Motofit – integrating neutron reflectometry acquisition, reduction and analysis into one, easy to use, package.

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Abstract. The efficient use of complex neutron scattering instruments is often hindered by the complex nature of their operating software. This complexity exists at each experimental step: data acquisition, reduction and analysis, with each step being as important as the previous. For example, whilst command line interfaces are powerful at automated acquisition they often reduce accessibility by novice users and sometimes reduce the efficiency for advanced users. One solution to this is the development of a graphical user interface which allows the user to operate the instrument by a simple and intuitive "push button" approach. This approach was taken by the *Motofit* software package for analysis of multiple contrast reflectometry data. Here we describe the extension of this package to cover the data acquisition and reduction steps for the Platypus time-of-flight neutron reflectometer. Consequently, the complete operation of an instrument is integrated into a single, easy to use, program, leading to efficient instrument usage.

1. Introduction

Neutron scattering instruments at modern facilities are now able to collect large volumes of high quality data faster than ever before. A large amount of effort is spent on constructing the complex instrumental hardware, with additional resources being used to develop software to acquire (operate), reduce and analyse data from the instrumentation. One example is the approach used in the DANSE project [1] which, in part, was initiated to develop software infrastructure for the reduction and analysis of data from the high intensity Spallation Neutron Source facility.

The software created for this purpose has to cope with complex data analysis problems that mirror the sophisticated nature of a neutron scattering experiment. Existing analysis tools have been more than adequate but often show deficiencies, such as their inability to cover new technique aspects, or the use of a command line interface to control the program. This latter point is often invisible to expert users, but can be a huge stumbling block for novices. At best this leads to inefficient use of the instrument, at worst the user obtains bad data and may not return.

The *Motofit* reflectometry analysis package [2] was originally designed to solve such a problem, offering sophisticated analysis of multiple contrast data, but in an easy to use manner.

Recently we faced the ease-of-use problem during the construction of the new *Platypus* time-of-flight (TOF) neutron reflectometer [3] at OPAL. To address this *Motofit* was extended and is now an integrated approach for the acquisition, reduction and analysis of reflectometry data. This integration means that the user is only ever exposed to a single program throughout the experiment lifecycle,

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leading to simple operation, a better understanding of the data and efficiencies in preparing data for publication. *Motofit* was designed to operate in the *Igor Pro* (Wavemetrics Inc) data analysis program [4], offering rapid development using the instrinsic data analysis functionality already present.
Here we describe each of the modules of *Motofit* to give an overview of how Platypus operates.

2. Acquisition module – FIZZY

The Platypus reflectometer [3], like most instruments at the OPAL facility, is operated using a server-client paradigm. The instrumental hardware is controlled by a command line SICS control server [5], which is responsible for moving motors, speaking to the detector acquisition electronics and software, as well as saving the data in NeXUS format. The FIZZY module was designed to provide a user interface (GUI) for a generic SICS server and have the following functionality: 1) easy visualisation and control of instrument parameters (motor positions, etc), 2) single button press data acquisition and alignment (figure 1a), 3) realtime visualisation of multidimensional detector images (figure 1b) and 4) batch mode for measurement of multiple samples.
Figure 1 demonstrates the simplicity of the user interface. There are no other menus to FIZZY, with all instrument operation taking place in a single multi-tabbed window. Even the potentially difficult batch mode operation is simplified via popup suggestions for the different kinds of instrument operations available.
Behind the scenes FIZZY communicates with SICS using the *Sockit* and *EasyHttp* plugins for IGOR [6], which enable TCP/IP and http communication. FIZZY simply abstracts the SICS command line functionality into GUI controls, such as buttons.

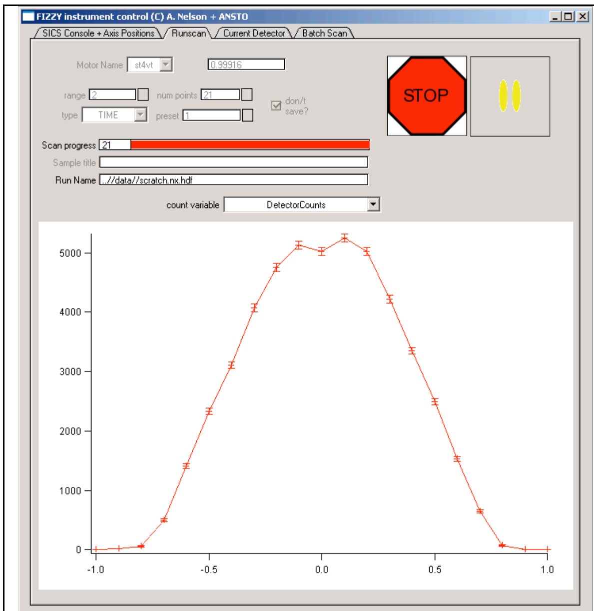

Figure 1a) Alignment scans and acquisitions require a single button press

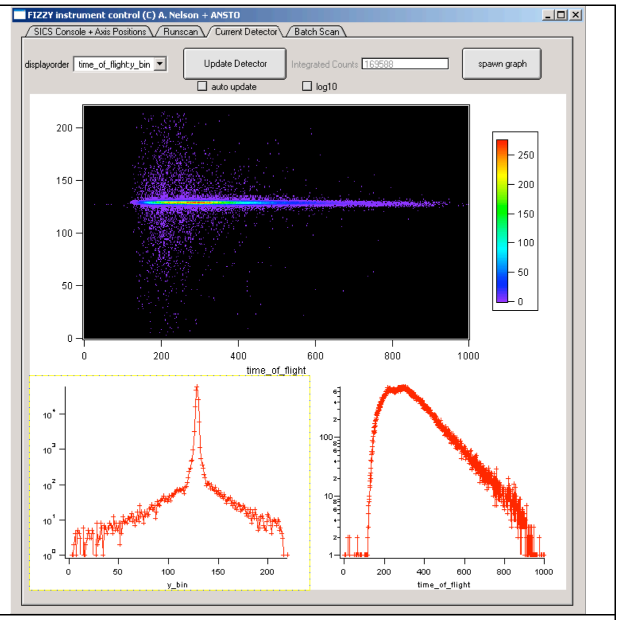

Figure 1b) Real time detector view showing 2D image (ypixel vs TOF) with projections along each of the axes.

3. Reduction module – SLIM

Whilst most of the data analysis is done offline, real-time assessment of the data streaming off the instrument is vital, as this often determines the course followed in an experiment. The SLIM module offers this access in a simple manner. All the user has to do is select the runs they need to visualise, with reflectivity curves being generated automatically. The user has many different choices for the plot system, both 1D (R vs Q, R vs lambda, R vs TOF, Intensity vs TOF, Intensity vs lambda, etc) and 2D detector images.

The SLIM module accepts NeXUS files as input and outputs both specular and offspecular reflectivity. The output files are text based and have two forms, a columnar dat file and an XML file that is related to the canSAS XML format for SAS data. All data files contain experimental uncertainties - standard deviation for reflectivity and full width half maximum for Q resolution.

The exact reduction process will be detailed in a later paper, although we give a short overview here. Both direct and reflected 2D (detector y pixel vs TOF) spectra are corrected for spatial detector efficiency. A gravity correction is applied to both spectra, as Platypus is a vertical scattering plane instrument and the angle of incidence is wavelength dependent. Since data is oversampled in time-of-flight the 2D spectra are rebinned using dT/T bins that reflect the instrumental resolution. The data are then converted to a wavelength axis. The actual angle of reflection is calculated using the positions of the specular reflection and direct beam on the detector. An instrumental background is subtracted by linear fit between regions either side of the spectral ridge, for a given wavelength bin (although constant Q subtraction is being developed).

The direct beam wavelength spectrum is then obtained by summing detector y pixels over the incident beam width, for a given wavelength.

In contrast each pixel in the reflected beam image has a Q_z, Q_y value calculated for it, with the pixel intensity being divided by the direct beam intensity for that wavelength. Rebinning of pixels with equal Q_z in the specular beam yields a reflectivity curve. Experimental uncertainties are propagated throughout the reduction process, with the Q resolution calculation according to van Well [7].

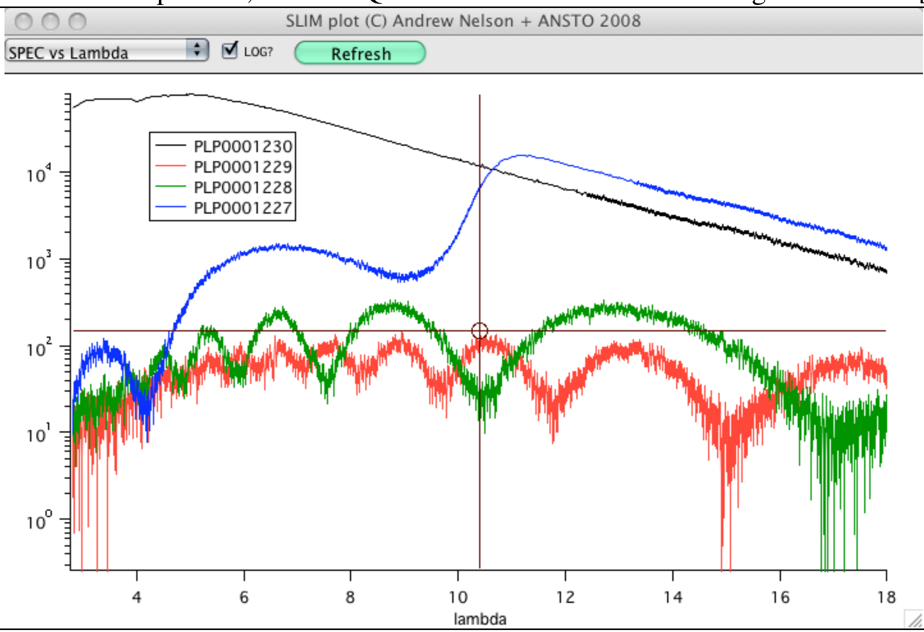

Figure 2) Realtime data visualisation of direct and reflected beams. The uppermost curve is a direct beam run, the other curves are reflection runs at different incident angles.

4. Analysis module - *Motofit*

The reflectivity analysis module was the first to be developed and is described in more detail by Nelson [2]. It's overriding design criteria were the simultaneous least squares analysis of multiple contrast neutron and X-ray reflectometry data, with an interface that was easy to use by novices and experts alike. Since the original description further functionality has been added to extend the analysis capabilities including: genetic optimisation [8], batch fitting of multiple datasets [9], monte carlo error analysis [10], exploration of χ^2 for different parameter combinations, analytical SLD profiles.

The main advantage of integrating all the aspects of the experimental software is that the data files from SLIM are immediately available for analysis in *Motofit*. However, data analysis in *Motofit* is not restricted to data obtained on Platypus, data from any neutron and X-ray reflectometry data can be also be used.

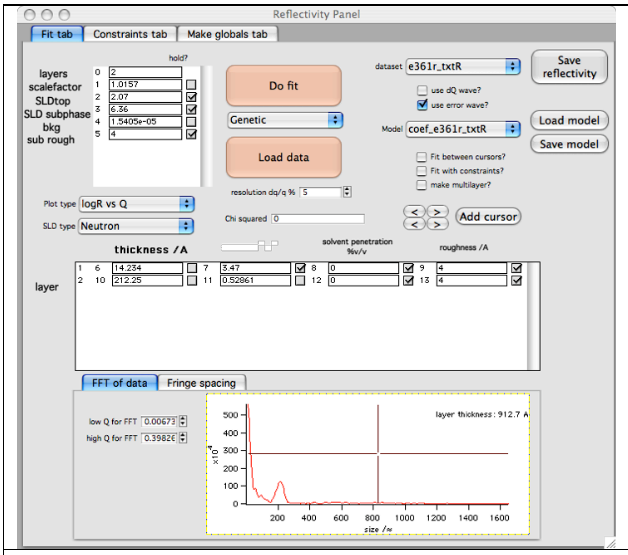

Figure 3a) *Motofit* analysis panel

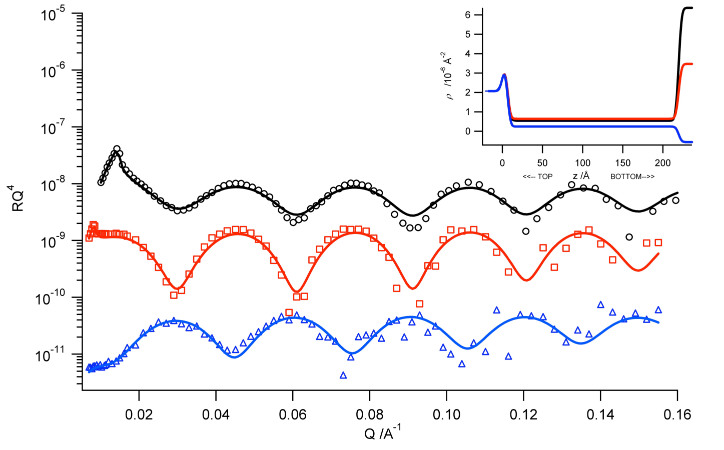

Figure 3b) Graphics from the co-refinement of multiple contrast data are publication ready.

5. Conclusions

We have streamlined the user operation of the Platypus neutron reflectometer by integrating data acquisition, reduction and analysis into a single program. This leads to efficient use of Platypus by novice and expert users alike.

The *Motofit* program is available from http://motofit.sourceforge.net or from http://dav1-platypus.nbi.ansto.gov.au.

6. References

[1] http://danse.us, The DANSE project

[2] Nelson A 2006 Co-refinement of multiple contrast neutron / X-ray reflectivity data using MOTOFIT *J. Appl. Crystallogr.* **39** 273-276

[3] James M; Nelson A, Brule A and Schulz J 2006 Platypus: A time-of-flight neutron reflectometer at Australia's new research reactor *Journal of Neutron Research* **14** 91-108

[4] http://www.wavemetrics.com IGOR Pro Wavemetrics Inc.

[5] Heer H, Konnecke M and Maden D 1997 The SINQ instrument control software system *Physica B* **241** 124-126

[6] available from http://www.igorexchange.com

[7] van Well A A and Fredrikze H 2005 On the resolution and intensity of a time-of-flight neutron reflectometer *Physica B* **357** 204-207

[8] Wormington M, Panaccione C, Matney K and Bowen D 1999 Characterization of structures from X-ray scattering data using genetic algorithms *Philosophical Transactions of the Royal Society of London*, **1999**, *357*, 2827-2848

[9] Mueller-Buschbaum P, Bauer E; Maurer E, Nelson A and Cubitt R. 2007 Competitive swelling and de-swelling of this polystyrene films by toluene *Physica Status Solidii - RRL* **1** 68-70

[10] Heinrich F, Ng T, Vanderah D, Prabhanshu S, Mihailescu M and Losche M 2009 A New Lipid Anchor for Sparsely Tethered Bilayer Lipid Membranes *Langmuir* **25** 4219-4229