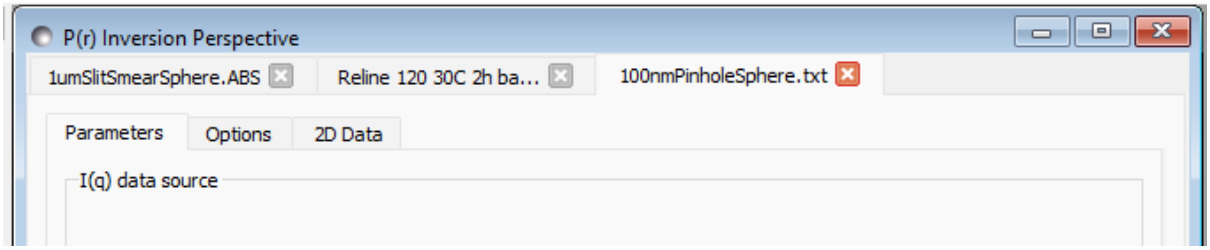
Notes and Reference Document for Pr interface

Introduction

I worked on batch processing, 2D slicing, batch tables, minor UI changes, and a few plots during my summer internship. The vast majority of these changes were made in the Pr Interface directory. I was also tasked with figuring out how to make Pr work with SVD-reduced data. However, I ran out of time and was unable to incorporate it into Sasview. The code for the SVD work I've done so far is available on one of my GitHub repositories.

At the time of writing this document the work I have done is still not merged to the main branch. Although most of the features for it is finalised, double checking, code cleaning and commenting is still yet to be completed.

Tabbing System



Tabs were one of the first things I implemented. This new tabbing system lets users to have numerous instances of the Pr interface opened at the same time. Furthermore, multiple sets of individual data, as well as batches of data and 2D slices, can be worked on at the same time without continually adding and removing data. The tab can be saved and/or closed if the user is happy with the calculations. Although tabs were not originally intended to be worked on, this was an increase in quality of life for the users as well as a good starting point for me to get familiar with the source code.

How To Use Tabs

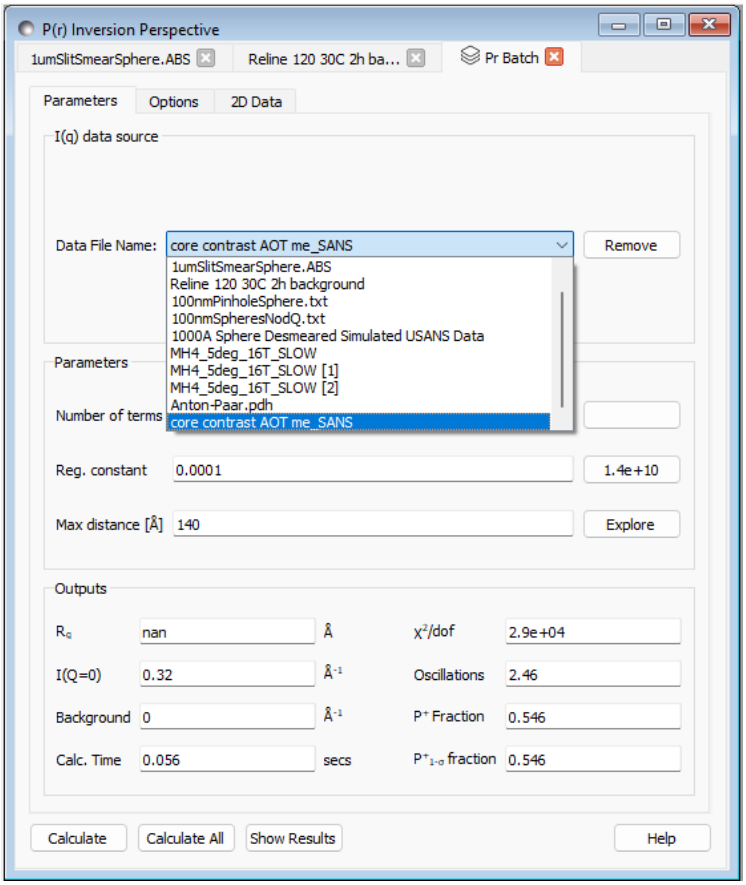
Open the Pr perspective and load either a single 1D Data file, a 2D Data file, or a set of 1D data files (Batch Mode must be checked). The Perspective should automatically set up the type of tab for the imported data. Once the tabs are created it can easily be scrolled through and calculated, and it can also be closed using the [x] button on the right of each tab.

Future improvements:

- [ ] Plots for the tab can be automatically closed when the tab is closed.

Batch Processing

Multiple sets of 1D data can be imported into the Pr perspective in Sasview using the data explorer widget. This can be done by checking the Batch Mode Checkbox. Once the data is sent to the PERSPECTIVE the Dropdown menu will be populated with the data. The user now can decide to keep the default parameters or scroll through and change the parameters for each of the files. The software should remember the parameter set by the user for that specific file. The user can then either calculate the current file from the dropdown or batch process all the files using the set parameters. If the parameters are not set default values will be used. Side Note: SVD was planned to be used here to automatically calculate some of the parameters primarily the Number of terms and regular constant.



Once calculated a table with all the outputs along with the parameters should be presented in a table using a pop-up window. This data can then be plotted or saved to an CSV file. IF the user is unhappy with the calculation, they can also remove that specific file form the perspective or recalculate the data using different parameters. This could be done using the calculate button. When this is done plots will also be presented unlike when batch processed where the plots are disabled. This was done to avoid Sasview from running slow or crashing due to multiple matplotlib plots (Which are slow to create). One of the biggest bugs that I am still facing in the writing of this document is that when batch processed the table shows duplicate calculations. The file name and parameter are however correct, but the calculation can duplicate. I believe this might be because calculations are done in parallel using multithreading. A way to get around this is by using the mouses scroller to scroll through the file from the dropdown menu which recalculates the data onload.

How To Use Tabs

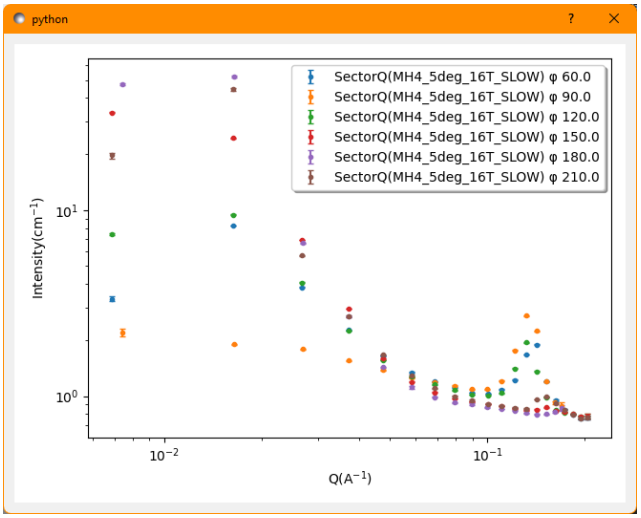
Any set of 1D data files can be passed to the perspective and be set to be batch processed using the data explorer. The user can then go through the items in the dropdown menu and set parameters for each of the file. using the “Calculate all” Button all the files withing the tab should be processed and a table with all the outputs should appear. The way this works is it goes through every interface, loads, calculates, and saves the data and does this until all the data in the tab is calculated. The data is then sent to the table where the user can decide if it needs to be exported to a CSV and/or plotted.

Future improvements:

[ ] Fix the Duplication Bug. The calculations for rows in the table duplicate when batch processed, and the user currently need to scroll back through each of the file (in the dropdown menu) for it to be fixed.

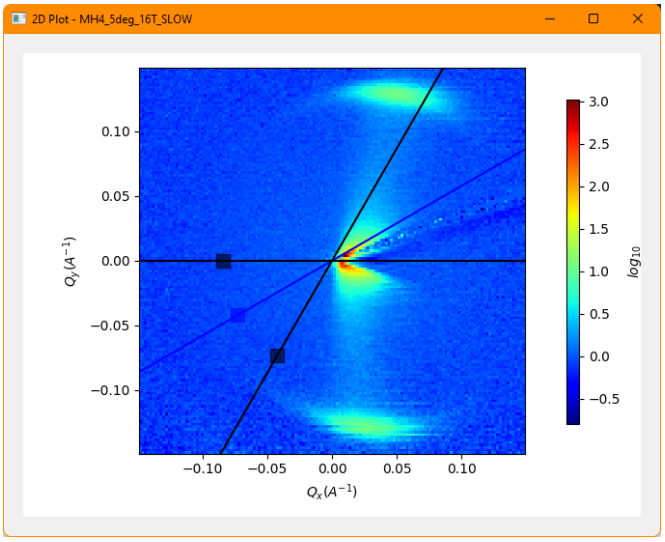
[ ] Plots for the tab are automatically closed when the tab is closed.

2D Slices

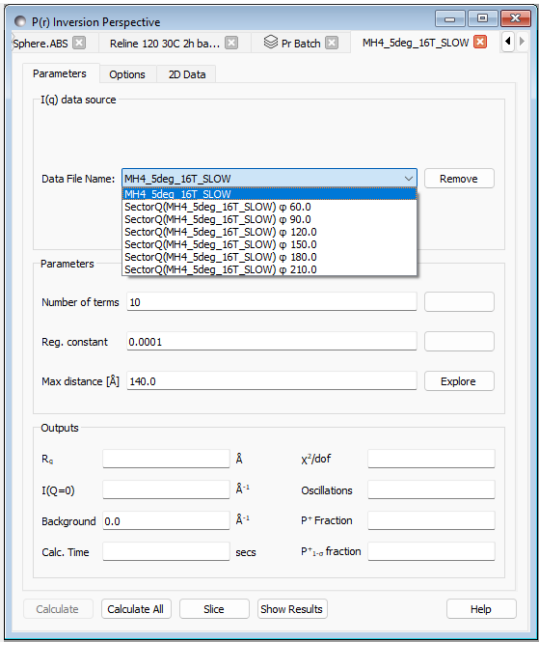


2D data can now be loaded into Pr perspective and should automatically be recognised. If 2D data is imported a 2D plot of the raw data will be presented. A new button will also be available to allow the user to slice the data. The parameters to slice the data will be accessible under the "2D data" tab. This will take in the Start Point, Number of slices and Q Bin and when sliced will produce a Pr plot with all of the 1D slices. The way this is sliced is by using the new muiltiSlicer() function which returns a list of slice plots and creates a Model Item using the Plot in the slice(). Once sliced the slices will be made visible in a table in the 2D Data tab as well in the Dropdown menu Which can be batch processed similar to 1D data.

How To Slice 2D data



When a 2D Data file is sent to the Pr perspective. A plot similar to the one on the left is displayed. To give the user a rough idea of what the data looks like. Additionally, a slice button is also made available. The user can then switch to the 2D data tab and set the parameters for the slicer and slice using the slice button. The sliced data will then be sent to the dropdown menu similar to the screenshots on the right. Users can select each of the slice, set parameters and calculate each of it individually or batch process all the slices together. A batch table with all the results should also be displayed.



Future Improvements

- [ ] Plots need to be within the window
- [ ] Plots need to close when data is deleted or the tab is closed.
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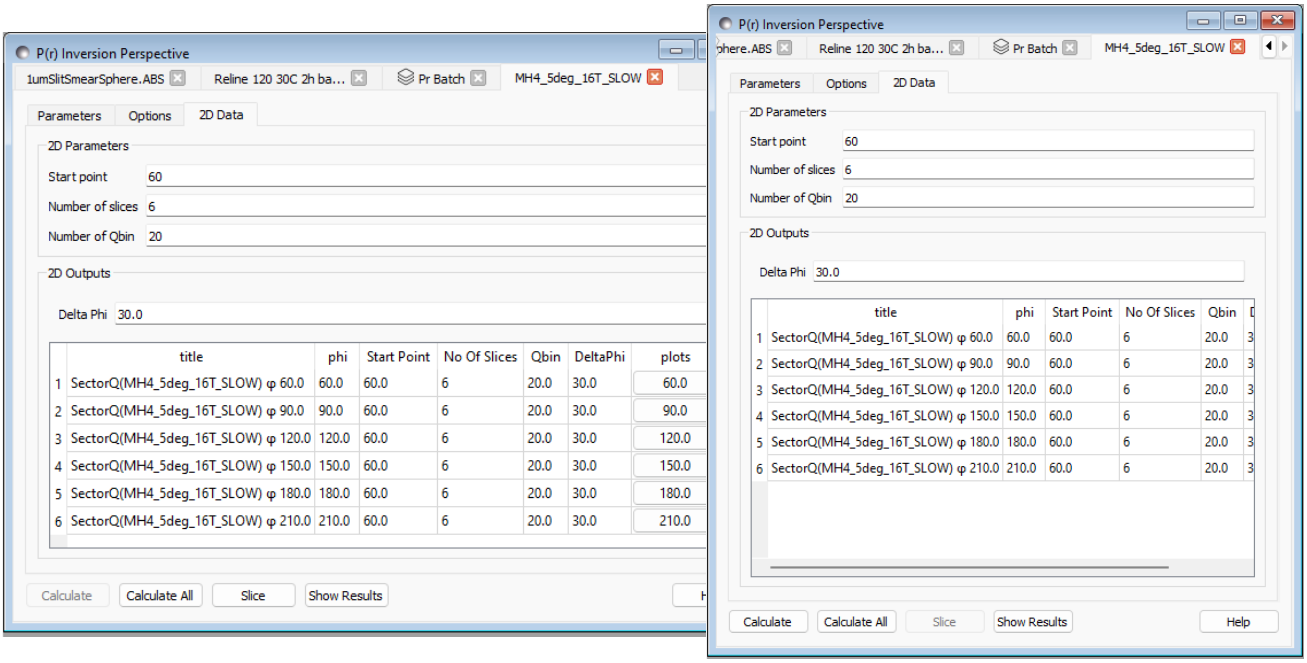
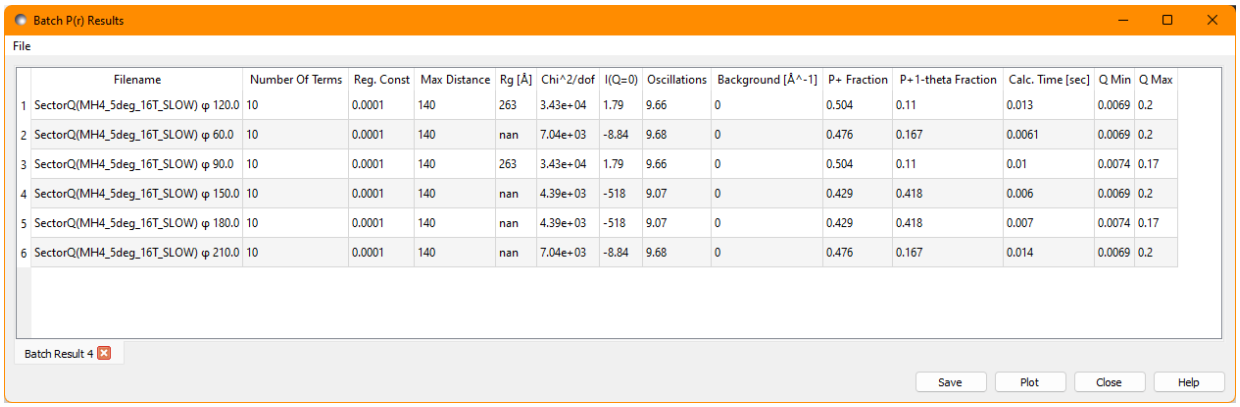


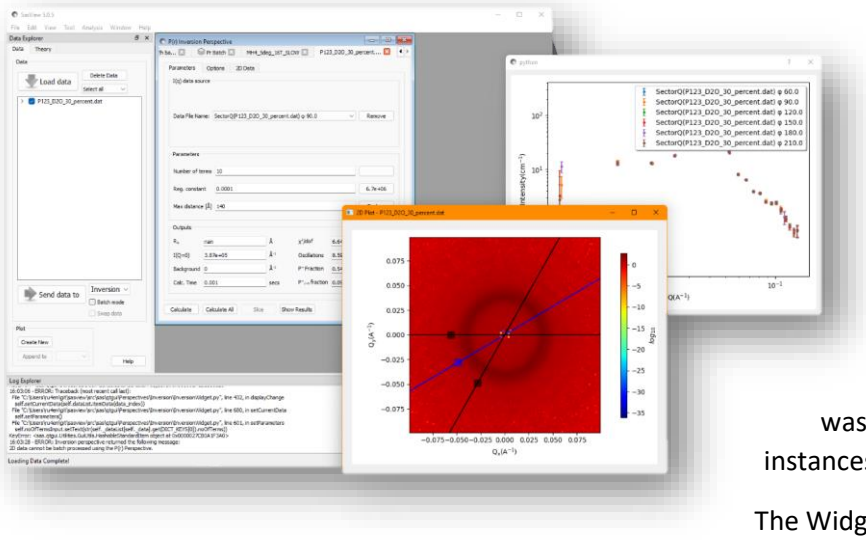
Batch Table

A table of the batch results will pop up after the “Calculate all” button is pressed. Additionally, a new tab of the data can be sent to batch table using the show results button. For Pr the Batch Table should show n number of rows n being the number of files imported and calculated. With columns showing the Filename, Number of Terms, Reg. Constant, Max Distance, Rg [Å], Chi^2/dof, I(Q=0), Oscillations, Background [Å^-1], P+ Fraction, P+1-theta Fraction, Calc. Time [sec], Q Min and Q Max. Batch Results also support tabbing and multiple iteration of results can be saved and navigate to if the user decides to make changes to the calculations.

Withing the Batch Table interface data can be exported to a CSV file using the save button. Furthermore, a 2D plot can also be created by selecting the rows and using the plot button.



Minor UI Changes



Minor Ui changes were made to accommodate the tabs. The file InversionPerspective.py was split into 2 one keeping the main window InversionPerspective.py) the other the inner parts of the tabs which the user used to calculate (InversionWidget.py). This was done to allow multiple instances of Pr.

The Widget was also changed a bit, A major change that can be noticed is the new tab to allow setting parameters for 2D data slicing. Minor changes were also made to the buttons. With the addition of "Calculate all", "Slice" and the "Show Results" Button.

New Plots

There have been a few changes to the way plots behave. With addition to a few more plots. Originally Pr had 2 types of plots Pr plots and I(Q) plots. These 2 Plots now can be displayed only of the "Calculate" button is pressed. This means If the data is calculated during loading or whilst batch processing the plot are hidden to reduce computation. There has also been an addition of 2 new plots. Once data is loaded a 2D plot of the raw data is displayed. The other is a 1D Pr plot of all the slices. Which can be viewed individually by clicking the buttons in the Plot column in the slice table.

Bug Table

Description	Note	Status
Duplicate Data in the batch Results Panel.	In Batch Mode if calculate all button is pressed the results in the batch results table shows duplicate Rows. This is "Probably" a multi-Threading issue. The outputs however are calculated correctly using the interface. The table can be "fixed" by scrolling through this recalculates which also updates the outputs in the table.	
Data does not save from Batch Results Panel to CSV	When save is pressed the function that gets the data cannot find the _data for the current tab.	Fixed
Plots and Batch Results Panel Pops out of SasView Interface.	New Plots and Tables show as its own window and not within the Sasview interface.	

Single Value Decomposition

Although I didn't get time to implement Single Value Decomposition into Pr. I have been working on a script to use Sasview data loader to load, process its Sv and calculate the P of r using Sasview calculator. I also might work on this past my summer placement. The code for this is available on my GitHub repository https://github.com/ru4en/sasview-Pr-SVD