Manual of SuPerRod_v1.0 software

Canrong(Jackey) Qiu, kiel University, Kiel, Germany
crqiu2@gmail.com

"It doesn't matter how good your software is, because if the documentation is not good enough, people will not use it." — Daniele Procida

Table of Contents

1. Motivation of software development

I have been dreaming of a user-friendly and powerful software for CTR fitting since 2010 when I embarked on CTR work as a PhD student at University of Alaska Fairbanks. Unlike many other X-ray techniques, eg. X-ray absorption spectroscopy, GISAXS, for which there are already numerous nice software from which you can pick to do the modeling work, the available software to fit CTR data is very limited. I started my PhD program with Prof. Tom Trainor in Alaska in 2010. My PhD project involved resolving metal binding mechanism on hematite(1-102) surface using CTR technique. To start with my CTR modeling, I first used ROD, which is written in C language. It runs fast, and it is still used by some groups nowadays, but the limitations of ROD are apparent. Firstly, it doesn't have a GUI interface but works with a bunch of commands in terminal, which makes things obscure especially for beginners. In addition, it is cumbersome to start a model fit with ROD. Furthermore, it does not support constraints, eg. bond valence constraints, during the fit. The biggest drawback, in my opinion, is the fit algorithm that is based on non-linear least square routine, which comes up with solutions probably representing local minimum. After a while of using ROD, I learned of GenX software, which was first developed for fitting both X-ray/neutron reflectivity data. The functionality of the software had been extended to also fit CTR data afterwards. GenX is written in Python scripting language by Matts Bjorck, who is now working for Swedish Nuclear and Fuel Management Company. Once I started using GenX, I cannot stop using it. The software is user-friendly with a wxpython-based GUI. It becomes very easy to get a good hand on it. In addition, GenX is equipped with a powerful fitting engine based on differential evolution algorithm, a global optimization algorithm aiming to find solutions of global minimum. The software is well written with highly modularizable functionalities, which can be extended and/or customized easily. For example, I made some contributions to this software during my PhD years, when I parallelized the code to allow for running a model on a supercomputer cluster systems thanks to the mpi4py Python package. GenX is fit for users of different levels. For beginners, you can always follow the logics while playing with the GUI widgets; for advanced users, you can customize the functionality accordingly to live up to your full potentials to accomplish different purpose. The transition from beginner to advanced user is a matter of time, which should be relatively short for a heavy user.

I have been a heavy user of GenX until the end of my first postdoc position in HZDR in Dresden, Germany. Five CTR papers (one is under second run of review) have been published, where I used GenX for CTR modeling work. Since I started my postdoc position in Kiel, I have been getting involved in several projects, which required a wealth of scripting work. Not long ago, I started with GUI programming using PyQt5. Three GUI applications (CTR, XRV, PXRD, all shipped with DaFy) have been developed for processing synchrotron data. Having accumulated some GUI programing experience, I was amazed by the fact that how much better you feel when you are using a program with nice GUI compared to working with pure code files. GUI programming with pyqt5 is much simpler than I thought, and the signal/slot protocol employed in PyQt5 is not only simple but also efficient for signal transfer among GUI widgets compared to "callback" mechanism used in wxPython. I don't intent to make detailed comparisons between PyQt5 and wxPython in terms of the performance for GUI programing, but there is a nice article if you want to learn more (https://opensource.com/article/17/4/pyqt-versus-wxpython). As said in the article, both have pros and cons, but I myself prefer the advantages PyQt5 has to those coming with wxPython. I can endure the disadvantages of PyQt5 without pain.

I realized the speed issue of wxPython-based GUI program when I was using GenX. That's also the reason why I developed the mpi code to speed up the model running with GenX. Except for the speed, I do like all the concepts of GenX software design and also the powerful fitting engine. Realizing these, a glimpse of crazy idea came to my mind one day, "How about equipping GenX's powerful heart with a PyQt5-GUI shell to improve the script performance?". Since the fit engine is already hard coded in GenX, I only need to pull the program apart into pieces of modules, and re-assemble them into the new GUI shell. After around 3 month coding work, I made a brand new SuPerRod application with a PyQt5-based GUI, where all nice concepts found in GenX are maintained. More than just making a new skin, I optimized some central modules from bottom in SuPerRod, and some new features are implemented during the software development. Upon comparing the performance between SuPerRod and GenX, I have a strong feeling that SuPerRod runs much faster than GenX(more than 10 times faster). In a word, SuPerRod consists of GenX's central fitting codes and a new GUI based on PyQt5.

2. Glimpse of SuPerRod software

The purpose of SuPerRod may be misunderstood by its name, which sounds like a tool to fit rod data. In reality, SuPerRod provides a platform to solve all general scientific problems, where model fitting is required to get the answers. SuPerRod is like a powerful car, which runs on different roads. As mentioned above, SuPerRod is shipped with the powerful fitting engine taken from GenX. The differential evolution (DE) fitting algorithm will be discussed later. DE algorithm can be used to achieve solutions of global minimum, and it also features an intrinsic metadata structure that can be easily employed in a parallelized computation to improve the fit performance. While SuPerRod can be used as a general fitting tool, it does provide a fully functionable API that is dedicated to resolve CTR modeling, e.g structure factor calculation, dealing with water layering structure, consideration of surface roughness, just name a few. If you are fitting CTR data, numerous functions/modules are already available to help you set up your model in no time. If you would like to fit other data, and you have implemented the calculation of the variable you need to fit, then it is trivial to set up your model in SuPerRod (refer to later section for details). If you start your project from scratch, you won't miss all the fun parts to crank your codes, since Python is the easiest, if not the best, programing language in the world. At last, enjoy your SuPerRod trip. Be bold, and you will get there soon.

3. Benchmark features of SuPerRod

Not just having a new GUI-shell, SuPerRod comes with some new benchmark features that do not belong to GenX. First, SuPerRod uses a thread program to separate the manipulating GUI widgets from the fitting processes. As a result, the main GUI won't freeze during fitting process, since the GUI widgets reside in a separated thread. In addition, the burden of the fitting process (most computation expensive) is distributed to different processers in a multiple-core architecture CPU system, which is usually equipped in modern PC's. In addition, you can modify your script easily by pushing some buttons rather than making edits directly in the script editor panel. The idea is you predefine different sorbates, which are wrapped and collected inside the sorbate module. Then by tagging through the standard script with unique name-tag, which you use to locate the corresponding code block, you can locate and replace the code block in a way defined by the given sorbate tag. Speaking of model script, the figure of merit function is structured to return a tuple, that contains a simulated result and a penalty factor. You are free to define the penalty factor as a constraint for the fitting process. Constraining your fit is a very robust way to avoid overfitting. Having said that, let me say something about fit parameters. Clinging to the concept of user-friendly concept, I implemented in SuPerRod auto-filling fit parameters in the parameter panel. Now setting up a model in SuPerRos is really a few easy steps away: loading data, modifying script, and defining parameters, which are (semi)-automatic process. Last but not least, a Python terminal widget is imbedded to allow for exploration of modules, variables and many others on your model. It is a nice/easy way for either debugging or testing new feature on SuPerRod. All these features will be detailed in later sections.

4. Targeted users of SuPerRod

SuPerRod targets users, who are working on a complicated fitting problem, which means large number of fit parameters (let's say >8). In reality, the heavier your duty is, the better performance we can achieved with SuPerRod. It is not recommended to use SuPerRod to fit simple problem (although it can), e.g Gaussian peak fitting, since you can accomplish the fit with a much lighter code, e.g scipy.curve_fit, lmfit, etc. The user should have some basic knowledge of Python scripting language. Some site-packages, like numpy, pandas, scipy, are heavily used in SuPerRod, so it is recommended to master these packages.

5. Installation/setup guide

Install Python 3 (at least>3.5, 3.7 is the best) first.

Install following Site-packages:

- PyQt5: GUI package
- pyqtgraph: GUI package for graphing
- qdarkstyle: GUI decoration tool
- numpy
- matplotlib
- scipy
- pandas

I didn't check the compatibility of these packages of different versions, but it should be safer to install the newest version to avoid compatibility issue. One combination that is working on win32 system may fail on Linux system. You need to try this out by yourself. Location of DaFy/SuPerRod package: https://github.com/jackey-qiu/DaFy. You can run 'git clone https://github.com/jackey-qiu/DaFy' in your terminal or download the package directly. You don't need further installation of DaFy. After you unzip the DaFy package, in a terminal you change directory to superrod folder (DaFy/projects/superrod), and run "python SuPerRod_GUI.py". Then you should be able to see the main GUI pop out like below. Read more below to learn further steps after this.

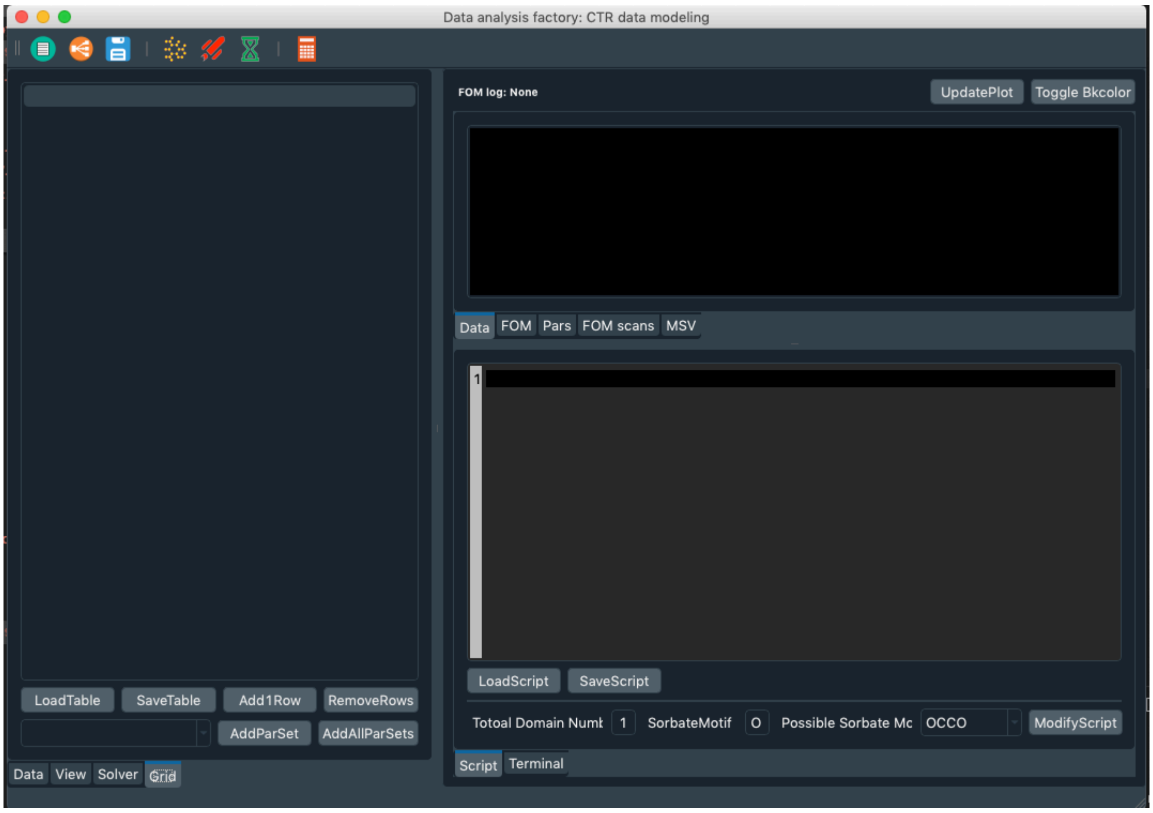
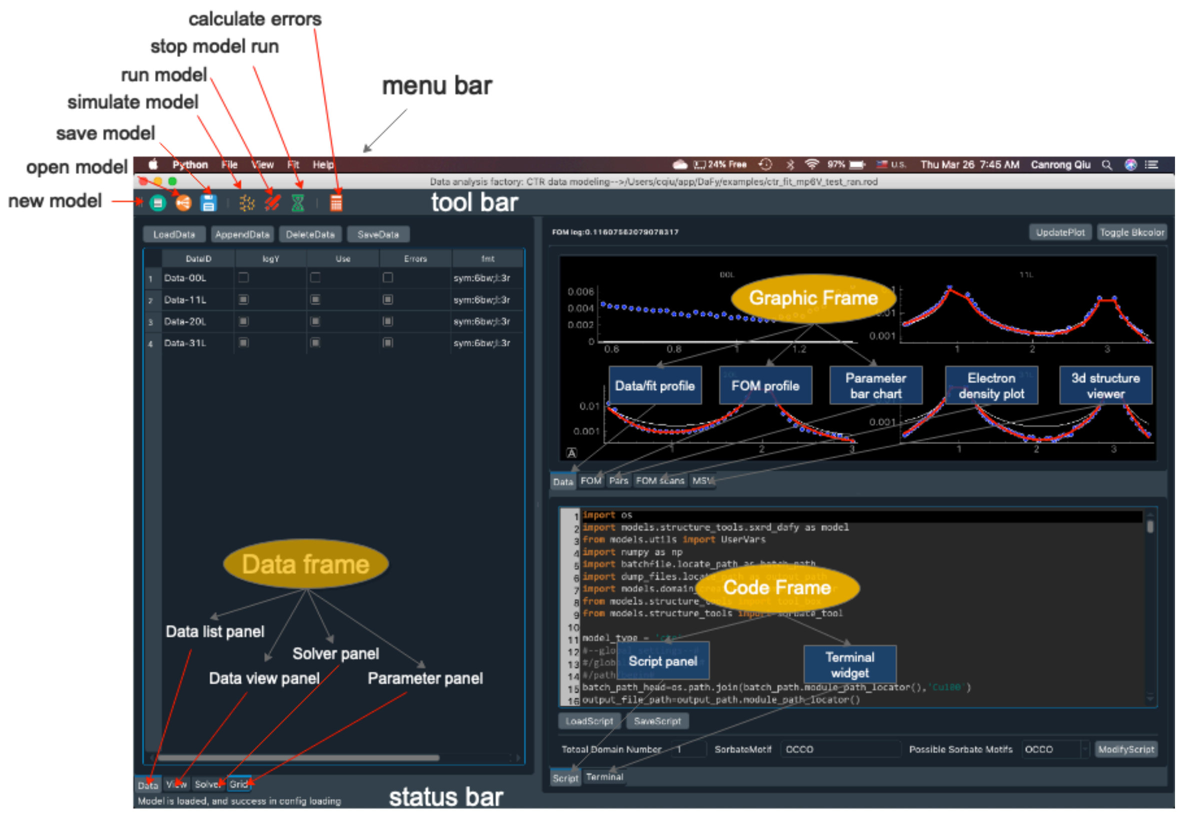


Figure 1. Main GUI frame popping out upon launching SuPerRod program.

6. Operation guide

In this section, the functions of different components will be illustrated, including widgets, modules (data, script and parameter instance). Understanding these components will help you understand the underlying logic of working with SuPerRod.

(1) Introduction of widgets



	DataID	logY	Use	Errors	fmt
1	Data-00L	☐	☐	☐	sym:6bw;l:3r
2	Data-11L	▣	▣	▣	sym:6bw;l:3r
3	Data-20L	▣	▣	▣	sym:6bw;l:3r
4	Data-31L	▣	▣	▣	sym:6bw;l:3r

```
import os
import models.structure_tools.sxrd_dafy as model
from models.utils import UserVars
import numpy as np
import batchfile.locate_path as batch_path
import dump_files.locate_path as output_path
import models.domain_creator
from models.structure_tools import tool_box
from models.structure_tools import sorbate_tool

model_type = 'ctr'
#--global settings--#
#/global
#/path
batch_path_head=os.path.join(batch_path.module_path_locator(),'Cu100')
output_file_path=output_path.module_path_locator()
```

Totoal Domain Number: 1 SorbateMotif: OCCO Possible Sorbate Motifs: OCCO ModifyScript

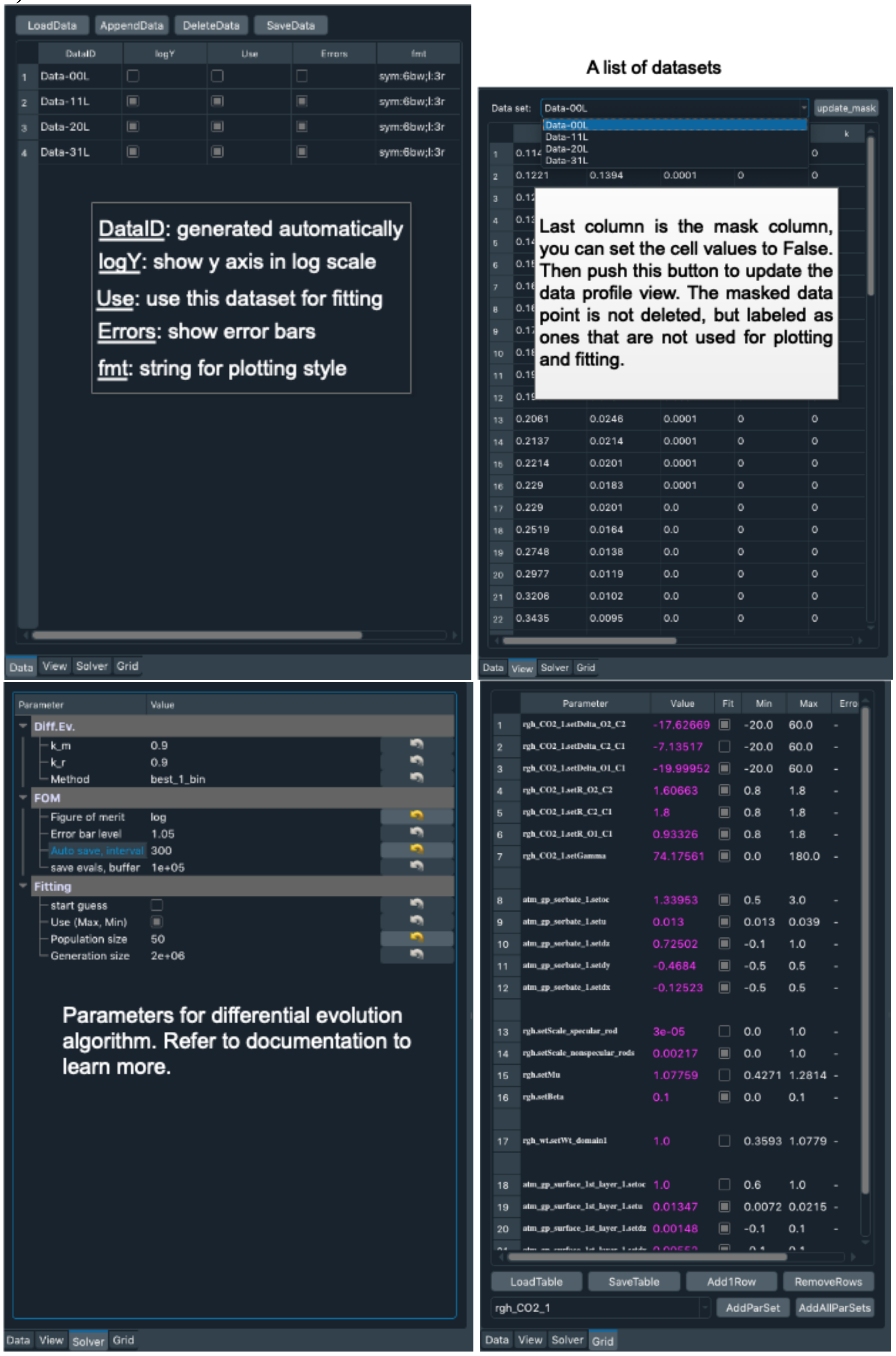
Figure 1. Layout of main GUI frame, three main widget frames, including Dataframe, Graphicframe and Codeframe, are labelled along with the associated constituent tab-widgets.

The main GUI frame consist of three tab-widget frame, including Dataframe, Graphicfram and Codeframe, as illustrated above. You can hide or show these frame by clicking the associated menu item in View tab. On the tool bar, you can find tool icons for, from left to right,

- **initializing a new model**: this will empty all the metadata holding by the current model, and a dialog will be prompted to ask for saving current model or not.
- **opening a saved model:** this will load all metadata saved in a model file (*.rod). A model fit is a zip file, which archive data, script and parameter instance using pickle dump.
- **simulating a model:** script will be compiled, and the fit variable will be calculated. The fit results will be plotted in the Graphicframe. The model structure will also be updated.
- **running a model**: you launch a model run. Figures in Graphicframe will be updated lively (every 3 secs), so do the parameter values in the Parameter panel.
- **stopping a model run**: you stop a running model. The looping will be killed, and the associated timer will be stopped. The control is given back to user.
- **calculating the errors**: after you finish the model run, you press this button to calculate the errors for each fit parameter. Note the error bar values are only estimated from all intermediate fit results from all fit generations, and the error may not accurately represent the statistic errors. If you want to get statistical errors of each fit parameter, you can run a further NLLS fit using the best fit parameters, which is not implemented in SuPerRod.

To follow up, functions of widgets on each frame will be illustrated in detail.

1) Data Frame



LoadData AppendData DeleteData SaveData

	DataID	logY	Use	Errors	fmt
1	Data-00L	☐	☐	☐	sym:6bw;l:3r
2	Data-11L	▣	▣	▣	sym:6bw;l:3r
3	Data-20L	▣	▣	▣	sym:6bw;l:3r
4	Data-31L	▣	▣	▣	sym:6bw;l:3r

DataID: generated automatically
logY: show y axis in log scale
Use: use this dataset for fitting
Errors: show error bars
fmt: string for plotting style

Data View Solver Grid

A list of datasets

Data set: Data-00L update_mask

Data-00L
Data-11L
Data-20L
Data-31L

					k
1	0.114				0
2	0.1221	0.1394	0.0001	0	0
3	0.12				
4	0.13				
5	0.14				
6	0.15				
7	0.16				
8	0.16				
9	0.17				
10	0.18				
11	0.19				
12	0.19				
13	0.2061	0.0246	0.0001	0	0
14	0.2137	0.0214	0.0001	0	0
15	0.2214	0.0201	0.0001	0	0
16	0.229	0.0183	0.0001	0	0
17	0.229	0.0201	0.0	0	0
18	0.2519	0.0164	0.0	0	0
19	0.2748	0.0138	0.0	0	0
20	0.2977	0.0119	0.0	0	0
21	0.3206	0.0102	0.0	0	0
22	0.3435	0.0095	0.0	0	0

Last column is the mask column, you can set the cell values to False. Then push this button to update the data profile view. The masked data point is not deleted, but labeled as ones that are not used for plotting and fitting.

Data View Solver Grid

Parameter	Value
Diff.Ev.	
k_m	0.9
k_r	0.9
Method	best_1_bin
FOM	
Figure of merit	log
Error bar level	1.05
Auto save, interval	300
save evals, buffer	1e+05
Fitting	
start guess	☐
Use (Max, Min)	▣
Population size	50
Generation size	2e+06

Parameters for differential evolution algorithm. Refer to documentation to learn more.

Data View Solver Grid

	Parameter	Value	Fit	Min	Max	Erro
1	rgh_CO2_1.setDelta_O2_C2	-17.62669	▣	-20.0	60.0	-
2	rgh_CO2_1.setDelta_C2_C1	-7.13517	☐	-20.0	60.0	-
3	rgh_CO2_1.setDelta_O1_C1	-19.99952	▣	-20.0	60.0	-
4	rgh_CO2_1.setR_O2_C2	1.60663	▣	0.8	1.8	-
5	rgh_CO2_1.setR_C2_C1	1.8	▣	0.8	1.8	-
6	rgh_CO2_1.setR_O1_C1	0.93326	▣	0.8	1.8	-
7	rgh_CO2_1.setGamma	74.17561	▣	0.0	180.0	-
8	atm_gp_sorbate_1.setoc	1.33953	▣	0.5	3.0	-
9	atm_gp_sorbate_1.setu	0.013	▣	0.013	0.039	-
10	atm_gp_sorbate_1.setdz	0.72502	▣	-0.1	1.0	-
11	atm_gp_sorbate_1.setdy	-0.4684	▣	-0.5	0.5	-
12	atm_gp_sorbate_1.setdx	-0.12523	▣	-0.5	0.5	-
13	rgh.setScale_specular_rod	3e-05	☐	0.0	1.0	-
14	rgh.setScale_nonspecular_rods	0.00217	▣	0.0	1.0	-
15	rgh.setMu	1.07759	☐	0.4271	1.2814	-
16	rgh.setBeta	0.1	▣	0.0	0.1	-
17	rgh_wt.setWt_domain1	1.0	☐	0.3593	1.0779	-
18	atm_gp_surface_1st_layer_1.setoc	1.0	☐	0.6	1.0	-
19	atm_gp_surface_1st_layer_1.setu	0.01347	▣	0.0072	0.0215	-
20	atm_gp_surface_1st_layer_1.setdz	0.00148	▣	-0.1	0.1	-

LoadTable SaveTable Add1Row RemoveRows

rgh_CO2_1 AddParSet AddAllParSets

Data View Solver Grid

Figure 2. Layout of each constituent tabWidget in the DataFrame, including Data widget(top left), Viewer widget (top right), Solver widget (bottom left) and Grid widget (bottom right).

Dataframe contains one tabWidget, which consist of a Data widget, a Viewer widget, a Solver widget and a Grid widget.

- **Data widget:** a table widget of 5 columns, most are self-explainable. DataID assigns the id of each dataset taking the naming rule of form "Data-HKL". fmt column by default are occupied by string of "sym:6bw;l:3r", which can be changed to the plotting style you want. The first part of the string before ";" specifies the symbol size (6 here) and symbol filled color ("w") and symbol edge color ("b"). The second part of the string specify the line color ('r') and line width (3) for simulated profiles. Change these string tags accordingly. Acceptable color tags are: "r", "b", "k", "w", "y", "m", "g".
- **View widget:** a table widget to show the selected dataset, including 8 columns. X column is L column for CTR data, but it can represent other physical variables for other data type. Y column is the intensity column for CTR data. Error column displays the error values. dL and BL column are used for calculating Robinson's roughness factor. BL is the first Bragg peak L values in a rod, while dL is the L spacing between two adjacent Bragg peaks in a rod. The last column is mask column, which takes bool values (True, or False). A mask value of True means the associated data point will be displayed and used for fitting, while a data point with a False mask value will be masked out for plotting and fitting. But note that masking a data point will not delete the data point.
- **Solver widget:** this is a parameter tree widget to specify the intrinsic parameters for performing differential evolution fitting. Refer to last part of this section to learn of the meaning of k_r, k_m, and methods. (1) Figure of merit function is the cost function you use for model optimization. To fit ctr data, we most often use chi2bar cost function. It is also common to use diff and log cost functions for problems of general purpose. Refer the DaFy/util/fom_funcs.py to learn more details about the definition of different cost functions. (2) Error bar level (>1) is used to estimate the error bars for fit parameters. (3) "Auto save, interval" define the frequency of save model during model run. (4) "Save evals, buffer" defines the maximum generations allowed. It is a huge number by default. (5) Under Fitting branch, you will see a check box of "start guess", which toggle the two different ways to initialize the values of fit parameter in the first fit generation, either based on random generation (unchecked) or taking current values in the parameter panel. For a new model, we should always uncheck this button, while for a half-done model it may be wise to check it. In addition, (6)"Use(Max,Min)" checkbox should be always checked to tell the fit algorithm search for values within the boundary you define in the parameter panel. It is always better to set boundary for each fit parameter. (7) Population size and generation size define the size of model refinement (refer to last part of this section). Model runs with larger population size converge more slowly but could essentially avoid finding local minimum. Rule of thumb is the population size should be at least 8 times higher than the total number of independent fit parameters. You can set an arbitrary large generation size, and stop the model run whenever you see FOM profile has converged to a flat line.
- **Grid widget:** this is a table widget of 6 columns, where you define all fit parameters in terms of set function names, boundaries, fit or freeze check. In the parameter column, we provide the set function names for all fit parameters. For example, a function name of rgh.SetA1 will mean a parameter instance rgh containing an attribute A1 to be set by function rgh.SetA1. Therefore, remember the first column is not the name of a fit parameter but the name of a set function for setting the value of the associated parameter. In value column, the current best fit parameter values will be displayed in this column. When setting your model, ensure that the value of a parameter should be within the boundary you set for the parameter. The last column is

the error column, which will be filled after the model run is finished. Don't forget the push the button (a calculator-like push button found on the tool bar) to calculate the error values.

2) Graphic Frame

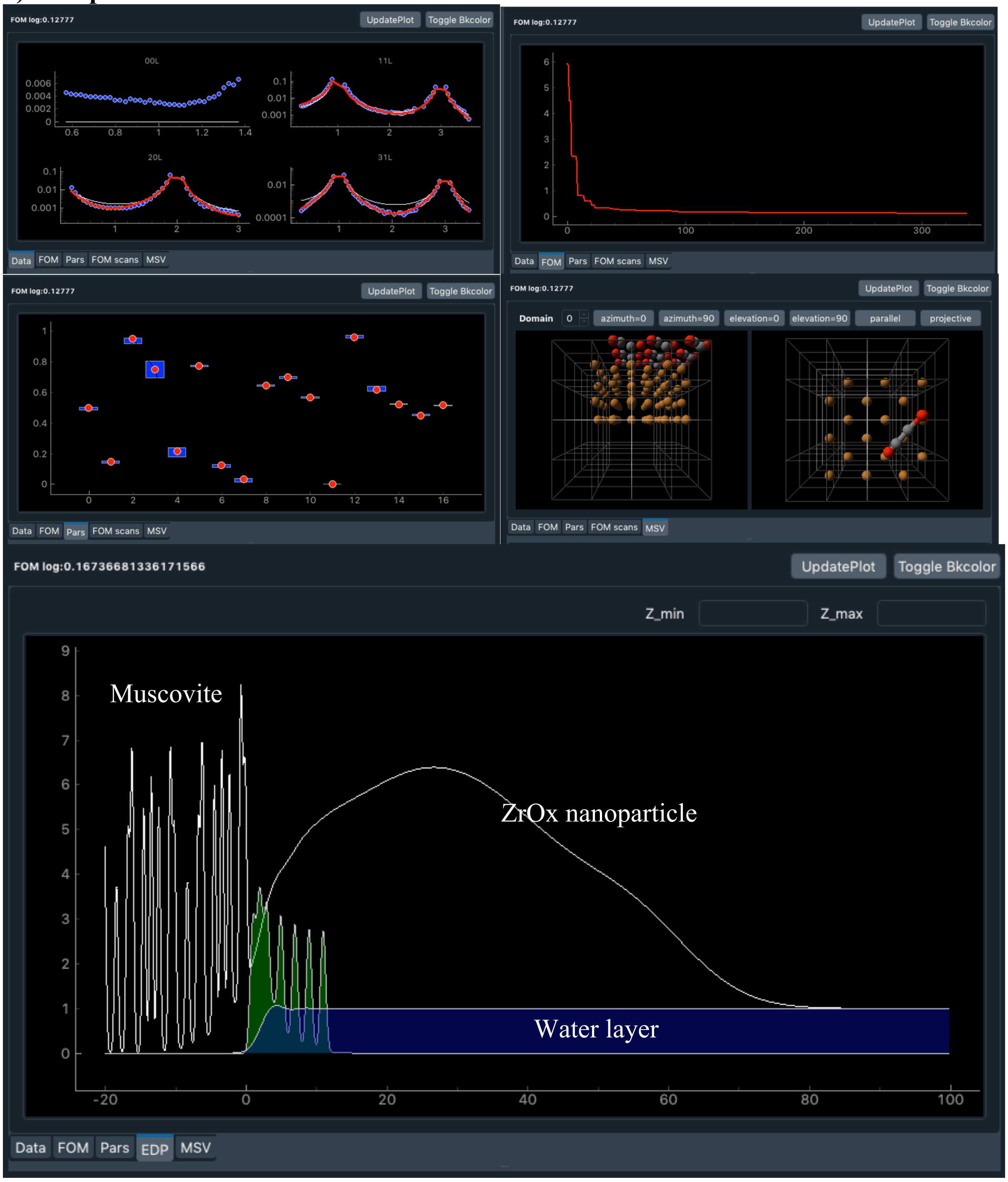


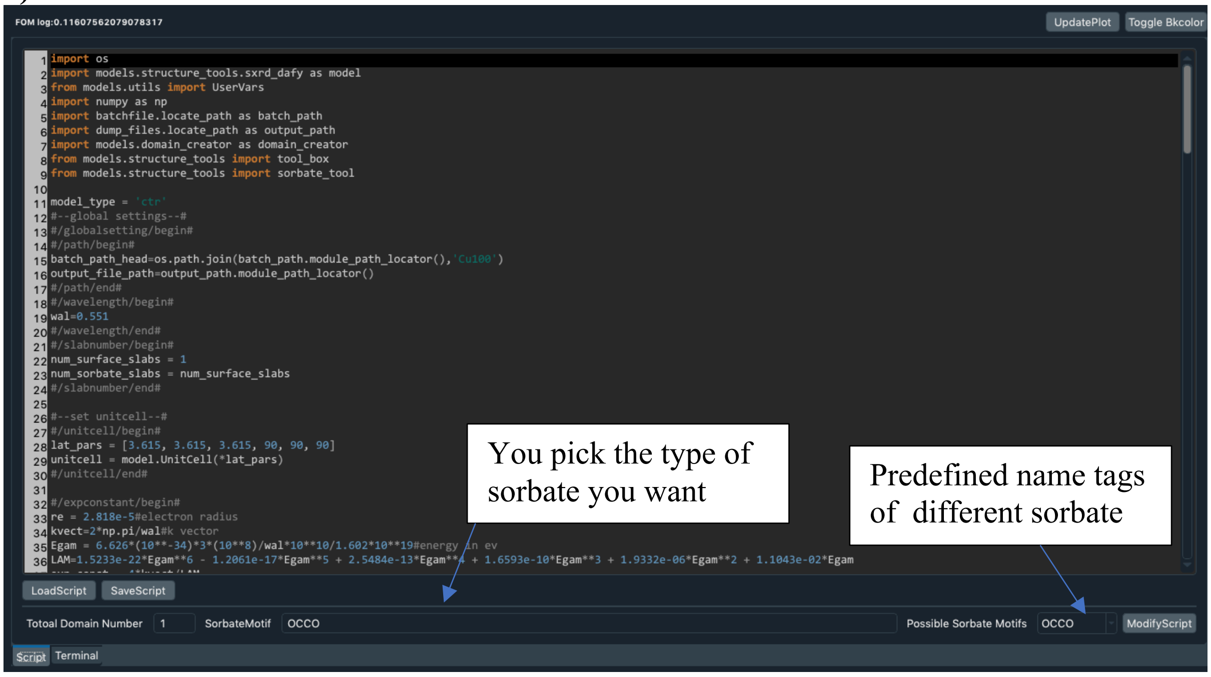
Figure 3. Layout of each constituent tabWidget in the GraphicFrame, including Data widget(top left), FOM widget (top right), Pars widget (middle left), MSV widget (middle right) and EDP widget (bottom).

The Graphic Frame contains a tab Widget, which consist of Data widget, FOM widget, Pars widget, FOM scan widget (not implemented yet) and MSV widget.

- **Data widget:** display the data profiles with filled circle symbols, simulated profiles in solid red lines (color can be changed), and calculated profiles for unrelaxed structure (for CTR data only). The figure layout will be expanded accordingly when more datasets are loaded.

- **FOM widget:** display the evolution of FOM (figure of merit) values during model running. It is a nice way to tell whether or not the model optimization is converged. You will see a more or less straight line spanning most part of the profile if the model fitting has converged.
- **Pars widget:** display the current best fit values of fit parameters in red filled circles. The values are normalized to range from 0 to 1 using the boundary of each parameter. Besides that, the bar chars illustrate the searching range at the current generation. An aggressive searching corresponds to a long searching bar. When a model is converged, you will most likely see all searching bars converged to a narrow line. This means you cannot improve your fit anymore, and you can stop the model run now.
- **MSV widget:** visualize the molecular structure on the side view (left) and top view (right). You can change the view angle by pushing those buttons on the widget panel. If you have defined several domains, you can also switch to a different domain by tweaking the spin box. The molecular structure in side view does not show chemical bonds, which give you an overview of how sorbate atoms are registering at substrate surface. The structure on top view only display the atoms on the top substrate layer and one sorbate molecule, and the chemical bonds are displayed in the sorbate molecule. From sideview structure, you can quickly tell the geometrical relationship between the sorbate and the substrate surface.
- **EDP widget:** draw the electron density profile of the system you are fitting. The substrate surface is at z=0. Electron density above z=0 is attributed to sorbate adsorption including layered water structure (blue filled curves), specific elements (green curves). The total electron density is displayed as white solid line. Note the total electron density profile is normalized to bulk water. You need to implement your script for drawing electron density profile. What you see above is showing the EDP pattern for Zr nanoparticle adsorption on muscovite(001) surface.

3) Code Frame


FOM log:0.11607562079078317
UpdatePlot
Toggle Bkcolor
LoadScript
SaveScript
You pick the type of sorbate you want
Predefined name tags of different sorbate
ModifyScript
Script
Terminal

```
import os
import models.structure_tools.sxrd_dafy as model
from models.utils import UserVars
import numpy as np
import batchfile.locate_path as batch_path
import dump_files.locate_path as output_path
import models.domain_creator as domain_creator
from models.structure_tools import tool_box
from models.structure_tools import sorbate_tool

model_type = 'ctr'
#--global settings--#
#/globalsetting/begin#
#/path/begin#
batch_path_head=os.path.join(batch_path.module_path_locator(),'Cu100')
output_file_path=output_path.module_path_locator()
#/path/end#
#/wavelength/begin#
wal=0.551
#/wavelength/end#
#/slabnumber/begin#
num_surface_slabs = 1
num_sorbate_slabs = num_surface_slabs
#/slabnumber/end#

#--set unitcell--#
#/unitcell/begin#
lat_pars = [3.615, 3.615, 3.615, 90, 90, 90]
unitcell = model.UnitCell(*lat_pars)
#/unitcell/end#

#/expconstant/begin#
re = 2.818e-5#electron radius
kvect=2*np.pi/wal#k vector
Egam = 6.626*(10**-34)*3*(10**8)/wal*10**10/1.602*10**19#energy in ev
LAM=1.5233e-22*Egam**6 - 1.2061e-17*Egam**5 + 2.5484e-13*Egam**4 + 1.6593e-10*Egam**3 + 1.9332e-06*Egam**2 + 1.1043e-02*Egam
```

Totoal Domain Number: 1
SorbateMotif: OCCO
Possible Sorbate Motifs: OCCO

Figure 4. Layout of each constituent tabWidget in code frame.

Code Frame is the place where you display, modify your script. The main widget here is a plaintext editor, which has been styled to highlight Python key words. To use the modifyscript button, you need to define sorbate types, which are stored in a script module to be loaded in main GUI name space. In addition, you should also define name tags in the standard script file, so that the script block for defining sorbate can be located. It is a handy feature, but you don't have to use it if you don't know how to get around with the coding trick. It should be noted that you cannot mix-use tab-space and normal space in the editor, otherwise error will be prompted. Therefore, you should always use normal space for indentation.
The script will be compiled upon model simulation through "exec script_string". After compiling, the variables and functions will be stored in the name space of model.script_module, which is defined in the main GUI frame class. I will elaborate below the guides to setup the script for model fitting.

(2) Data format

Data loader loads data file of contents in a special format. Data file is a normal ascii file, which must contain 8 columns of space separated numeric values. When the data file is loaded, the data loader will split the data values into multiple date sets according to the values of second and third columns. The rows with same values in both 2nd and 3rd columns will be grouped into one dataset. For example, rows with the 2nd column values of 0 and 3rd column values of 0 will be assigned to a separated data instance, which will be named as Dataset_00L. For each dataset, a special name will be assigned to each column in the associated data instance. From column 1 to column 8, the corresponding names are 'x', 'h', 'k', 'Y', 'y', 'error', 'BL' and 'dL'. While 'x', 'y', 'error' are direct attributes of the data instance, the others are stored in the extra_data attribute, which is a normal Python dictionary. For example, if we define a data instance with a name of *data*, one-to-one corresponding match between the original column in the data file and the name space defined in *data* instance is as follows:

1st column←→*data*.x,
2nd column ←→*data*.extra_data['h'],
3rd column←→*data*.extra_data['k'],
4th column←→*data*.extra_data['Y'],
5th column←→*data*.y,
6th column←→*data*.error,
7th column←→*data*.BL,
8th column←→*data*.dL.

When dealing with **CTR/RAXR data**, you stick to the data format as follows:

1) For CTR data, x column is L column, Y column is filled with 0
2) For RAXR data, x column is energy column, Y column is L column
3) h, k columns are holding H, K values
4) y column is holding background-subtracted intensity of CTR signal
5) BL and dL are two values for roughness calculation, of which BL represents smallest Bragg peak L along one rod, dL represents L interval spacing between two adjacent Bragg peak.

If the data you want to load is **not in CTR format**, to make successful loading, assure:

1) your data file has 8 columns
2) columns are space-separated (or tab-separated)
3) you can add comment lines heading with "#"
4) if your data has <8 columns, then fill the unused columns with 0

5) to assess your data column, you should use the naming rule described above, although
the real meaning of each column, eg x column, could be arbitrary depending on your data.
For example, if you put frequency values to the first column(x column), then to access this
column, you use *data*.x to achieve the frequency values.

Data file of 8 columns should be enough to cover many different data format situations. You can freely format your datafile, as long as you remember which column corresponds to what and how to extract them from a data instance. If you fill, for example, frequency data in first column, then to extract them using *data*.x. If you do it differently by filling the frequency data in 8th column, the to extract them using *data*.extra_data['dL'], which has no literal connection with the name "dL" to the meaning of your values (frequency). If you know the naming rule for a data instance, you should know how to extract the data column you would like to use in your model script.

(3) Script module

Script module (named *script_module*) is a module attribute of the *model* instance, which is defined in the main GUI object. *script_module* holds a name space, which include all object variables defined in your script. Besides that, it also holds the data list (named *data*), which is a list dataset instances. For example, you can achieve the first dataset instance using *model.script_module.data[0]*. Then obviously, *model.script_module.data[0].x* will return the first column of this dataset. As a user, you don't need to manipulate script module for your modeling, but it can help you understand the logic flow map shown below.

(4) Fit parameters

Defining fit parameters is an indispensable part of setting up a model. It is extremely flexible and convenient to define a fit parameter in SuPerRod. All you need to do is implementing the associated set function for one parameter attribute residing in different object. In other words, the parameter attributes can live in different objects. Let's take one class instance objects (*obj1*) as an example here. I define and initialize an attribute named *attr1* in this object through:

```
self.attr1 = 1
```

At the same time, I also define the associated set function for this attribute.

```
def setattr1(self, val):
    self.attr1 = val
```

With these steps, you have already defined a fit parameter and its set function. In the parameter table (Figure 2, bottom right), you can filled one row of the first column with the set function name, i.e *obj1.setattr1*, then the program knows you want to fit the attribute attr1 living in the name scope of *obj1*. Besides this way, there is a built-in class object (*UserVars*) you can import to quickly setup a fit parameter. In your script, you can simply import it through *from models.utils import UserVars*. Then the same work shown above can be done in a much more concise and easier way:

```
obj1 = UserVars()
obj1.new_var("attr1",1)
```

In summary, you can create your fit parameters through defining the attribute of any class object along with its set function or using built-in class object (*UserVars*). Both ways could be helpful in different situations.

(5) Logic flow map

With the knowledge of script module, data format and fit parameter, let's put them together in one snapshot to understand the underlying logic flowing path while the program is running. As shown in Figure 5, SuPerRod is highly modularized with different objects living inside different name space. Data exchange between different object makes all the logic flowing pattern shown in Figure 5. The main GUI object is the place you enter when you launch this program. The main GUI object holds the GUI widgets, which live in one of the three qt frames: Dataframe, Codeframe and Graphicframe. In addition, the main GUI object define a *model* attribute, which stores information of data, parameter, script and model fit configurations. We have discussed all these components above, so refer to the associated section if anything is unclear to you. To accomplish the fitting, run_fit is defined as well in the main GUI object. In run_fit, there is a solver attribute that connect to the defined model attribute. The fit looping is triggered by a switch (run button widget on the tool bar). Once the fit looping starts, a new thread is open for the optimization, where the calculation task will be chopped into sub-tasks being completed in parallel by different processors if available. The optimization evolves through many generations. After each generation, a pyqt signal will be emitted to be caught by main frame widgets. To respond to the signal, the fit parameter values will be updated. To avoid potentially long overhead time caused by 3D structure visualization, a timer is created to connect the signal, when it is emitted the first time. The connection is open only once, and then will be close. Once the timer starts, it will trigger the updating of molecular structure rendering every 3 seconds. The optimization looping will continue moving forward until receiving a stop run signal, which can be triggered by pressing the stop model button on the tool bar.

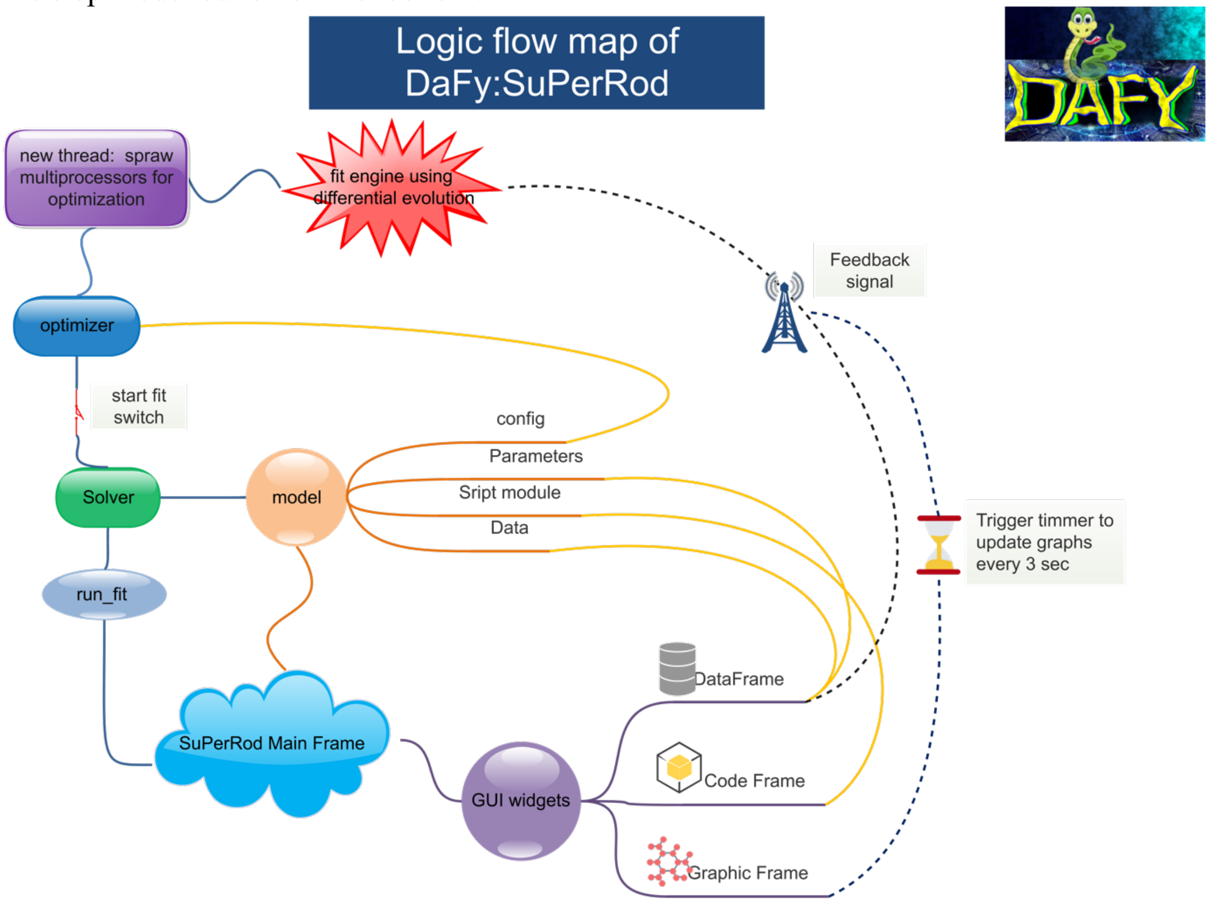

Logic flow map of DaFy:SuPerRod
DAFY
new thread: spraw multiprocessors for optimization
fit engine using differential evolution
Feedback signal
optimizer
start fit switch
config
Parameters
Sript module
Data
Solver
model
run_fit
Trigger timmer to update graphs every 3 sec
DataFrame
SuPerRod Main Frame
Code Frame
GUI widgets
Graphic Frame

Figure 5. Logic flow map of SuPerRod. Solid lines indicate sharing name spacing between objects, dashed lines are signal transmitting path.

7. Setup a model from scratch

To set up a model, you need a data file of specific format (refer to Data format section before), model script, and fit parameters. You should define the fit parameters inside the model script. Play with those two examples below to get yourself being more familiar with model setup. To run your model script well, you need two minimum components in your script. First is the definitions of fit parameters, and second is a function named *Sim* at the end of the script. This *Sim* function is mandatory. It takes the first argument of *data*, which is a list of dataset instance. The body of *Sim* function is the place where you implement the calculation of the *y* variable (eg. structure factor for CTR model) you want to fit. This function should return a three-member tuple. The 1st tuple member is a list of y variable values calculated from the model, 2nd tuple member is a penalty factor, which should be set to 1 if you don't have any penalty function of place a constraint. The last tuple member is a list of weighting factors scaled to the calculated FOM value for each dataset. You can assign different weighting factos for different datasets during fit. This way, the fit subroutine will bias towards making better fit to the dataset with larger weighting factor. You can simply set the scaling factor to 1 for each dataset to disable the weighting strategy.

8. Three examples

Three examples rod files are already created for you to play with. You can locate these files and load it using open model button.

(1) Multi-Gaussian peak fitting problem

The model file is located in DaFy/examples/ four_gaus_peaks.rod The data is a simulated multi-Gaussian peak model. Four overlapping Gaussian peaks are summed up to produce the datafile. From this example, you will learn how to set up a model with a non-CTR dataset.

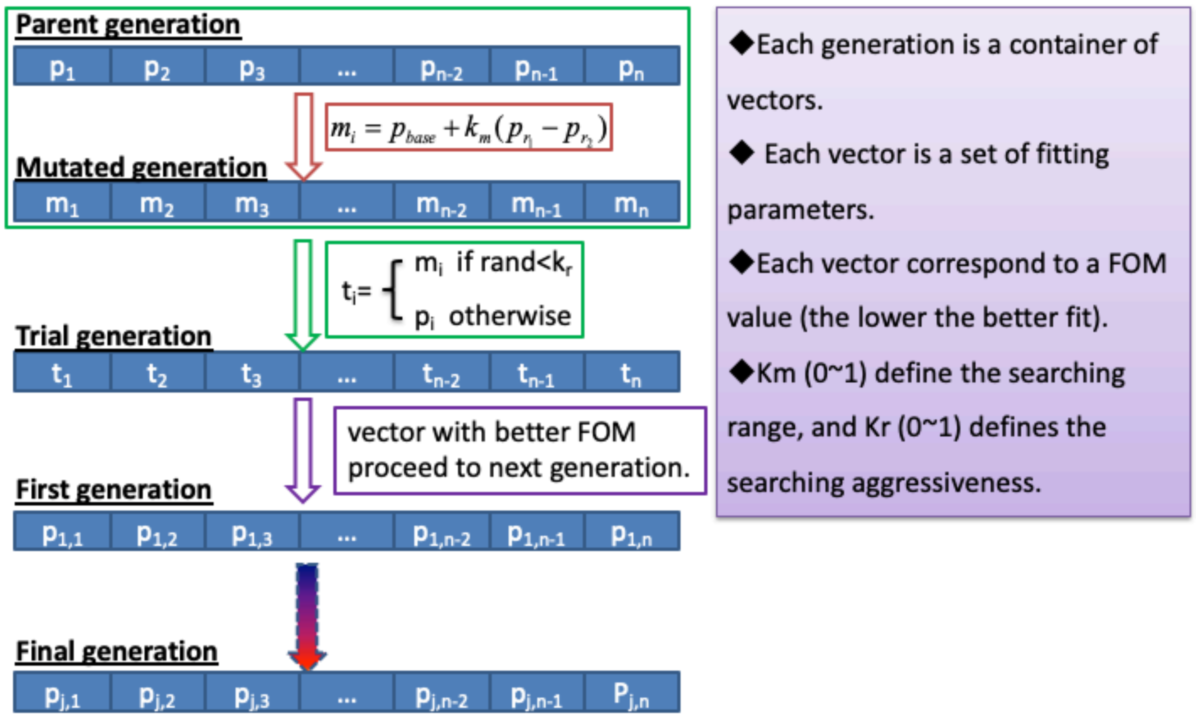
(2) CO2RR on Cu(100) surface

The model file is located in DaFy/examples/ ctr_fit_mp6V_test.rod. This model deals with the adsorption of CO2 reduction product on Cu(100) surface under operando condition at reductive potential -0.6 V (w.r.t Ag/AgCl reference electrode). The data quality is not good enough to resolve the binding structure, but this example provide some insights into setting up CTR model.

(3) Zr nanoparticle on muscovite surface

The model file is located in DaFy/examples/ ctr_example_muscovite.rod. This model deals with X-ray reflectivity data to solve the adsorption of ZrOx nanoparticle on muscovite(001) surface. In this example, you will learn how to implement electron density profile visualization in your model.
Read more at https://pubs.acs.org/doi/10.1021/acs.langmuir.8b02277

9. Introduction of differential evolution



Parent generation
p_1 p_2 p_3 … p_{n-2} p_{n-1} p_n
$m_i = p_{base} + k_m(p_{r_1} - p_{r_2})$
Mutated generation
m_1 m_2 m_3 … m_{n-2} m_{n-1} m_n
$t_i = \begin{cases} m_i & \text{if } rand<k_r \\ p_i & \text{otherwise} \end{cases}$
Trial generation
t_1 t_2 t_3 … t_{n-2} t_{n-1} t_n
vector with better FOM proceed to next generation.
First generation
$p_{1,1}$ $p_{1,2}$ $p_{1,3}$ … $p_{1,n-2}$ $p_{1,n-1}$ $p_{1,n}$
Final generation
$p_{j,1}$ $p_{j,2}$ $p_{j,3}$ … $p_{j,n-2}$ $p_{j,n-1}$ $P_{j,n}$

◆Each generation is a container of vectors.

◆ Each vector is a set of fitting parameters.

◆Each vector correspond to a FOM value (the lower the better fit).

◆Km (0~1) define the searching range, and Kr (0~1) defines the searching aggressiveness.

Figure 6. Differential evolution mechanism

The optimization algorithm used in SuPerRod is differential evolution, which is a method that optimizes a problem by iteratively trying to improve a candidate solution with regard to a given measure of quality. In this process, new generation with better fitting quality will be generated from the parent generation. Some basic concepts are listed here.

- Each generation is a container of vector, and each vector is a set of fit parameter values. Each vector corresponds to a FOM value, which determines the fitting quality. The population size is arbitrarily set.
- To start with, the parent generation is created on a random basis.
- Then each vector in the parent generation will be mutated by applying a mutation rule. The p_{base} here is the vector with best fit quality, K_m is a fit factor, ranging from 0 to 1, which determines the searching range. P_{r1} and P_{r2} are randomly selected from the parent generation.
- With this mutation step, we come up with the mutated generation. Now we apply a selection rule to each vector in the mutated generation to compute the trial generation. Here the K_r is the selection factor, ranging from 0 to 1, which defines the searching aggressiveness. *Rand* is a random number from 0 to 1.
- As the last step, we simply compare the FOM value of each vector in parent generation to that in the trial generation. The vector with better FOM will proceed to the next generation.
- We repeat the mutation and trial method on the new generation to come to next generation. This process will be repeated again and again until we arrive at the final generation.

As you can see, the new generation always has a better FOM value than the old generation. That way, we get a better and better fit in differential evolution. This is basically how DE works.