Reel1.0 Quick Guide

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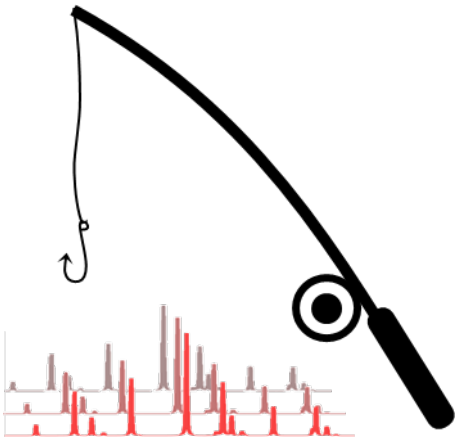
May 2021



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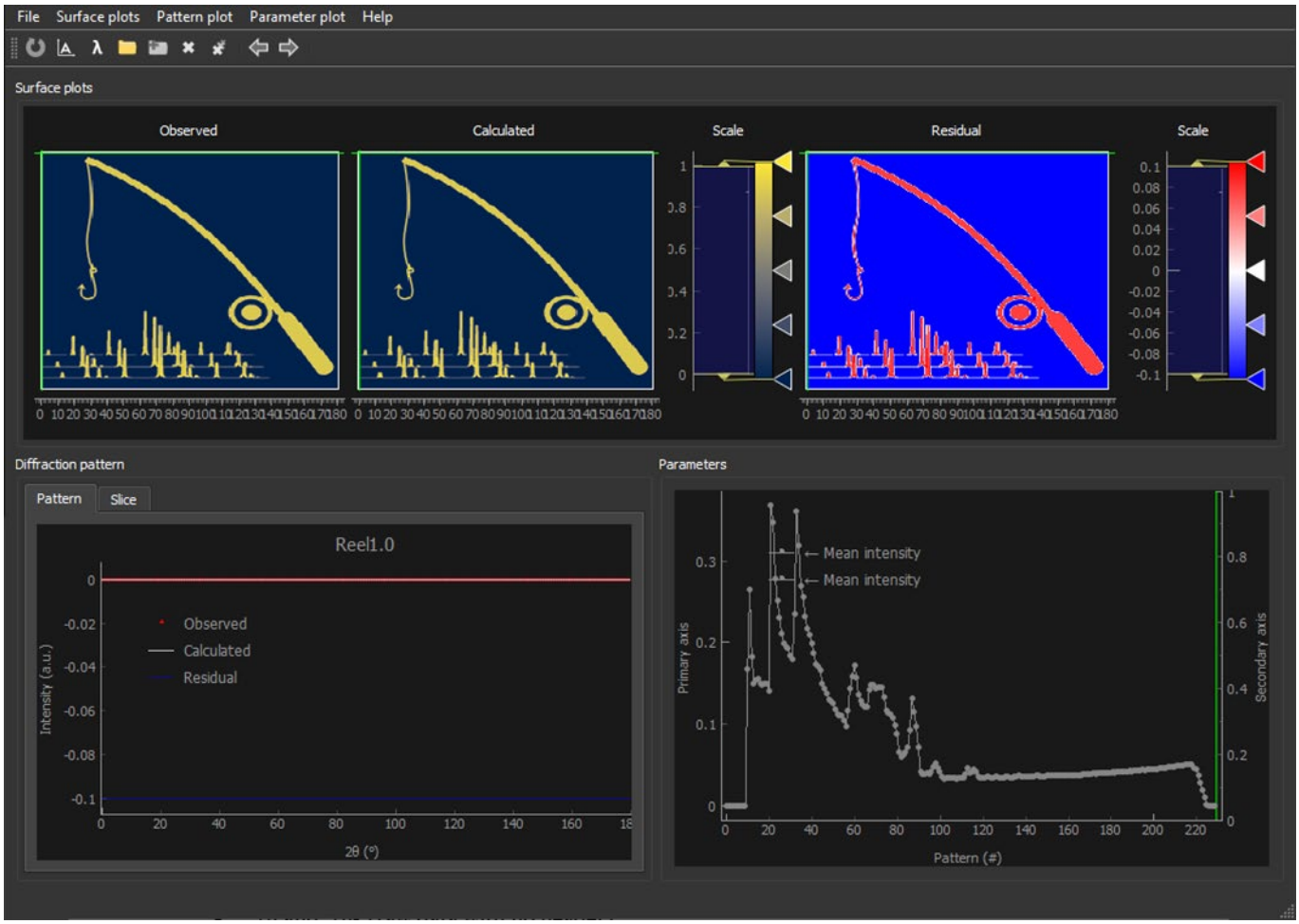


Welcome

Reel1.0 is a visualization tool for diffraction data and refinement results, intended for *in-situ, operando,* or similar larges datasets. The program allows the user to "Reel" through their data and quickly asses the quality of a multitude of refinements. While the idea for the program came from parametric refinements, it is equally applicable for sequential refinements or even raw data. Reel1.0 is written in Python and is open-source and free for all to use, however, I kindly request that it is not distributed with commercial intend. I hope that you enjoy the program and encourage any and all feedback.

-Frederik

Installation (Windows)

Reel1.0 comes as a collection of python files, and as such, require the user to install Python 3 and a few non-built-in modules. All the modules can be installed using *pip install* or *anaconda*. The latest version-requirements are: (May 2021)

Python 3.8.3

Non-built-in python modules:

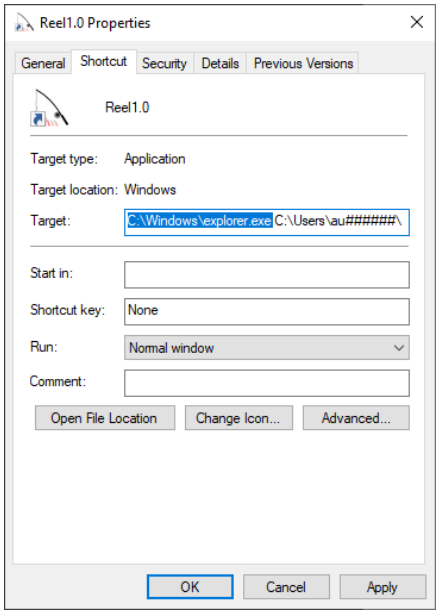
Module	Version	pip install command
PyQt5	v. 5.14.2	pip install PyQt5
pyqtgraph	v. 0.11.1	pip install pyqtgraph
matplotlib	v. 3.3.3	pip install matplotlib
numpy	v. 1.19.5	pip install numpy
scipy	v. 1.6.0	pip install scipy

+ Requirements imposed by the modules. Use *pip show [module]* for information about your current version.

Once all the required modules are installed, run the *setup.bat*. This will make the *run_Reel.bat* file and a *Reel1.0* shortcut. Open the program by double-clicking the short-cut or the *run_Reel.bat* file. If the program does not open, check that the path to *python.exe* in *run_Reel.bat* line 5 is valid.

Pinning the shortcut to start/toolbar

In order to pin the shortcut to the windows toolbar or start menu, right-click the *Reel1.0* shortcut, go to *properties*, add *C:\Windows\explorer.exe* in front of the *target* path, and click *OK*. Right-clicking the shortcut will now allow you to pin the shortcut to the start menu and the toolbar.



Installation (MAC)

There are no shortcut or batch files for mac-users, instead, open a terminal window, navigate to the *Reel1.0* folder, and run the *Refinement_evaluator_ver1.0.py* in python.

Getting started

New files are opened by clicking the *Open* button and selecting the desired file format in the dialog box.[1] Open several datasets by clicking the *Add dataset* button, and change between the opened datasets by clicking their names, the *Next* or *Previous* buttons, or with (ctrl+arrow keys). Update the current dataset by clicking *Update* or the hotkey (F5). Remove one or all dataset(s) by clicking the *Remove* buttons.

"Reel" through frames by dragging the green *Reel cursor* lines, either in the *Surface* plots or in the *Parameter* plot, or by using the arrow keys.

Select which parameters to plot and which axis to plot them on in the *Parameter plot* menu. Likewise, choose available sub plots from the *Pattern plot* menu.

You can scale the intensities separately for the *surface* plots and the *pattern* plots in the *Surface plot* and *Pattern plot* menus. Notice that scaling one will not affect the other. Adjust the colormap scaling by moving the yellow upper and lower boundaries in the *scale bar histograms* in the *surface* plot.

There are several options for zooming and panning in the plots. Change between the zoom modes for a given plot by right-clicking in the plot and selectin *Mouse Mode*. Auto-scale the range for all plots by clicking *auto-range* or using the hotkeys (A) or (space).

You can manually set the wavelength by clicking the *Set wavelength* button.

You can change the user defined default settings by editing the *ReelUserSettings.py* file in the *_lib* folder, and restore the default settings from the *Help* menu in *Reel1.0*.

[1] **NB:** The file order might depend on the sorting order of the current folder!

Data formats

Reel accepts several common data formats, but for the full range of option, use the *.xyy* format, as described below. The accepted data formats are:

- *.xyy* (custom Reel1.0 format)
- *.prf* (FullProf, prf=3)[2]
- *.prf* (JANA)[3]
- *.par* (+ associated *.fit* files, MAUD)
- *.dat* (FullProf, ins=0, 10)[4]
- *.xy* and *.xye* (raw data with no header)
- *.csv* (2θ in the first line and intensities in consecutive lines)

Custom *.xyy* file format for Reel1.0

The following is a guide to the custom *.xyy* file format intended for *Reel1.0*.

The header is separated in several parts. It starts with a *mandatory* filename on the first line. Then follows a section of *keywords* ending on a colon and followed by a *value*. There are three keywords of special significance: *R_wp:, Temperature (K):,* and *Wavelength (Å):*. Any additional colon-separated *keywords* and *values* are read by the program and can be plotted in the *parameter plot*.

The *keyword* section is terminated by the beginning of the comments section. The comment section is started with *COMMENTS*, and any additional lines will be ignored by the program, until the *END OF HEADER* line.

The data columns start with a column label, followed by the data. *Reel* expects the following *mandatory* columns: "*tth Y_obs Y_calc Y_res Background*". Any additional columns will be added as *sub plots* with their corresponding label.

```
File_name
R_wp: 4.702
Temperature (K): 373.500
Wavelength (Å): 2.52098
Counts: 834837.00
COMMENTS
Any additional comments or metadata provided by the user
END_OF_HEADER
    tth       Y_obs      Y_calc      Y_res     Background    Phase_1    Phase_2    Phase_3    Phase_4
  9.970    8039.000    8305.591   -266.591    8287.333    8294.666    8298.258    8287.333    8287.333
 10.070    7999.000    8283.805   -284.805    8264.862    8272.764    8275.903    8264.862    8264.862
 10.170    8045.000    8262.288   -217.288    8242.581    8251.130    8253.740    8242.581    8242.581
 10.270    7960.000    8241.055   -281.055    8220.490    8229.776    8231.768    8220.490    8220.490
 10.370    8221.000    8220.122      0.878    8198.587    8208.722    8209.986    8198.587    8198.587
 10.470    8110.000    8199.512    -89.512    8176.871    8187.989    8188.394    8176.871    8176.871
 10.570    7990.000    8179.257   -189.257    8155.342    8167.607    8166.992    8155.342    8155.342
 10.670    8104.000    8159.391    -55.391    8133.999    8147.613    8145.777    8133.999    8133.999
 10.770    7990.000    8139.962   -149.962    8112.840    8128.054    8124.748    8112.840    8112.840
 10.870    7894.000    8121.036   -227.036    8091.865    8108.997    8103.905    8091.865    8091.865
 10.970    8187.000    8102.705     84.295    8071.073    8090.531    8083.246    8071.073    8071.073
```

Mandatory
Special

[2] FullProf manual p. 73
[3] JANA2006 cookbook p. 773
[4] FullProf manual p. 74