RhoChi:

1. Input files
2. Program structure
3. ToDo

19.03.2019

Input files

1. Experimental data:
    - single crystal: list of hkl reflections
    - powder: 1D, 2D diffraction profiles and background

2. Model parameters:
    - ".cif" or STAR-like file (International Tables vol. G)

3. Handbook values:
    - space group
    - magnetic form-factors ($\langle j_0 \rangle$, $\langle j_2 \rangle$)
    - neutron scattering length

Experimental data

single crystal:

```
#wavelength 1.40
#field  0.000 0.000 1.000
#orientation 0.6468462   -0.6860854   0.3300297 0.2141139
-0.2557555   -0.9343334 0.7319312   0.6810804    -0.0183183
#   h   k   l        FR       sFR
    0   0   8   0.64545   0.01329
    2   0   6   1.75682   0.04540
...
```

1D powder diffraction:

```
#wavelength 2.35
#field 0.0 0.0 5.0
# ttheta      IntUP     sIntUP    IntDOWN   sIntDOWN
    7.80    0.74282    0.55201    0.24785    0.29666
    8.00    0.18608    0.18170    0.16548    0.17133
...
```

2D powder diffraction:

```
#wavelength 2.35
#field 0.0 0.0 5.0
#IntUP
                                                    2θ
       241         4.00000         4.20000      ...   ──►
 -40.00000       -85.31322         7.54655      ...
 -39.50000       -53.87826        59.90163      ...
       ...             ...             ...      ...
 ϕ
 ▼
```

background:

```
# ttheta   IntBKGR
    8.20   0.11000
   80.40   0.18300
...
```

Model parameters -- ".rcif"

- phase (totally correspond to .cif description)
- experiment
- refinement

```
global_filerhochi

data_nacaalf
_cell_length_a 9.88888773144
_cell_length_b 9.88888773144
...
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_b_iso_or_equiv
 F1  F  0.13847  0.30656  0.12052  1.0  0.0
...
```

phase

refinement

```
data_ref
_refinement_file_name_output 'full.lis'

loop_
_refinement_param1
 $pnd_$nacaalf_pd_phase_scale
...
```

```
data_pnd
_2dpd_file_name_bkgr 'full.bkg'
_2dpd_file_name_input 'full.dat'
...
loop_
_2dpd_phase_name
_2dpd_phase_scale
_2dpd_phase_igsize
_2dpd_phase_extinction_radius
_2dpd_phase_extinction_mosaicity
 nacaalf  0.0110321630859  0.0  0.0  0.0
```

experiment

It can be directly used to plot the structure

Handbook values

space group: ‘itables.txt’

coefficients for $<j_0>$, $<j_2>$: ‘formmag.tab’

neutron scattering length: ‘bscat.tab’

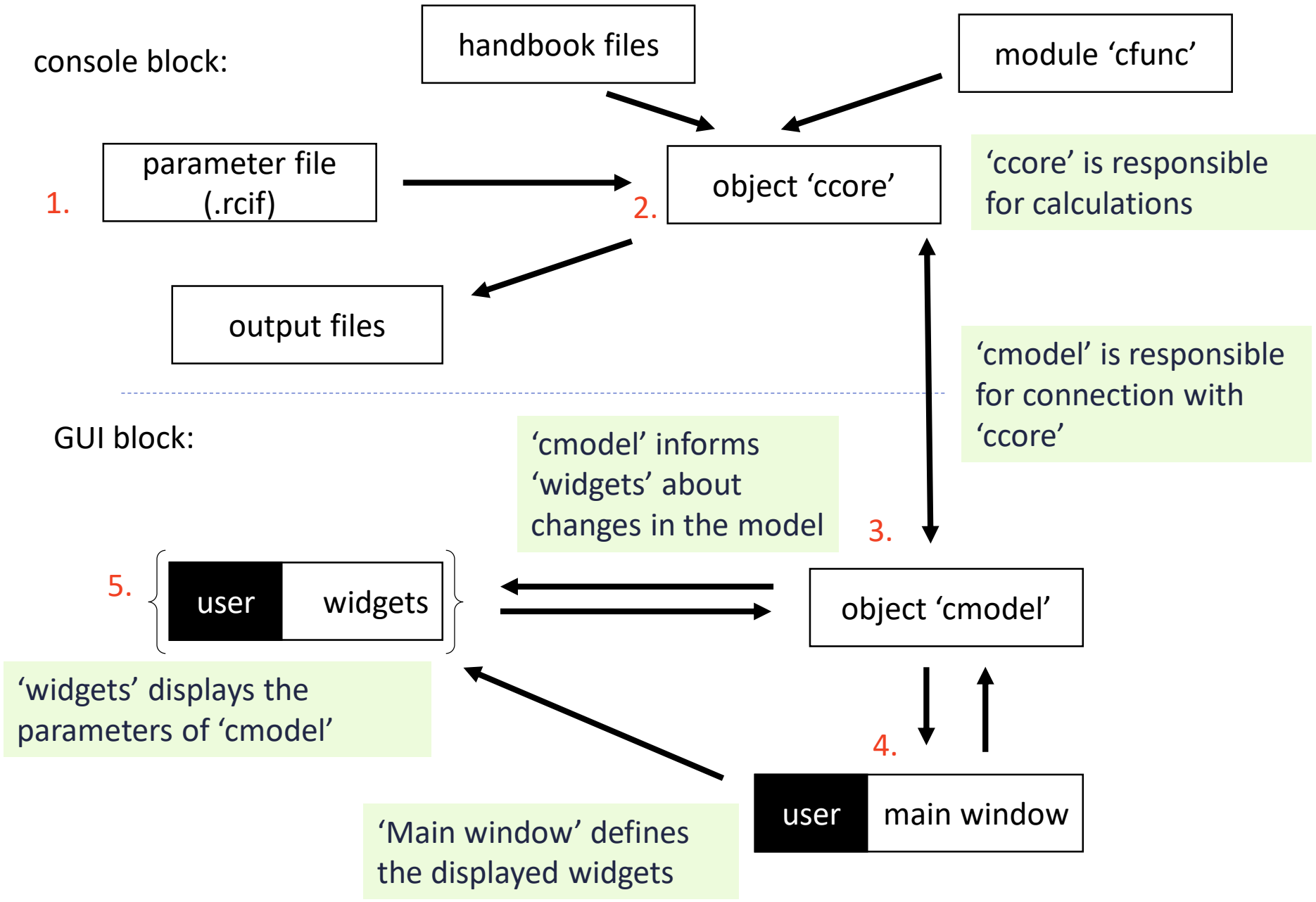
```
203 Fd-3            Cubic
choice: 1
centr: true
pcentr: -0.125,-0.125,-0.125
symmetry: x,y,z
symmetry: -x,-y,z
symmetry: -x,y,-z
symmetry: x,-y,-z
symmetry: z,x,y
symmetry: z,-x,-y
symmetry: -z,-x,y
symmetry: -z,x,-y
symmetry: y,z,x
symmetry: -y,z,-x
symmetry: y,-z,-x
symmetry: -y,-z,x
```

```
Z <j0> form factors for 3d transition elements and their ions
Z
F Sc0  0  0.2512 90.0296  0.3290 39.4021  0.4235 14.3222 -0.0043
F Sc1  0  0.4889 51.1603  0.5203 14.0764 -0.0286  0.1792  0.0185
F Sc2  0  0.5048 31.4035  0.5186 10.9897 -0.0241  1.1831  0.0000
F Ti0  0  0.4657 33.5898  0.5490  9.8791 -0.0291  0.3232  0.0123
...
```

```
#Neutron scattering lengths and cross sections
#!Isotope  conc     Coh b     Inc b    Coh xs    Inc xs    Scatt xs      Abs xs
 H          ---   -3.7390      ---     1.7568    80.26      82.02       0.3326
 1H      99.985   -3.7406   25.274     1.7583    80.27      82.03       0.3326
...
```

Program structure

Principal scheme

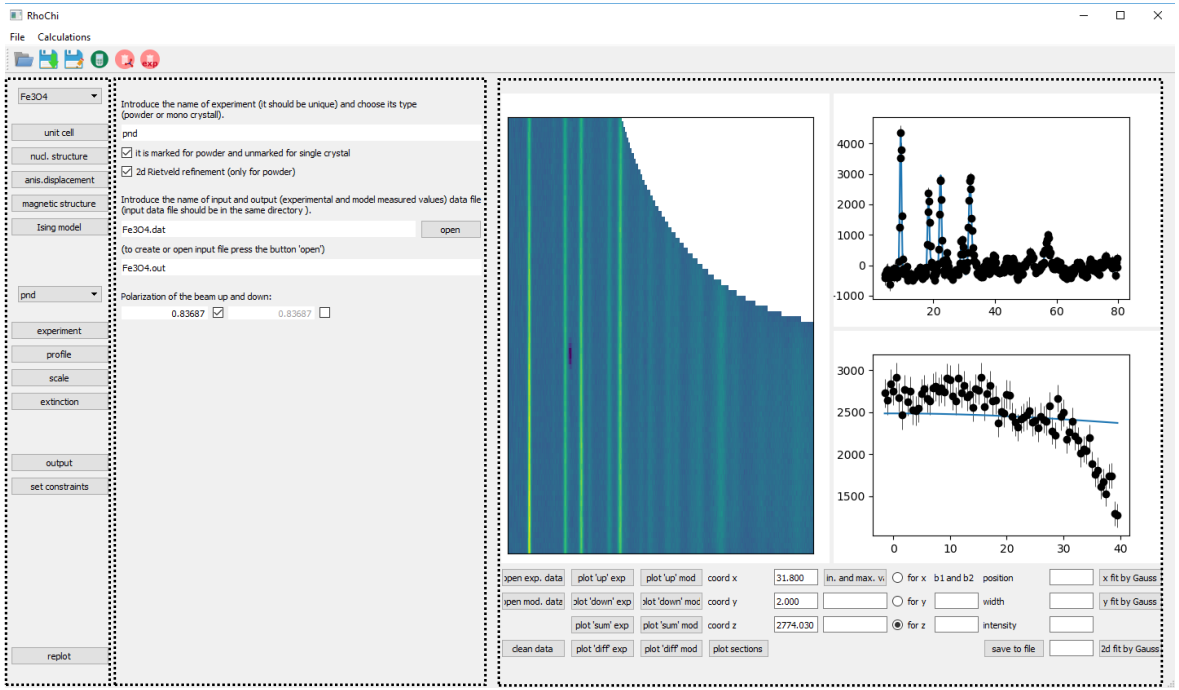


'Main window' (defined in the file 'rhochi.py')

The widgets:

- widg_cpanel
- widg_left
- widg_right

The widget description is given in separate files.



info about 'cmodel' output files

Task:

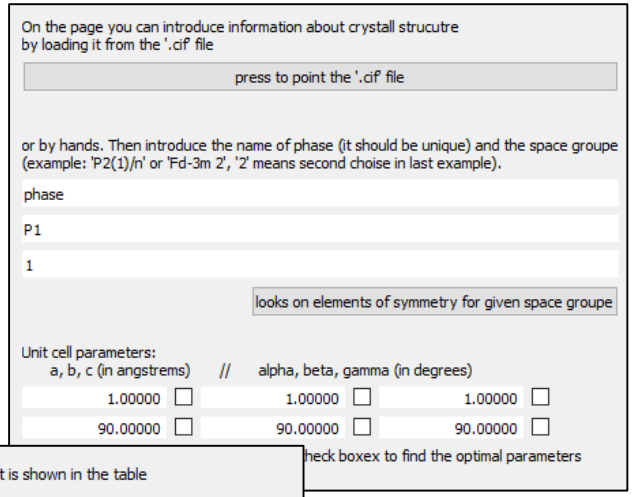
- the widgets arrangement

'Widgets' interacting with 'cmodel'

List of widgets (each in the separate file '.py'):

- widg_adp
- widg_const
- widg_exptype
- widg_extinction
- widg_magn
- widg_magn_ising
- widg_nucl
- widg_output
- widg_param
- widg_profile
- widg_results
- widg_scale
- widg_cb_exp
- widg_cb_ph
- widg_cb_ph_exp
- widg_sconstr
- widg_spgr

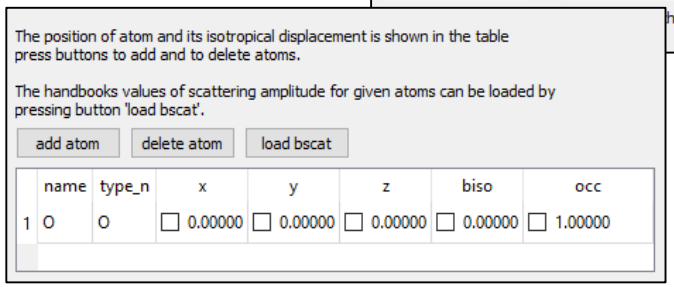
example: widg_spgr.py



Common elements:

- QCheckBox
- QLineEdit
- QTableWidget

example: widg_nucl.py



Parent class:

- widg_min

(defined methods to interact with 'cmodel')

Object ‘cmodel’ (‘cmodel.py’)

- cmodel
  - cmodel_ph
    - cmodel_at
  - cmodel_exp
    - cmodel_exp_ph
  - cmodel_ref:

‘cmodel’ has information about the model parameters

‘cmodel_ph’ has information about a phase

‘cmodel_at’ has information about an atom

‘cmodel_exp’ has information about an experiment

‘cmodel_exp_ph’ has information about a phase contributing in the experiment

(the classes are defined in the file ‘cmodel.py’)

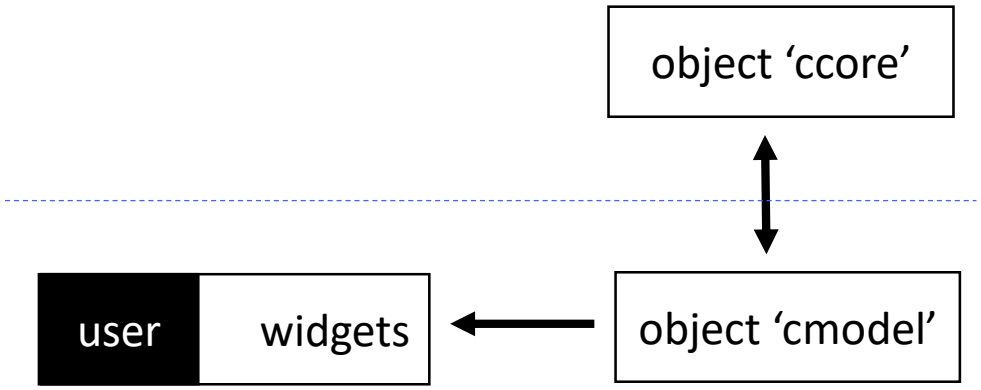
Tasks:

- interaction with ‘widgets’
- interaction with ‘ccore’

Parent class:

- cmodel_min

(defined methods to interact with ‘widgets’)



Object 'ccore' ('ccore.py')

- ccore
  - ccore_ph
    - ccore_at
  - ccore_exp
    - ccore_exp_ph
  - ccore_ref:

Tasks:
- load exerimental data
- calculations

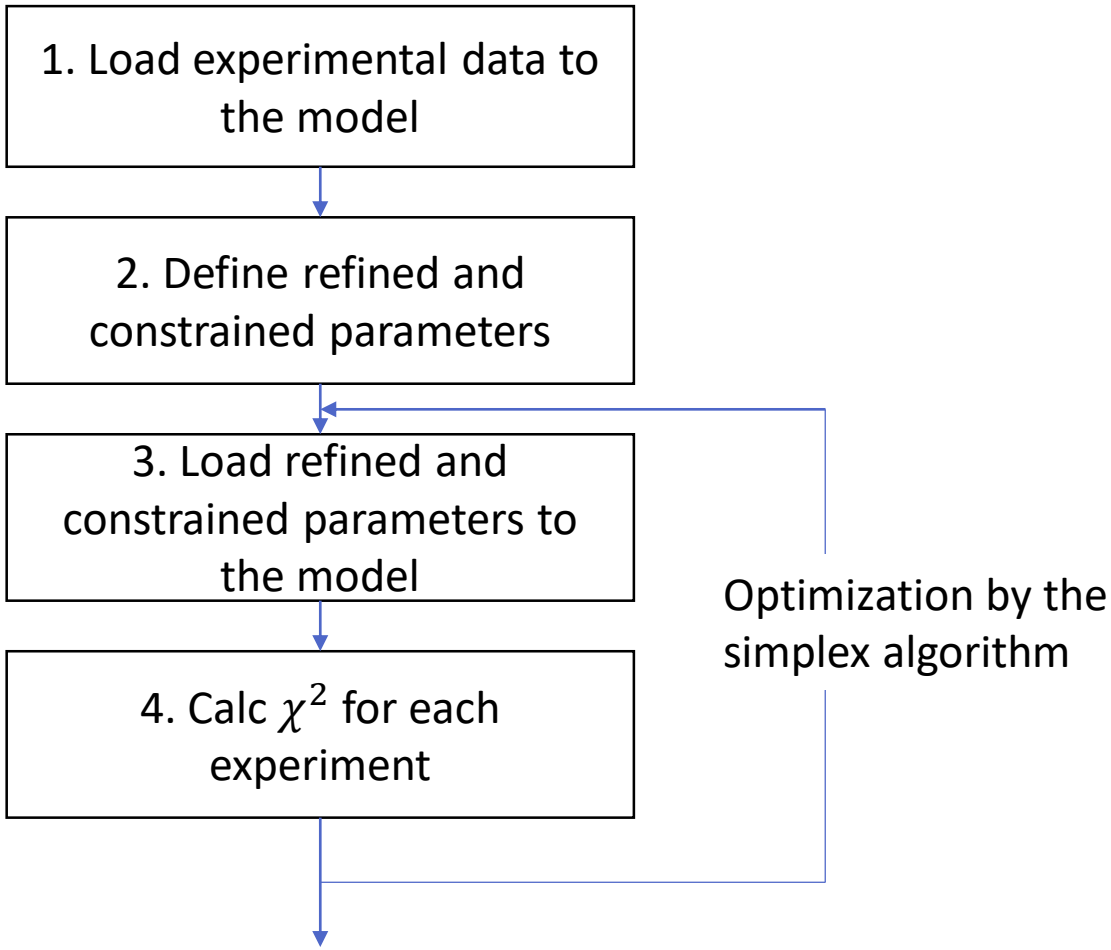
The main methods:

ccore:
- run_refinement
  refinement, by simplex method
- run_errors
  estimation of errorbars by calculation of Hessian

ccore_exp:
- load_exp_data
  make prelimiary calculations and load experimental data before refinement
- *calc_chi2*
  calculation of chi2 for one experiment

ccore_ph:
- calcFNhkl
  calculation of the nuclear structure factor
- calcSFThkl
  calculation of the structure factor tensor

Structure of refinement



ToDo:

1. Executable file
2. Organization of file location
3. Least square refinement

Thank you for your attention.