

Welcome

Reel1.0 is a visualization tool for diffraction data and refinement results, intended for *in-situ*, *operando*, or similar large datasets. The program allows the user to “Reel” through their data and quickly assess 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 intent. 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.

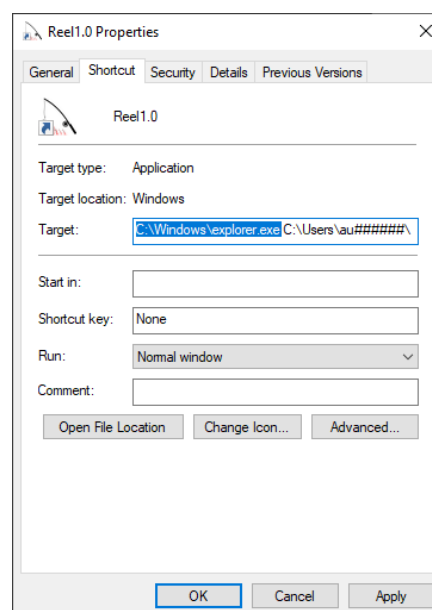
Once all the required modules are installed, run the *setup.bat*. This will make the *run_Reel.bat* file and a *Reel1.0* shortcut. Open the program by double-clicking the short-cut or the *run_Reel.bat* file. If the program does not open, check that the path to *python.exe* in *run_Reel.bat* line 5 is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

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)

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_{up}*., *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" and "Y_obs" (case sensitive), and three optional columns with special meaning: "Y_calc", "Y_res", and "Background". Any additional columns will be added as *sub plots* with their corresponding label, separated by *space*.

```

1 File name
2 R wp: 4.702
3 Temperature (K): 373.500
4 Wavelength (Å): 2.52098
5 Counts: 834837.00
6 COMMENTS
7 Any additional comments or metadata provided by the user
8 END OF HEADER
9
10 tth Y_obs Y_calc Y_res Background Phase_1 Phase_2 Phase_3 Phase_4
11 9.970 8039.000 8305.591 -266.591 8287.333 8294.666 8298.258 8287.333 8287.333
12 10.070 7999.000 8283.805 -284.805 8264.862 8272.764 8275.903 8264.862 8264.862
13 10.170 8045.000 8262.288 -217.288 8242.581 8251.130 8253.740 8242.581 8242.581
14 10.270 7960.000 8241.055 -281.055 8220.490 8229.776 8231.768 8220.490 8220.490
15 10.370 8221.000 8220.122 0.878 8198.587 8208.722 8209.986 8198.587 8198.587
16 10.470 8110.000 8199.512 -89.512 8176.871 8187.989 8188.394 8176.871 8176.871
17 10.570 7990.000 8179.257 -189.257 8155.342 8167.607 8166.992 8155.342 8155.342
18 10.670 8104.000 8159.391 -55.391 8133.999 8147.613 8145.777 8133.999 8133.999
19 10.770 7990.000 8139.962 -149.962 8112.840 8128.054 8124.748 8112.840 8112.840
20 10.870 7894.000 8121.036 -227.036 8091.865 8108.997 8103.905 8091.865 8091.865
21 10.970 8187.000 8102.705 84.295 8071.073 8090.531 8083.246 8071.073 8071.073

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⁴ FullProf manual p. 74