EasyTexture: a new software for data reduction at POWTEX

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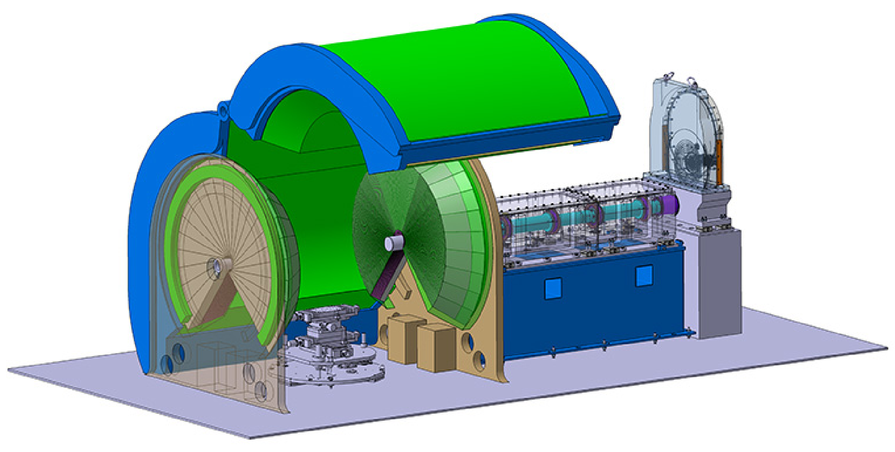
Motivation

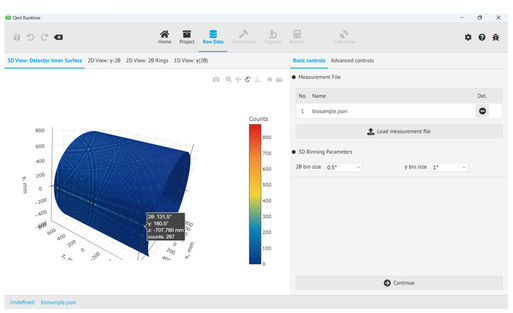


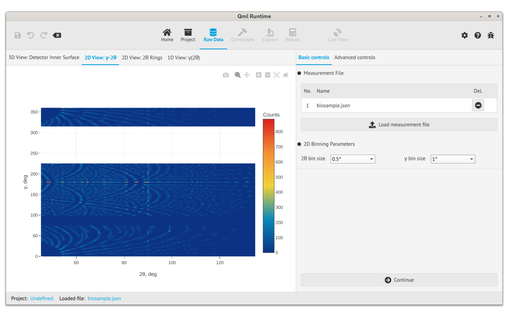
POWTEX is a high-intensity time-of-flight diffractometer at the FRM-II research reactor in Garching bei München, Germany [1]. The instrument will serve the needs of the solid-state chemistry, geoscience, and materials science communities through neutron scattering measurements on POWder and TEXture samples. In this poster, we present the current status of development of a new open-source software called EasyTexture, which will be used to reduce raw data for texture samples at POWTEX and prepare texture intensity resolved spectra for analysis within the MAUD package [2]. The graphical user interface of EasyTextrure is designed using the EasyScience framework [3] and the data reduction will be handled using Scipp and ScippNeutron [4] python libraries.

Highlights

The EasyTexture software is currently being developed to facilitate the data processing workflow at the POWTEX instrument at MLZ. The software will be characterized by the following features:

- It will implement a set of data reduction algorithms, which enable the users to correct the collected raw data by various experimental artifacts caused by the instrument and its environment.
- It will contain comprehensible tools for visualizations, which provide opportunities for the users to make quick and informed decisions in selecting best parameters for data analysis. The skeleton of the GUI is based on a Python/QML framework EasyScience, displayed below.
- It will provide means for exporting reduced data into a format, supported by the MAUD-software that can perform Rietveld texture analysis of measured samples.

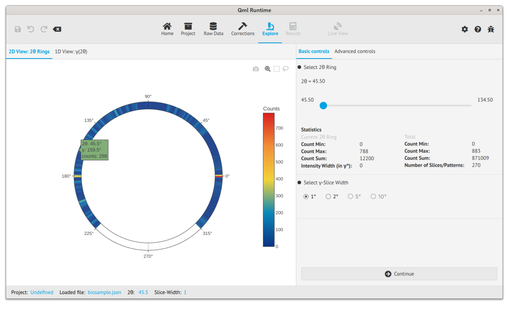


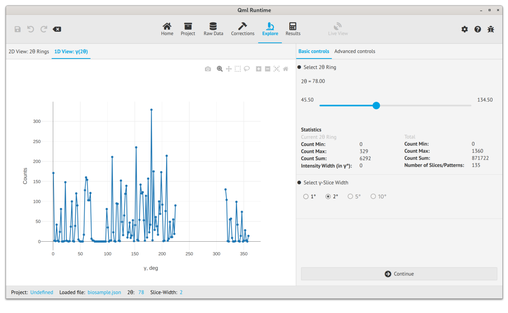


Current status and available features

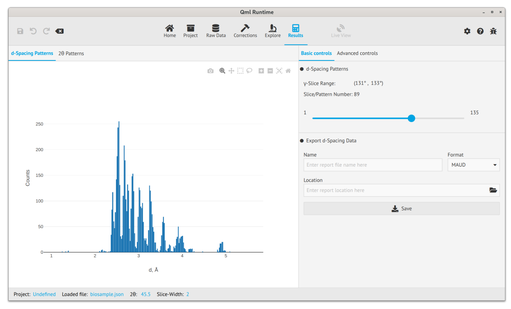
At the moment, the software is characterised by the following attributes:

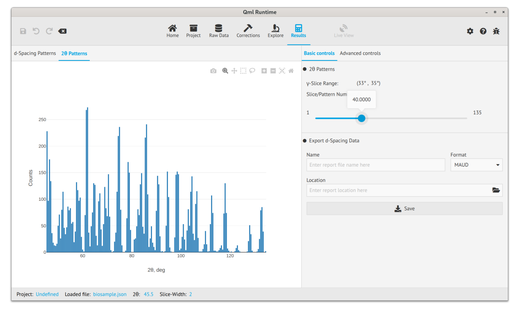
- Data processing workflow has been developed using the mockup dataset simulated in Vitess [5] and NumPy Python library.
- Main components of the workflow are established and are integrated into the GUI and users can select optimal binning for analysis.
- Outer detector layers are projected onto the inner-most detector mantel layer and the resulting counts information is shown to the users of software. Plotly library is used for visualizations.





The figures below display the layout of the "Results" tab, which contains user-friendly visualization tools for the final refinement of selected parameters and exporting obtained *d*-patterns for a subsequent processing with MAUD software.





EasyTextrure is being developed not only for performing offline data reduction, but it will also contain tools for on-the-fly tracking of data at the beamline, for which the "Live View" tab is being designed.

Further development

- Implementation of the workflow for processing detector voxels that belong to the top and bottom bases of the cylindrical detector surface.
- Development of the workflow for correcting raw angular- and wavelength-dependent event data using calibration measurements.
- Integration of a 1D peak finding algorithm for determination of an optimal width for γ-slicing.
- Implementation of the workflow for exporting the reduced data to a MAUD-supported format.
- Integration of Scipp and ScippNeutron libraries into software's data processing workflow.
- Development of exhaustive functionality for data exploration in "Live View" mode.

Acknowledgements

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References

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