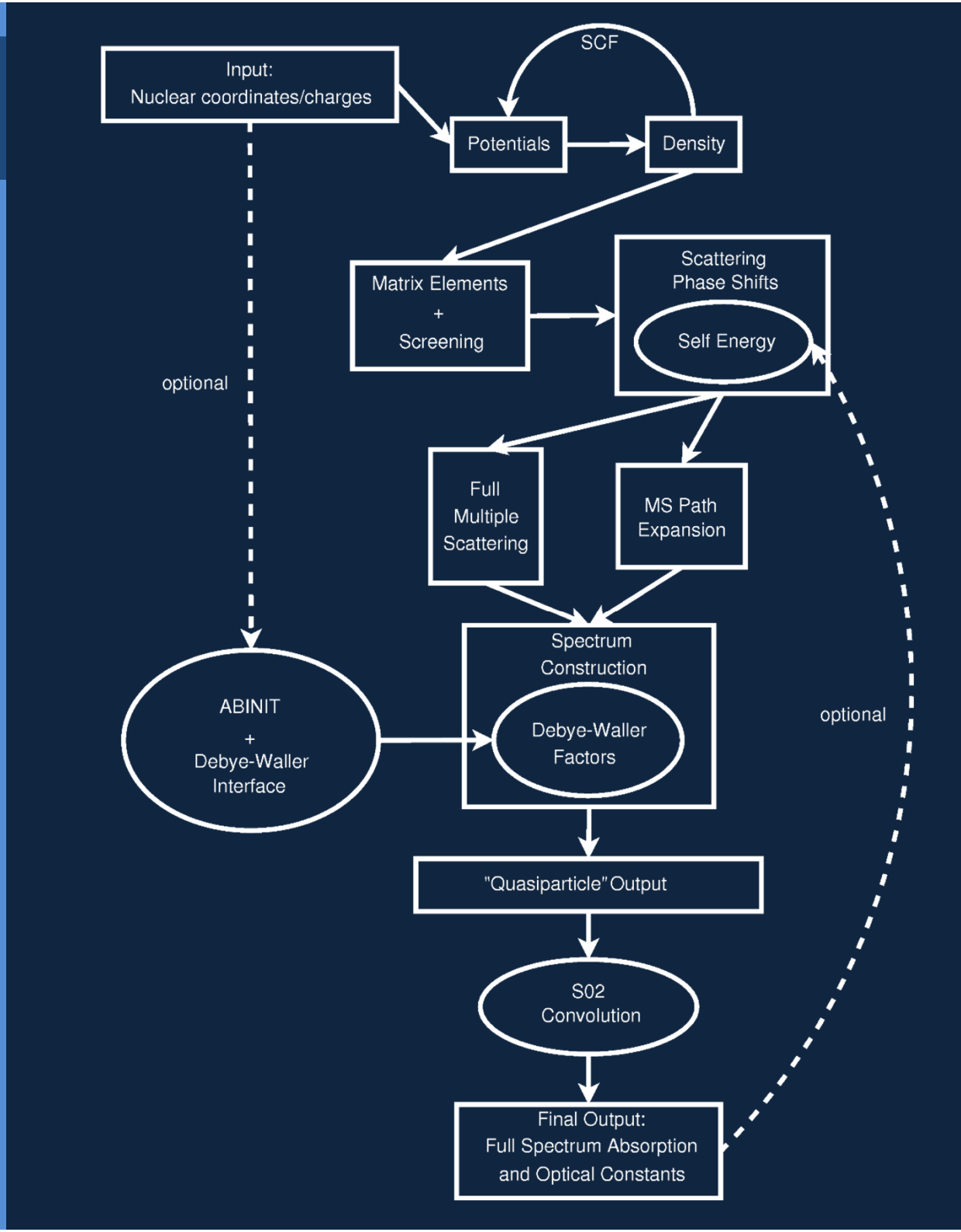
$$H_i R = E R$$
$$T^{ij}_{LL'} = t^i_{LL'} \delta_{ij}$$

XANES

$$G_{LL'} = \left[(1 - G_0 T)^{-1} G_0 \right]^{ij}_{LL'}$$

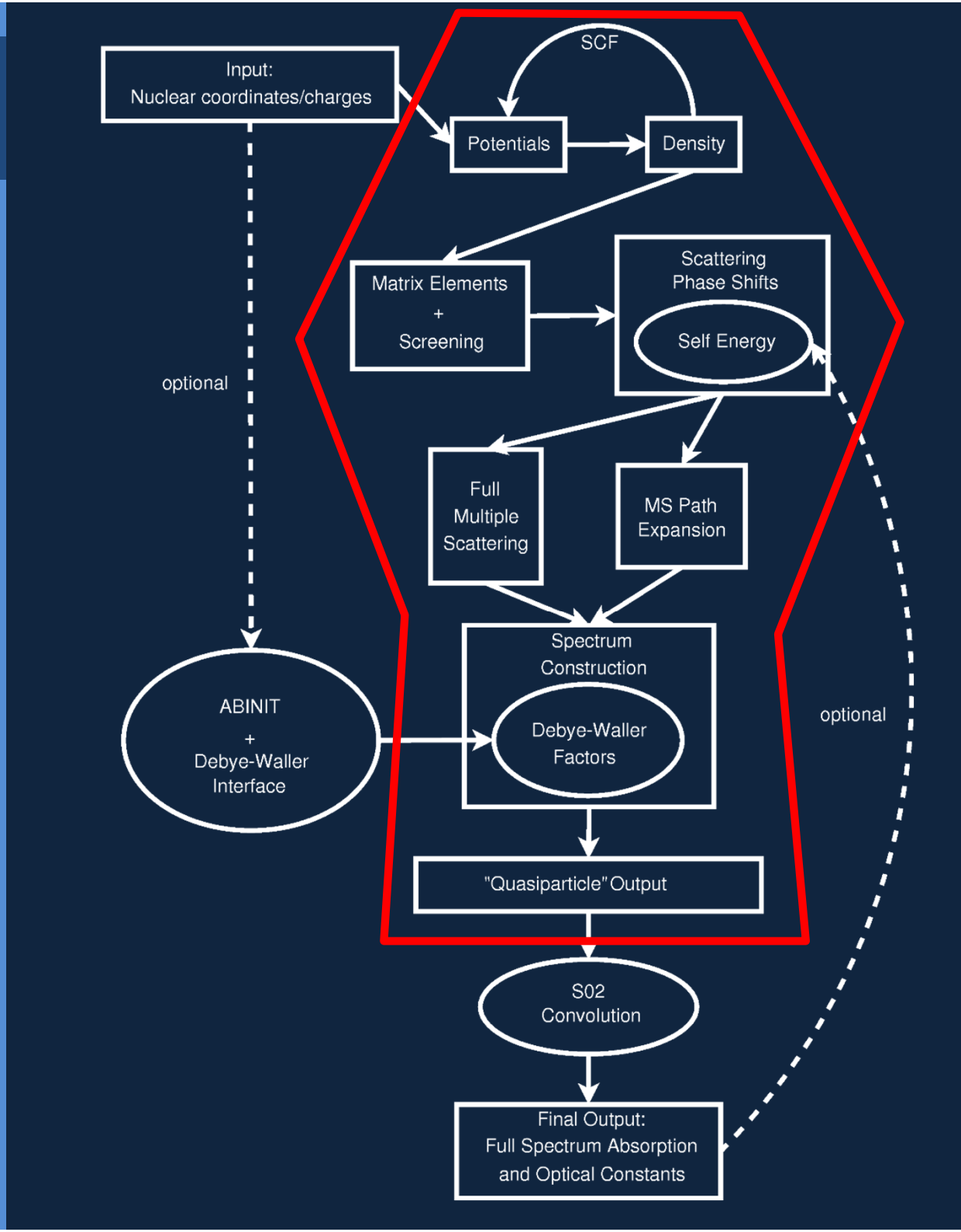
FEFF: Flow Diagram

GUI "hides" JFEFF workflow



FEFF: Flow Diagram

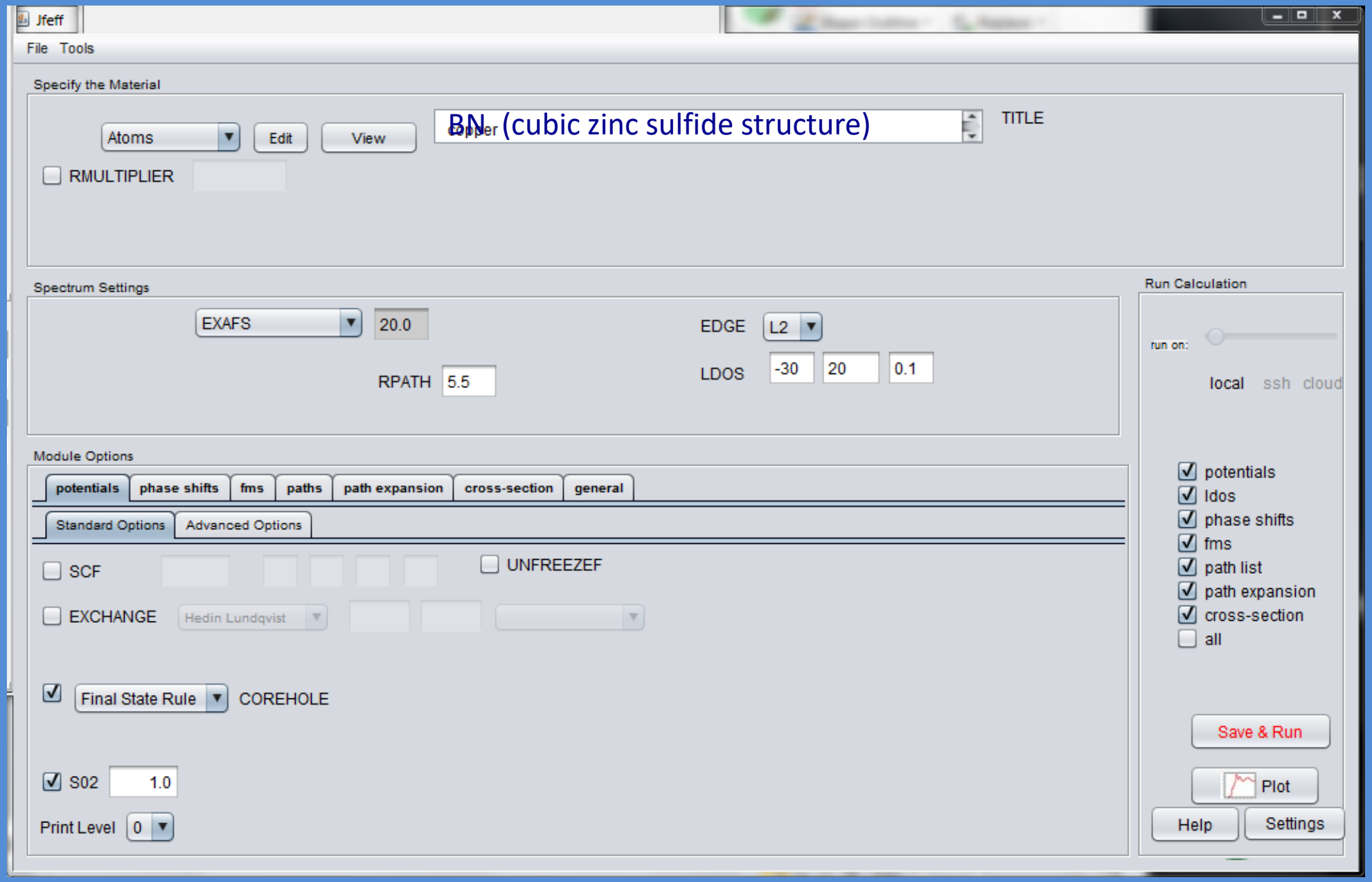
"Standard" FEFF run



FEFF10 code: Modules

rdinp	Read Input
dmdw	Standalone vib. properties
atomic	Solve atomic overlap problem
pot	Self-consistent scattering pot. solver
ldos	Calculate local projected DOS
screen	Screen potential (if requested)
crpa	RPA core-hole (if requested)
opconsat	Full spectrum setup (if requested)
xsph	Phase shifts, cross sections
fms	Full multiple scattering
mkgtr	Trace over Green's function
path	MS path expansion (EXAFS)
genfmt	Scattering amplitudes
ff2x	Build X-ray spectra
sfconv	Spectral function convol. (if requested)
compton	Compton spectra
eels	EELS spectra

JFEFF GUI: Example-03 BN



JFEFF GUI: Example_03

Load BN input file

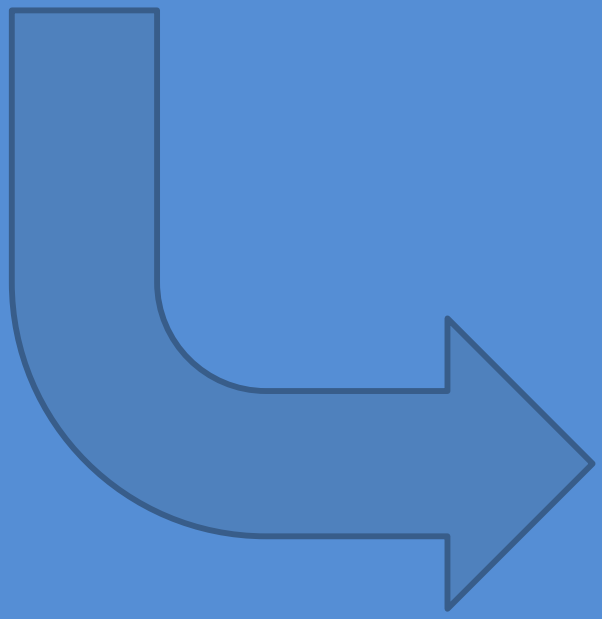
/home/feff10_examples/XANES/BN/feff.inp

Explore the different options available

- Spectroscopy
- Edge
- Hover mouse over boxes to see details

Look at all the different module tabs

Run the BN example - we can look at it later



Example_03

Overview of a typical FEFF input

```
TITLE BN  (cubic zinc sulfide structure)

EDGE K
XANES 4.0
LDOS -20 10 0.5

CONTROL 1 1 1 1 1 1
PRINT   5 0 0 0 0 0

EXCHANGE 0 0 1.0

S02 1.0
SCF 3.0
FMS 5.0

POTENTIALS
*    ipot    Z  element              l_scmt  l_fms   stoichiometry
       0     5   B                    2       2       0.01
       1     5   B                    2       2       1
       2     7   N                    2       2       1

ATOMS                          * this list contains 705 atoms
*   x          y          z       ipot  tag           distance
   0.00000    0.00000    0.00000  0    B1            0.00000     0
   0.90375    0.90375    0.90375  2    N1            1.56534     1
  -0.90375   -0.90375    0.90375  2    N1            1.56534     2
   ...
```

Why look at `feff.inp` text if we have a GUI?

THIS is what the GUI uses

"Whole run" settings in front of you

High end/performance runs are usually handled with text input (queuing in supercomputers)

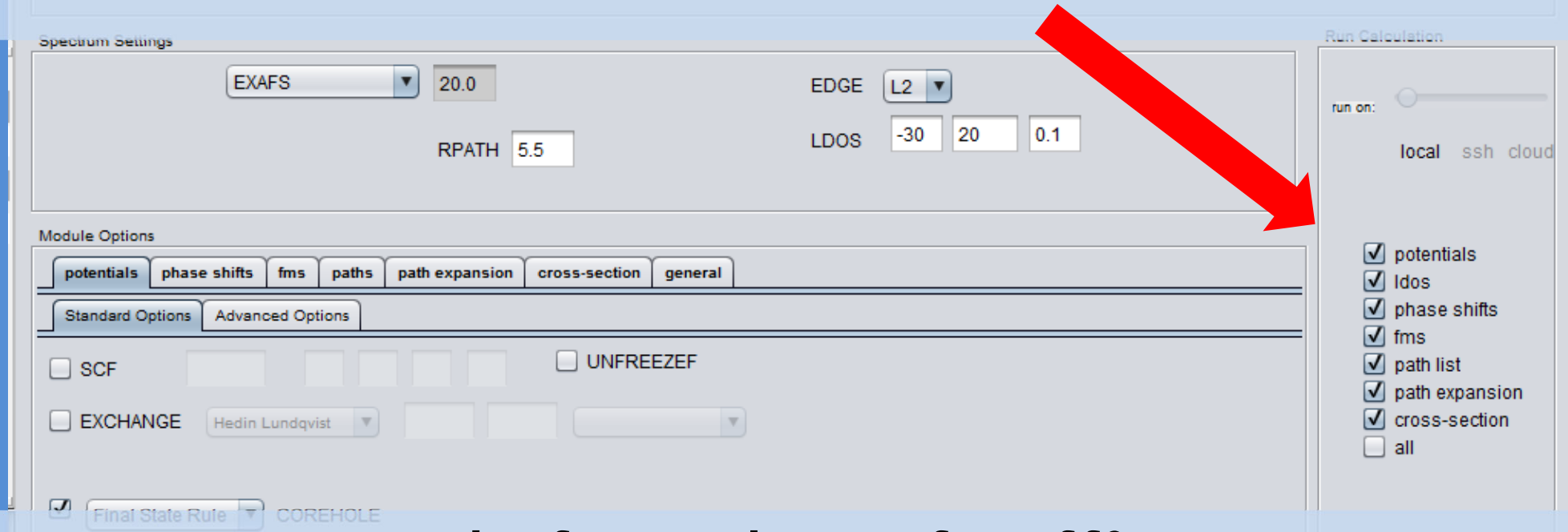
If you know what goes in the input files, you can make scripts to generate them and run them automatically

Because you are used to it

Program flow and printout cards

CONTROL ipot ixsph ifms ipaths igenfmt iff2x

Controls execution of the basic FEFF modules
Used to avoid repeated calculation
Closely related to JFEFF GUI buttons



PRINT ppot pxsph pfms ppaths pgenfmt pff2x

Controls print level of the basic FEFF modules

Main FEFF10 spectroscopy/property cards

```
EDGE      label [s02]
     Choose absorption edge

XANES     [xkmax xkstep]
     Do XANES up to xkmax with step xkstep

EXAFS     [xkmax]
     Do EXAFS up to xkmax

LDOS      emin emax eimag
     Compute projected DOS from emin to emax,
     broadened by eimag

XES       emin emax estep
     Compute emission spectra, from emin to emax with
     step estep
etc
```

Computational methodology cards

```
SCF             rscf [lfms1 ...]
     Self-consistent pot. with cluster of radius rscf
     lfms1: 0 for solids, 1 for molecules
FMS             rfms [lfms2 ...]
     Full multiple scat. with cluster of radius rfms
     lfms2: 0 for solids, 1 for molecules

COREHOLE        approximations
     Types of core hole: FSR, RPA, or none
RPATH           rpath
     Maximum effective EXAFS path length to use

EXCHANGE        ixc vr0 vi0 [...]
     Compute spectra using self energy type ixc, with
     rigid shift vr0 and broadening vi0
DEBYE           temp thetad [idwopt] [...]
     Add vibrational damping for temperature temp
     using Debye temperature thetad
```

Structure definition: Potentials and Angular momenta

```
 POTENTIALS
*     ipot    Z   element          l_scmt   l_fms    stoichiometry
         0     5    B                2        2         0.01
         1     5    B                2        2         1
         2     7    N                2        2         1
```

All atoms with the same potential are identical

Maximum *l* values determine quality of basis set

- Use -1 if not sure (sets defaults)
- Rule of thumb: (max. occupied *l*) + 1

Stoichiometry:

- Use 0.01 for absorber in solids
- Use 1 for absorber in molecules
- Rest should be number of atoms of type in unit cell or molecule

Structure definition: xyz coordinates

```
ATOMS                                * this list contains 705 atoms
*    x           y           z       ipot   tag          distance
    0.00000     0.00000     0.00000  0     B1           0.00000      0
    0.90375     0.90375     0.90375  2     N1           1.56534      1
   -0.90375    -0.90375     0.90375  2     N1           1.56534      2
    ...
```

Only Cartesian coordinates and potential types required

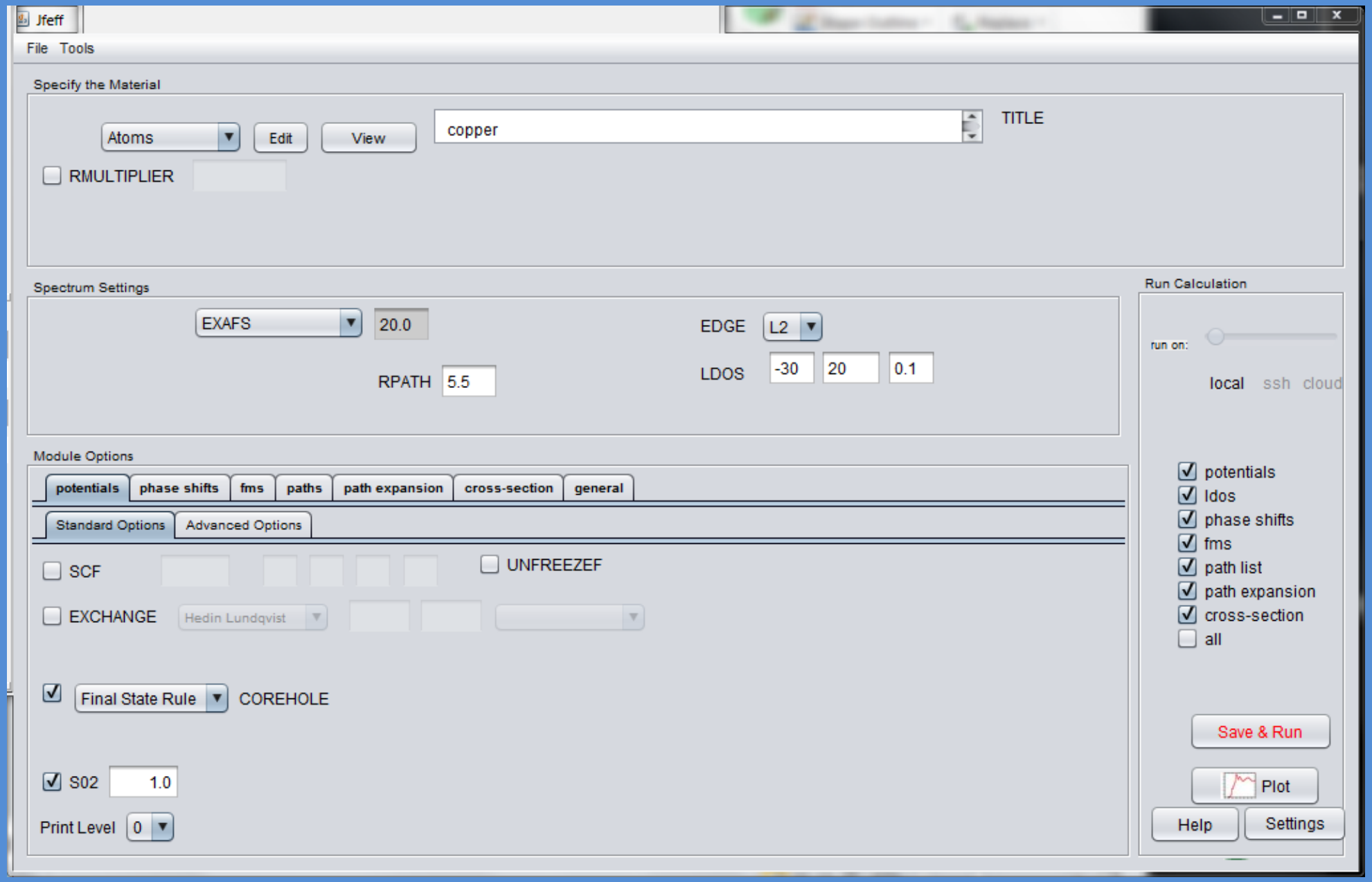
Tags and distances are useful

Put absorber in center of model cluster for optimal results

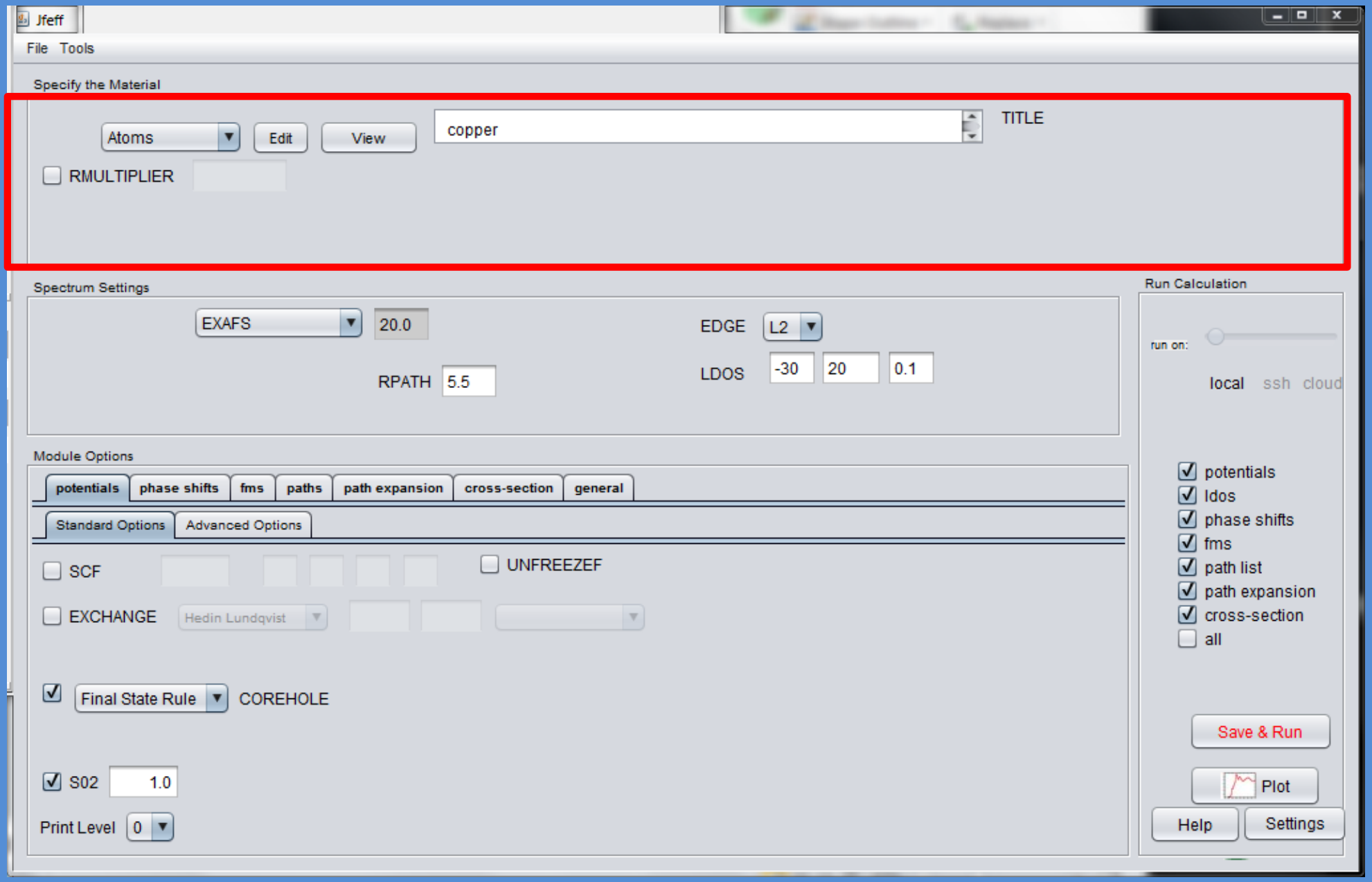
Good structures are essential to get good results

Structures with inequivalent atoms of the absorbing type must be done separately and averaged

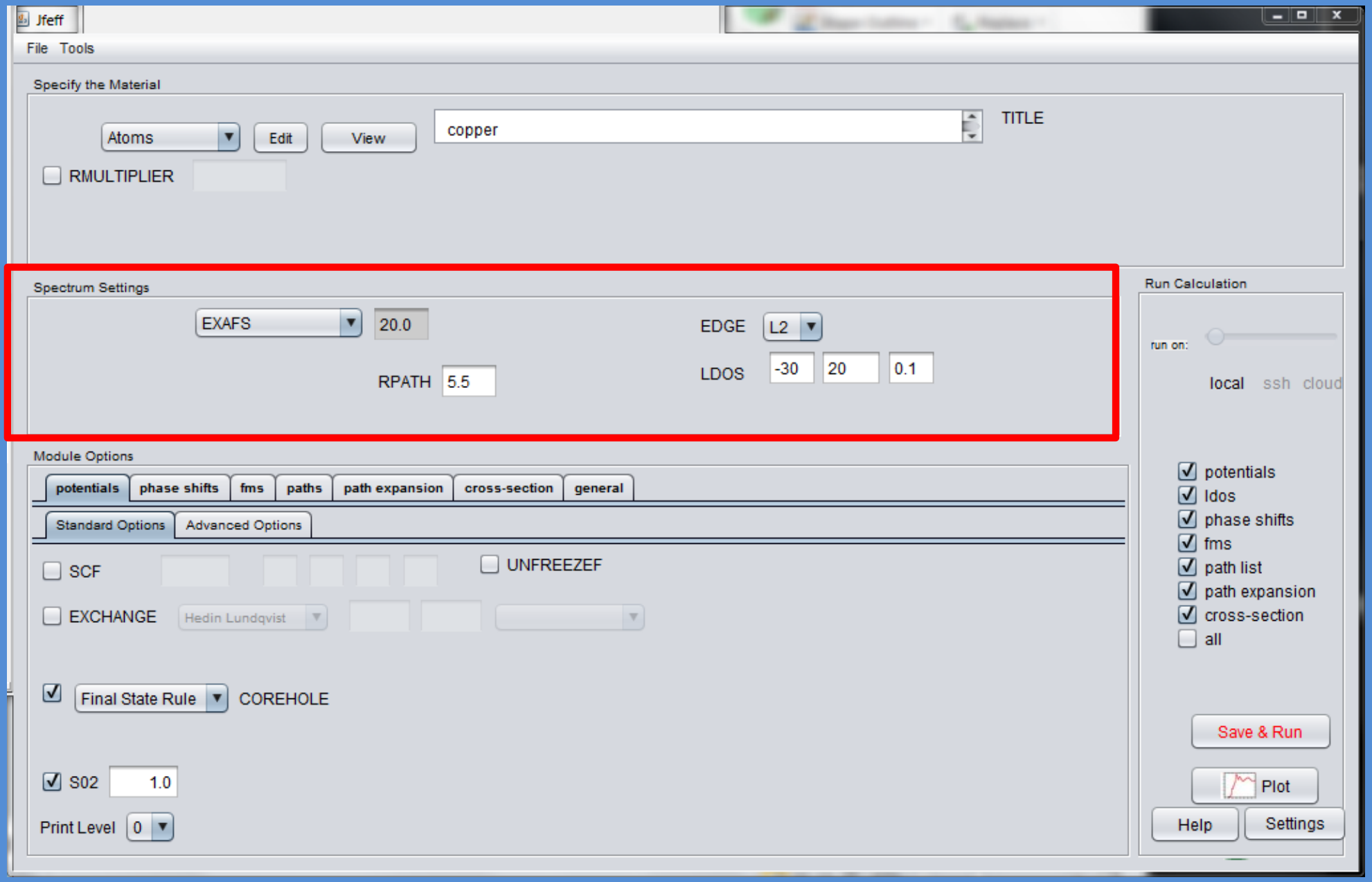
JFEFF: FEFF GUI Details



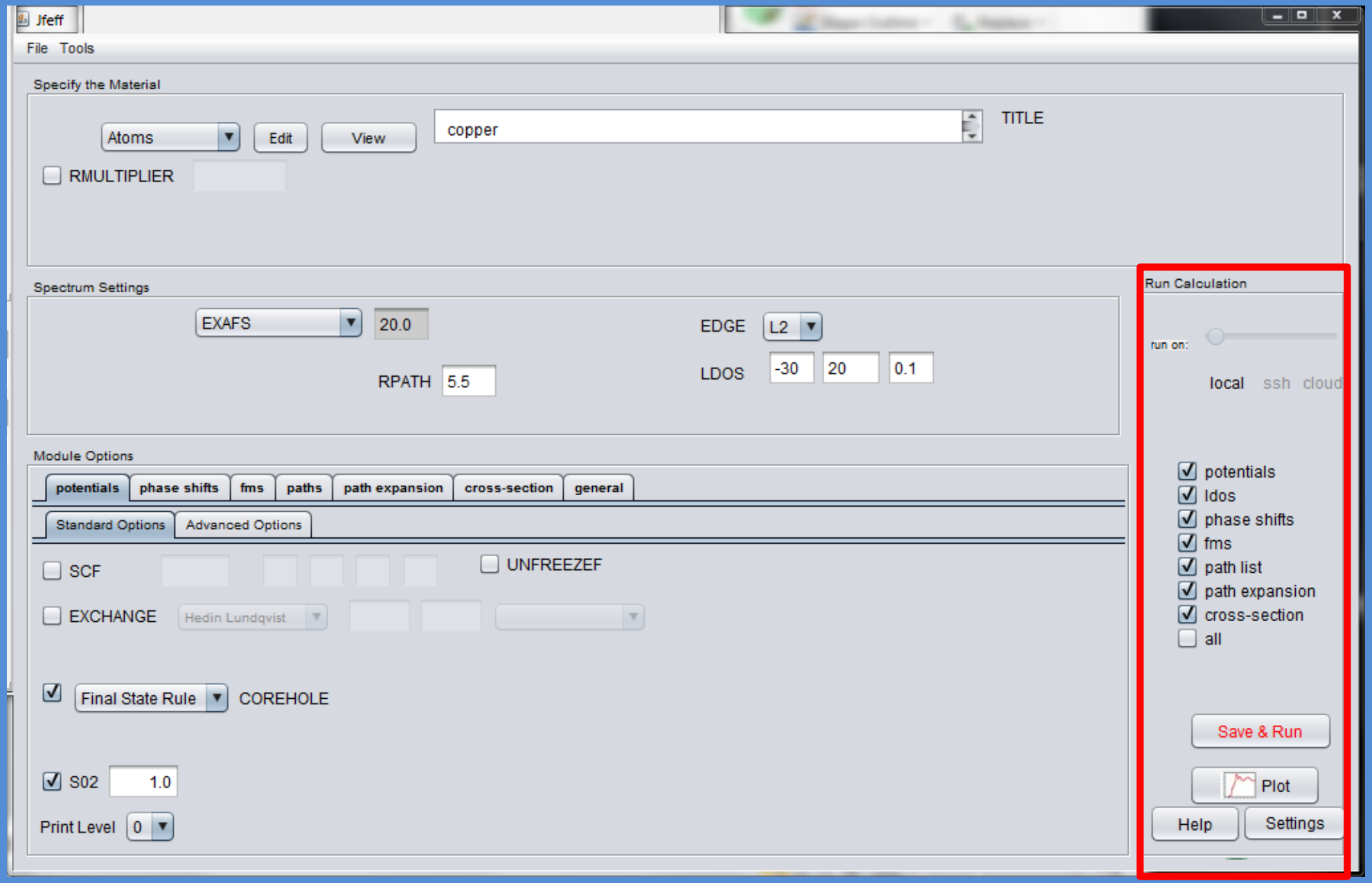
Material dashboard



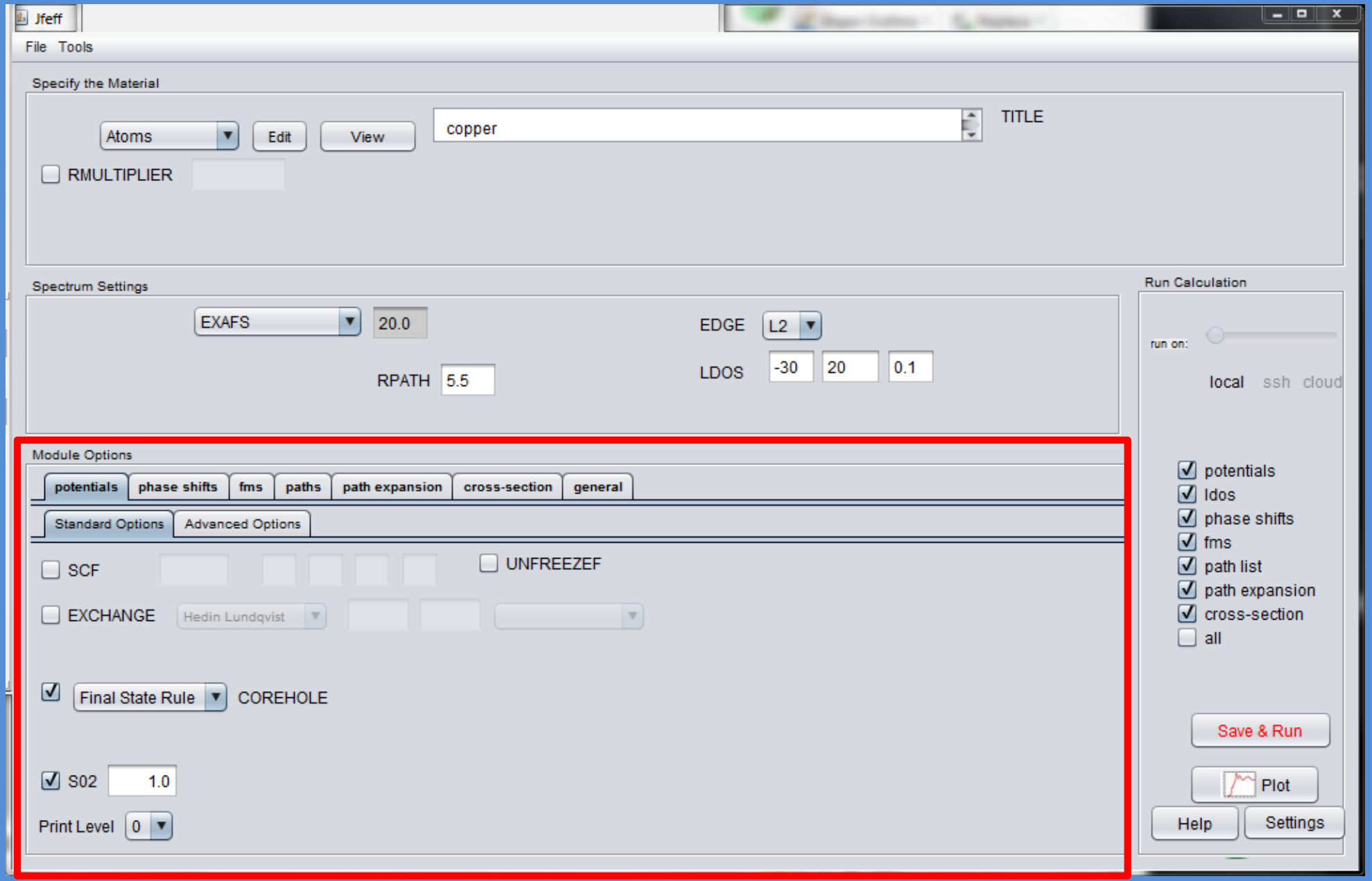
Spectroscopy dashboard



Control dashboard



Module options dashboard



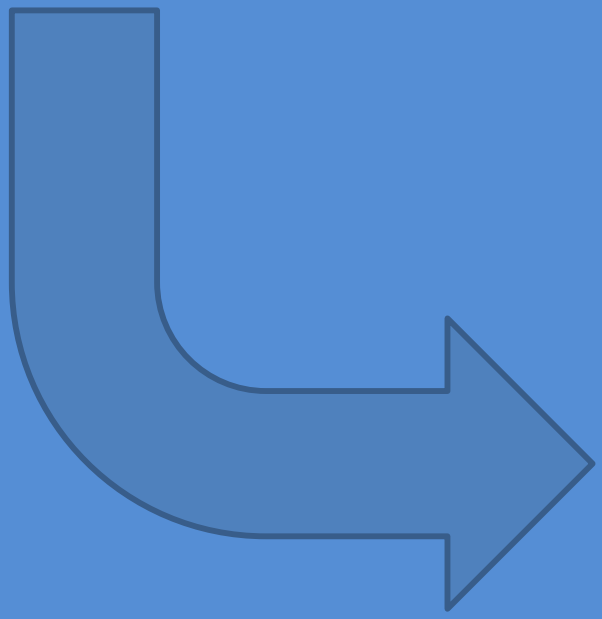
Where to get FEFF input files

WebAtoms

- Find material X
- Create input file
- Save to disk and load in JFEFF

Materials Project

- Find material with MP-ID
- X-ray spectra
- feff.inp
- MaterialsHUB



Web

Where to get info to build your own FEFF input

WebATOMS:

URL: https://millenia.cars.aps.anl.gov/webatoms
Get structures and FEFF inputs for common minerals
Build your own FEFF input from your data

Materials Project:

URL: https://www.materialsproject.org
Massive database of DFT optimized structures
Proto-interface for FEFF (MaterialsHUB)
Database of FEFF K-edge calculations and `feff.inp` files

Crystallography Open Database (COD):

URL: http://www.crystallography.net
Get Crystallographic Information Files (CIFs)
Experimental structures
Feed into FEFF or use data with Web ATOMS

Where to get info to build your own FEFF input

Comp. Chem. Comparison and Benchmark DataBase (CCCBDB):

- URL: http://cccbdb.nist.gov
- Get experimental and theoretical structures for many molecules
- Build your own FEFF input from your data

Others:

- Protein Data Bank (PDB)
- Cambridge Structural Database (CSD)
- Database of Zeolite Structures
- ChemSpider
- PubChem

FEFF output files

Where to find information: see feff10 doc for details

xmu.dat

x-ray spectrum, Fermi level, misc. info

logN.dat

Output for each module, depending on N

ldosNN.dat

Projected DOS local for pot. type NN

potNN.dat

Potentials and densities for pot. type NN

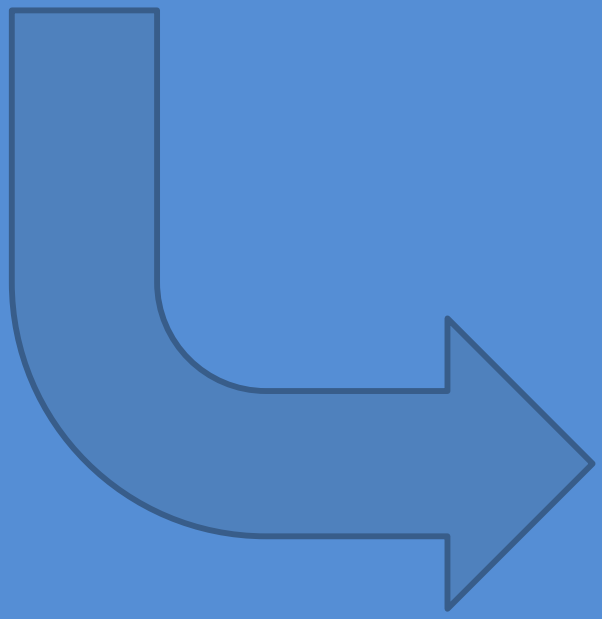
feffNNNN.dat

Path data for EXAFS

FEFF output

We will look at:

- `xmu.dat`
  - Plot spectrum
  - Find Fermi level
- logN.dat
  - `log1.dat`
    - Convergence and charges
- `ldosNN.dat`
  - Compare LDOS from 2 atoms
  - Get some chemical intuition
  - Broadly compare to XANES



Example_02

Default & reasonable settings for FEFF

SCF radius:

- Start with small clusters 2 shells or 30 atoms
- Always check convergence

FMS radius:

- Use mean free path rule or
- Start with 4 shells or about 50 atoms
- Always check convergence

Potentials:

- Too few → bad results
- Too many → poor SCF convergence
- Use chemical intuition l_{max} ~ max atomic $l + 1$
- Higher l_{max} → may improve results
- Too high l_{max} → heavy calculations

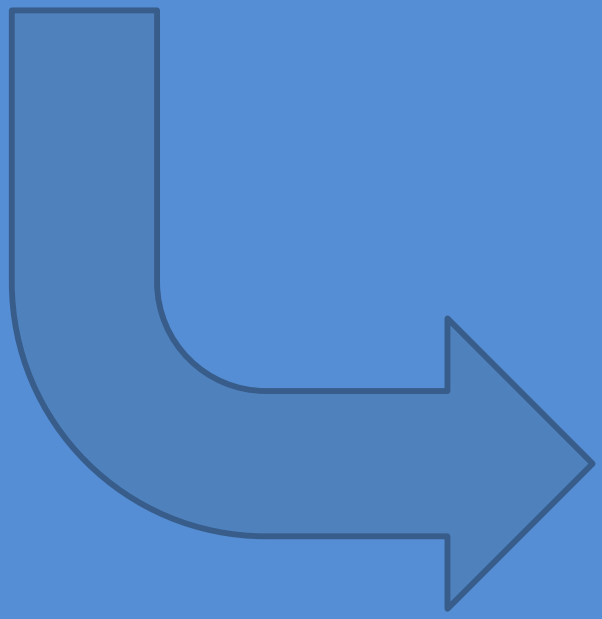
Command line FEFF and parallel versions

Parallel FEFF for SCF and FMS

- Much faster – MPI
- Essential for state-of-the-art modelling
- Commonly used in supercomputer centers

Need to get fortran source code
Need MPI compiler e.g. gfortran
Edit Compiler.mk to suit your sysem
Compile

Use "feff" script to run serial
Use "feffmpi" script to run parallel



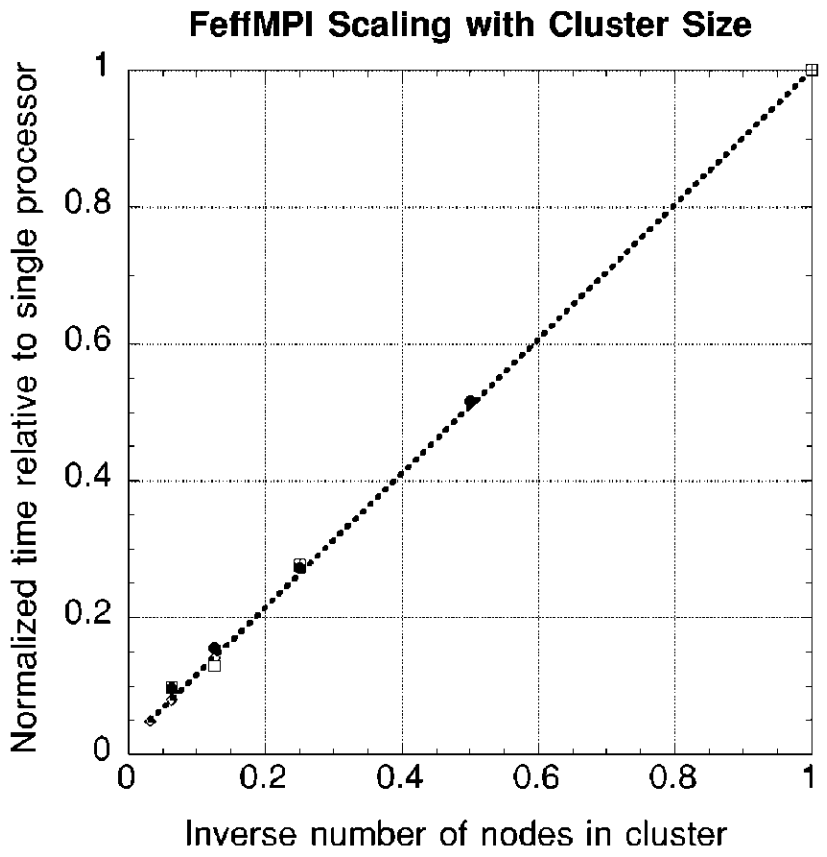
Linux shells

Parallel (MPI) FEFF

PHYSICAL REVIEW B, VOLUME 65, 104107

Parallel calculation of electron multiple scattering using Lanczos algorithms

A. L. Ankudinov,[1] C. E. Bouldin,[2] J. J. Rehr,[1] J. Sims,[2] and H. Hung[2]
[1]*Department of Physics, University of Washington, Seattle, Washington 98195*
[2]*National Institute of Standards and Technology, Gaithersburg, Maryland 20899*



MPI: "Natural parallelization"
Each proc. does a few energies

Needed for state-of-the-art XANES simulations

Summary part 1

Now you have or can:

- Install and run FEFF10 with JFEFF
- Know where to get structural information
- Make & understand FEFF input files
- Understand FEFF output
- Be ready for Practicum session

Part 2: Some challenging examples

1 Build an input file for and oxide of choice (eg WebAtoms)

Suggested: Cr_2O_3

Do NOT run the LDOS – not usually needed and takes time

Try a XANES Cr K edge calculation

Test SCF convergence

(start with rSCF ~ 4 shells)

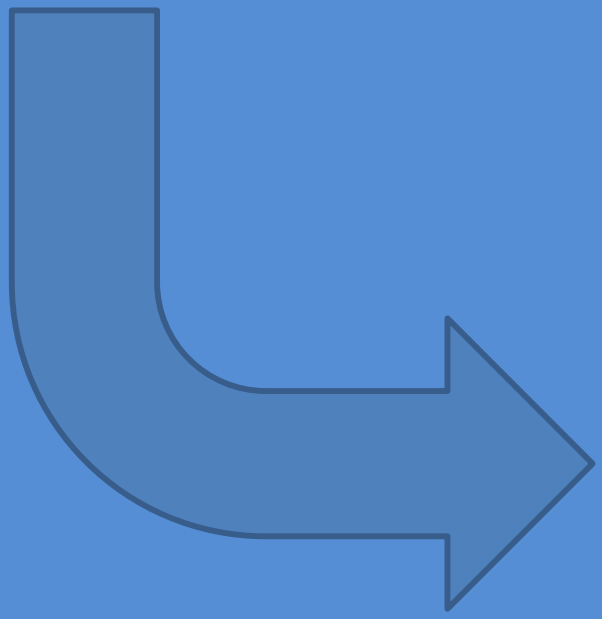
Test FMS convergence

(start with rFMS ~ 10 shells)

Visualize results

Find expt. results

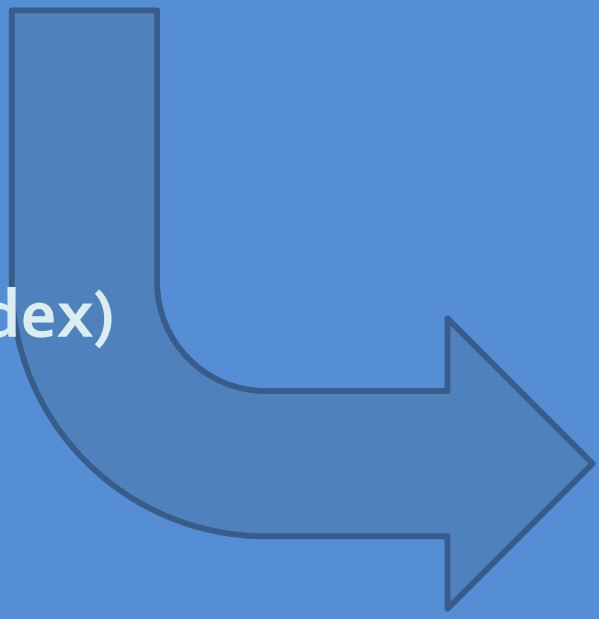
Try a quick Google Scholar search



Challenge_01

Some more challenging examples

2. Build a simple Pt nanoparticle: (Hint: WebAtoms again)
    - Suggested: About 19 atoms
    - Suggested: Use Pt crystal bond distances
- Use the L3 edge
- Use SCF and FMS radii to cover the whole particle
- From the initial feff.inp make inputs for
    - The atom in the center
    - An atom on a edge
    - An atom in a vertex
- (Hint: Just change the absorber potential index)
- Compute the XANES and compare
- Try to correlate XANES with:
    - Fermi level
    - Partial atom charges
    - LDOS



Challenge_02

Some challenging examples: Mn oxidation states

3. Make inputs for:
   - MnO
   - Mn_2O_3
   - MnO_2

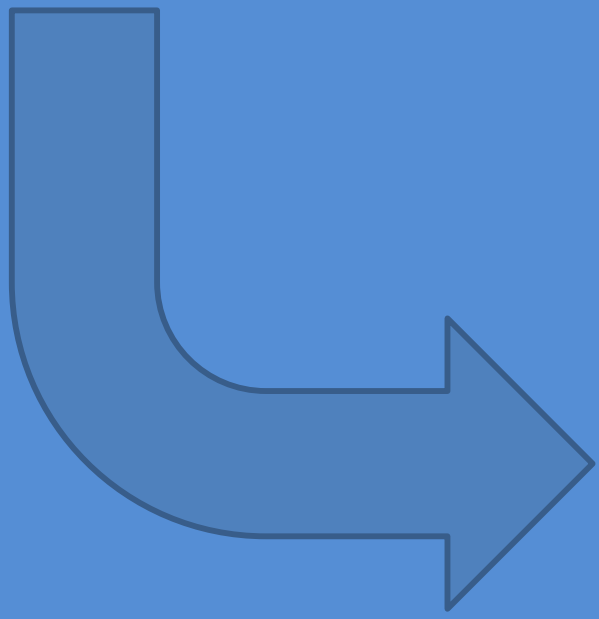
Use the K edge of Mn (Caveat: Mn_2O_3 has inequiv. Mn atoms)

Use consistent SCF and FMS radii
   - Suggested SCF: 4 Ang
   - Suggested FMS: 6 Ang
   - Keep complete shells

Compute the XANES

Estimate edge and white line position

Try to correlate with:
   - Fermi level
   - Formal oxidation state
   - Partial atom charges



Challenge_03

Using Ab Initio DW factors in FEFF – not discussed here

```
DEBYE Temp Debye_Temp [DW_Opt [dymFile DMDW_Order DMDW_Type DMDW_Route]]

          DEBYE    500.0  1073.0  5 feff.dym  6  0  1
```

DMDW_Type - Type of DW calculation, the possible values are:
0 - Parallel σ^2 (default)

DMDW_Route - Which paths to use in the dmdw module. These paths do not affect the path selection in the XAS calculations, they are used for the generation of an input for the independent dmdw module. The possible values are:

- 0 - Skip dmdw module (default)
- 1 - All SS paths from absorber
- 2 - Same as 1 + all DS paths from absorber
- 3 - Same as 2 + all TS paths from absorber
- 11 - All SS paths
- 12 - Same as 1 + all DS paths
- 13 - Same as 2 + all TS paths

The dynamical matrix file dym

```
   1                                                    # dym type
   3                                                    # Number of atoms
   8                                                    # Atomic numbers
   1
   1
    15.99491460                                         # Atomic masses (AMU)
     1.00782504
     1.00782504
   0.00000000   0.00000000   0.00000000                 # Cartesian coordinates (au)
   1.81679640  -0.23950080   0.00000240
  -0.23950080   1.81679640   0.00000240
   1   1                                                # Atom indices for FC block
  5.398996e-01 -1.171079e-01  5.031484e-07              # FC1x1x FC1x1y FC1x1z
 -1.171079e-01  5.399060e-01  9.690730e-07              # FC1y1x FC1y1y FC1y1z
  5.031484e-07  9.690730e-07 -1.841479e-03              # FC1z1x FC1z1y FC1z1z
   1   2
 -4.941835e-01  3.022460e-02 -6.064138e-07              # FC1x2x FC1x2y FC1x2z
  8.687800e-02 -4.571081e-02 -1.155657e-07              # FC1y2x FC1y2y FC1y2z
 -6.583932e-07  7.894155e-08  9.207451e-04              # FC1z2x FC1z2y FC1z2z
   1   3
 -4.571614e-02  8.688332e-02  1.032683e-07
  3.022992e-02 -4.941952e-01 -8.535212e-07
  1.552287e-07 -1.048028e-06  9.207340e-04
...
```

Typical DMDW output

```
Path Indices:    1    2
 pDOS Poles:
     Freq. (THz)     Weight
        7.609        0.00055
       14.776        0.00077
       24.890        0.00587
       31.463        0.00623
       33.972        0.70221
       34.762        0.28436

 pDOS Einstein freq (single pole) and associated temp:
 Freq (THz)    Temp (K)
  34.118       1637.35

 pDOS n Moments and associated Einstein freqs and temps:
  n      Mom (THz^n)    Freq (THz)      Temp (K)
 -2        0.00087       33.85132       1624.55
 -1        0.02941       34.00240       1631.80
  0        1.00000      ----------     --------
  1       34.09808       34.09808       1636.40
  2     1164.03434       34.11795       1637.35

 Path Length (Ang), s^2 (1e-3 Ang^2):  1.583    1.234
```

That’s all …