Reel1.0 - A visualization tool for evaluating powder diffraction refinements

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Summary

The ever-growing community for parameter-resolved X-ray and neutron diffraction, spurred by the rapid improvements in both detectors and sources for large-scale facilities, gives rise to the need for a fast and efficient evaluation approach for the large quantities of data produced during such experiments. As diffraction scientists, we need to be able to both visually and analytically compare our raw data and refined models in a consistent and user-friendly way. This is particularly true when refining in two dimensions, such as sequential or parametric refinements, where parameters such as time, temperature, field strength, pressure, etc. might be included in the models. Our proposed strategy, embodied in the Reel1.0 software, focuses on combined 1D and 2D visualizations (heatmaps) of the data, in order to qualitatively evaluate the observed, calculated, and residual data in parameter-space, with cross-comparison to key parameters. We accomplish this with a single-window interface, illustrated in Figure 1, where 1D and 2D data are easily compared with the moveable lines (or *Reel cursors*). Several datasets can be opened at once to quickly compare models. Using the simple customized *.xyy* file format allows any number of user-defined parameters to be plotted, such as temperature, pressure, R-values, or mean intensity.
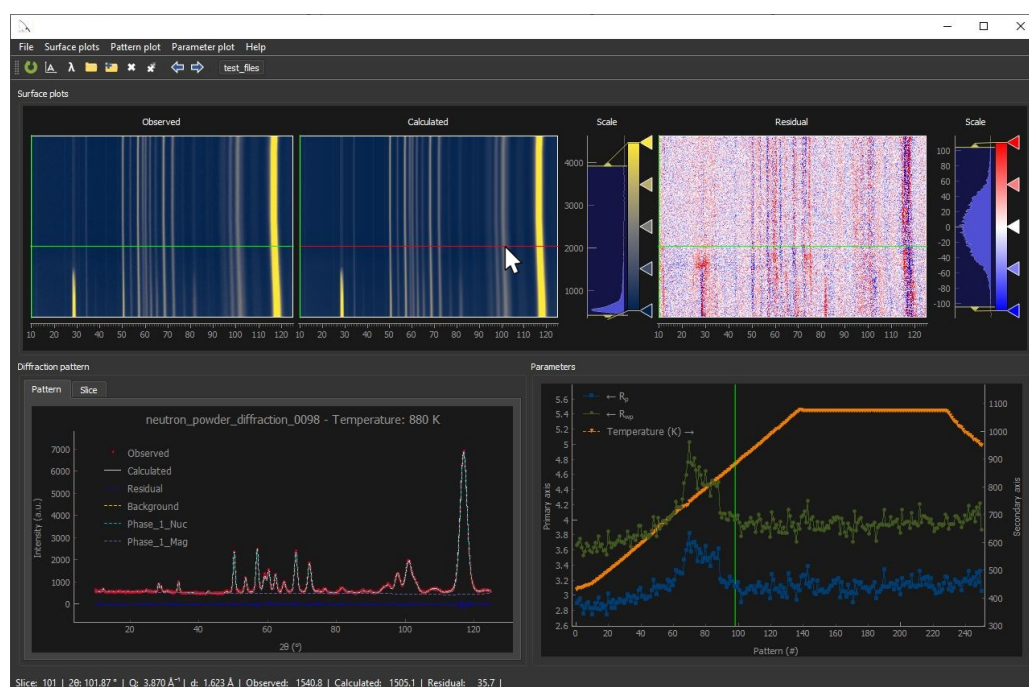
Figure 1: Illustration of the single-window interface of Reel1.0. The interface is divided in three main sections: 2D surface plots (heatmaps), 1D diffraction pattern plot, and 1D parameter plot.

Statement of Need

`Reel1.0` is a Python based GUI, based on the `PyQt5` and `pyqtgraph` packages (Campagnola, 2016). The graphical interface is intended to make `Reel1.0` appealing to a broad audience (within the community), even for users with limited programming knowledge. User-friendliness is a key feature, as `Reel1.0` is a visualization tool, intended to be used in combination with other refinement software, such as TOPAS (Coelho, 2018) or FullProf (Rodriguez-Carvajal, 1993), and with room for expansion in the future.

`Reel1.0` is intended for users working with large X-ray and neutron diffraction datasets, such as in-situ and operando studies, across several scientific fields (chemistry, physics, materials science). The visualization tools provided by the `pyqtgraph` libraries allow multiple datasets of several hundred patterns to be evaluated at once, without compromising the stability of the program. The simple interface, efficiency, and user-friendliness of `Reel1.0` will allow the powder diffraction community to pursue increasingly advanced parameter-resolved experiments and the modeling of these.

`Reel1.0` can be used at several steps in diffraction data processing, both for evaluating raw data and for evaluating and comparing refinement models. A suggested workflow for diffraction data evaluation using Reel1.0 is outlined in Figure 2. During data collection, the raw data can be evaluated to ensure that appropriate data quality is acquired. This includes evaluating parameters such as the signal-to-noise ratio, signal-to-background ratio, time-resolution, and angular resolution. During initial assessment, a more thorough pre-modeling evaluation can be performed. Here, the collected data is evaluated, in order to gather information needed for modeling. This includes phase transition, impurity formation, changes in background, mean scattered intensity, and external parameters (when available). The initial assessment also serves as a quick quality check, before the more time-consuming refinement is performed. The refinement is performed in an external software, e.g. FullProf or TOPAS, and the resulting output files are evaluated in `Reel1.0`. The modeling evaluation is particularly useful for direct visual assessment, both of 1D and 2D plots, but also for evaluating R-values and user-provided

parameters (only for the *.xyy* format). The 2D residual surface plot is an exceptional tool for identifying systematic deviations in the model, such as asymmetry, diffuse scattering, or incorrect background modeling.
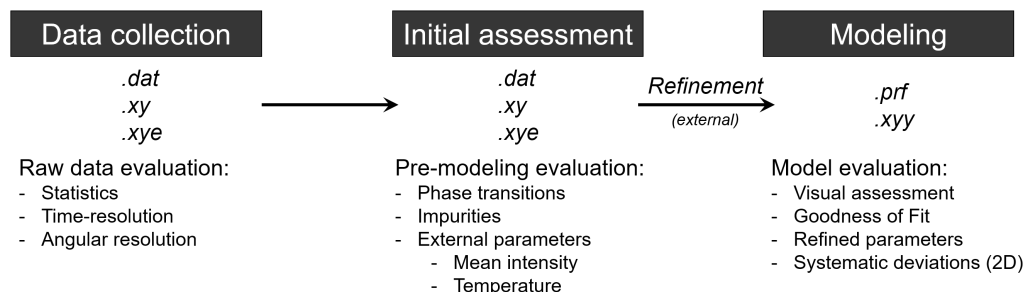

Figure 2: Example of a data processing flowchart using Reel1.0, along with examples of the associated data file formats. The formats .dat and .prf are based on standard FullProf formats, while the .xyy format is a custom file format, defined in the Ree1.0 Quick Guide.

State of the Field

To our knowledge, no other software in the community provides as easy and fast an evaluation of both 1D and 2D diffraction patterns. While refinement software, such as FullProf Suite, MAUD (Lutterotti et al., 2007), or TOPAS come with visualization tools for both 1D and 2D patterns, they lack the ability to combine the two. Examples of the visualization tools in FullProf Suite, MAUD, and TOPAS are illustrated in Figure 3.

The aesthetics of the visualizations are of course subjective, however, it has been shown that certain colormaps, such as "rainbow" maps, can be misleading and in the worst case, result in scientifically wrong conclusions. (Nuñez et al., 2018) As such, one should strive for using perceptually linear colormaps. Reel1.0 uses the perceptually linear and color vision deficiency friendly `cividis` colormap as default, but any colormap contained in the `Matplotlib` package is available.
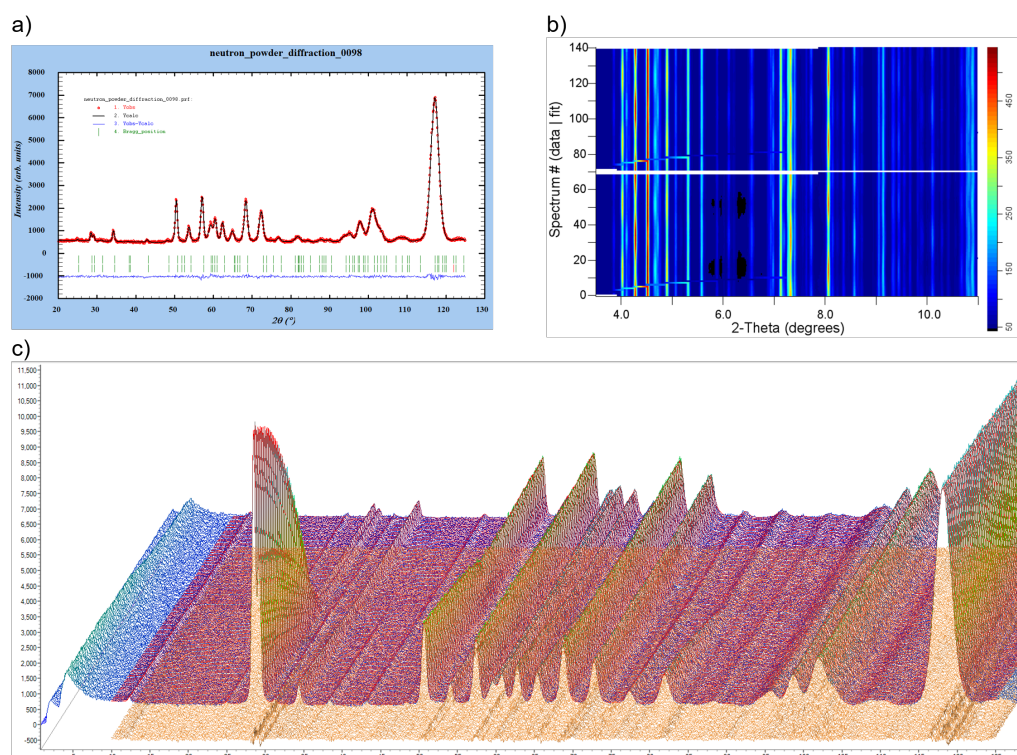
Figure 3: Examples of other visualization tools in the powder diffraction community. a) A 1D diffraction pattern as visualized in FullProf Suites WinPlotr. b) 2D observed-calculated heatmaps for 72 patterns as visualized in MAUD. c) Observed, calculated, and residual waterfall plot as visualized in TOPAS.

Acknowledgements

References

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