Journal of Physics: Conference Series

PAPER • **OPEN ACCESS**

A McStas simulation of the incident neutron beam on the VESUVIO spectrometer

To cite this article: A Di Giulio *et al* 2018 *J. Phys.: Conf. Ser.* **1055** 012014

IOP Conf. Series: Journal of Physics: Conf. Series **1055** (2018) 012014 doi:10.1088/1742-6596/1055/1/012014

A McStas simulation of the incident neutron beam on the VESUVIO spectrometer

A Di Giulio[1], M Zanetti[2], G Romanelli[3], M Krzystyniak[3,4], R Senesi[1,5,6] and F Fernandez-Alonso[3,7]

[1]Università degli Studi di Roma "Tor Vergata", Department of Physics and NAST Centre, Via della Ricerca Scientifica 1, Roma, 00133 Italy

[2]CNR, Department of Physical Sciences and Technologies of Matter, Piazzale Aldo Moro 7, 00185 Rome, Italy

[3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, UK

[4]School of Science and Technology, Nottingham Trent University, Clifton Campus, Nottingham NG11 8NS, UK

[5]Centro Fermi - Museo Storico della Fisica e Centro Studi e Ricerche "Enrico Fermi", Piazza del Viminale 1, Rome 00184, Italy

[6]CNR-IPCF Sezione di Messina, Viale Ferdinando Stagno d'Alcontres 37, Messina 98158, Italy

[7]Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

E-mail: `alexdigiulio@gmail.com`

Abstract. We present a Monte Carlo simulation of the incident neutron beam on the VESUVIO spectrometer at the ISIS Facility using the McStas code. As VESUVIO allows for concurrent measurements of neutron diffraction, neutron transmission, and deep inelastic neutron scattering, both incident and transmitted beams are characterized by a broad energy range, spanning over several orders of magnitude from fractions of meV to tens of keV. A transport simulation in the case of the VESUVIO spectrometer is a challenging task, for the McStas code has been traditionally applied to cold and thermal neutrons, and never used in the modelling of electron-volt neutron spectrometers, to the best of our knowledge. In this simulation study, we discuss the modelling of the collimation stages along the primary flight path so as to reproduce the absolute intensity of the incident neutron beam and its shape, both recently characterized experimentally. Finally, we show some preliminary results employing incoherent scattering samples so as to compare the epithermal component of the simulated backscattering spectra to experimental results from Pb.

1. Introduction

The design of new neutron instruments and the upgrade of existing facilities strongly depend upon simulation codes for neutron transport [1, 2]. A quick development of available software has enabled higher simulation speed and an increase of tools and features. One of the most used pieces of software in neutron-scattering-instrument simulations is the McStas code [3]. The package is based upon a special meta-language designed for Monte-Carlo ray-tracing calculations, and includes a library of highly-adaptable "components", with geometrical and physical properties that can be adjusted to the instrument design.

The development of these tools was supported with validation with experiments, however, only on a restricted dataset based on the most common kind of instruments. In many cases,

IOP Conf. Series: Journal of Physics: Conf. Series **1055** (2018) 012014 doi:10.1088/1742-6596/1055/1/012014

neutron instruments are designed so as to operate in a narrow range of energies, as for example diffractometers using cold neutrons and traditional spectrometers using thermal neutrons. As the operational energies of the instrument are fixed, the modelling of the incident and scattered neutron spectra can be verified over limited energy ranges, where reliable experimental data from the real instrument can be provided. In this scenario, the VESUVIO spectrometer [4, 5] at the ISIS pulsed neutron and muon source [6], represents a challenging instrument to be modelled. Owing to the absence of permanent energy filters on both the primary and the secondary paths, VESUVIO allows for concurrent measurements over a broad energy range from the fraction of meV to tens of keV. In recent years, VESUVIO has been referred to as an *epithermal and thermal neutron analysis station* [7, 8], as the same sample can be investigated using deep inelastic neutron scattering [9, 10], neutron diffraction [11, 12], neutron transmission [13, 14], and gamma dopplerimetry [8, 15].

In this article, we present some preliminary comparisons of the simulated incident neutron spectrum and beam profile against recent experimental characterisations [5]. Moreover, we show simulated backscattering time-of-flight spectra including both coherent and incoherent scattering from Pb. The development of McStas components able to reproduce VESUVIO spectra over a broad energy range is the first step in order to successfully simulate deep inelastic neutron scattering spectra within McStas.

2. McStas Model

Monte-Carlo calculations have been performed using McStas 2.4.1 [16]. Simulations were run on a local computer with Windows 10 operating system, as well as on the SCARF cluster [17]. The VESUVIO spectrometer, for which a detailed description can be found in Reference [5], was simplified in McStas with a moderator acting as the neutron source, a series of collimation slits along the incident neutron path, a sample at about 11 m from the moderator, and a monitor representing a ^{6}Li-doped scintillating detector in backscattering, as schematically showed in Figure 1. In particular,

- The moderator component used was Commodus_I [18] (the most recent version of viewModISIS [19]), in order to take into consideration the recent upgrade of the water moderator serving the VESUVIO instrument at the ISIS Target Station 1 [5]. This component can simulate the emission of neutrons from the moderator face with a proton current of $1\mu A$.
- The set of B_4C collimation slits in the range of distances 1.71 m to 9.66 m from the moderator were modelled by ideal "Slit" elements placed at the positions 1.71, 8.46 and 9.66 m. In particular, as the collimation stages are octagonal in transverse cross section, two square slits titled by 45 degrees with respect to each other were used.
- Images of the beam shape and intensity were obtained using virtual Position Sensitive Detector (PSD) components and virtual monitors "PSD_monitor" before and after the first slit, and at the sample position.
- A "Filter-gen" component at the sample position was used to take into account discrepancies between the simulated and experimental beam profiles prior to the scattering from the sample. The Filter_gen component reads a table generated from the left setup in figure 1, and corrects it to match the experimental one. The corrected flux is then back-traced to the last slit position and used to illuminate the sample. The table is an ASCII file where in the first column are listed the energy values and in the second column are reported correcting factors corresponding to the ratio of experimental-to-simulated intensities, so as to correct for the discrepancies in the two intensities.
- The components used to reproduce the backscattering data from a Pb sample were "PowderN" [20] and "Isotropic_Sqw" [21].

- The simulated spectra corresponding to a backscattering detector were recorded using a "Monitor_nD" component, and the count rate was corrected by the known efficiency of ^{6}Li-detector efficiency $\eta(E)$ according to

$$\eta(E) = 1 - e^{-n\sigma(E)d}. \tag{1}$$

where n is the atom density, $\sigma(E)$ cross section and d detector thickness.

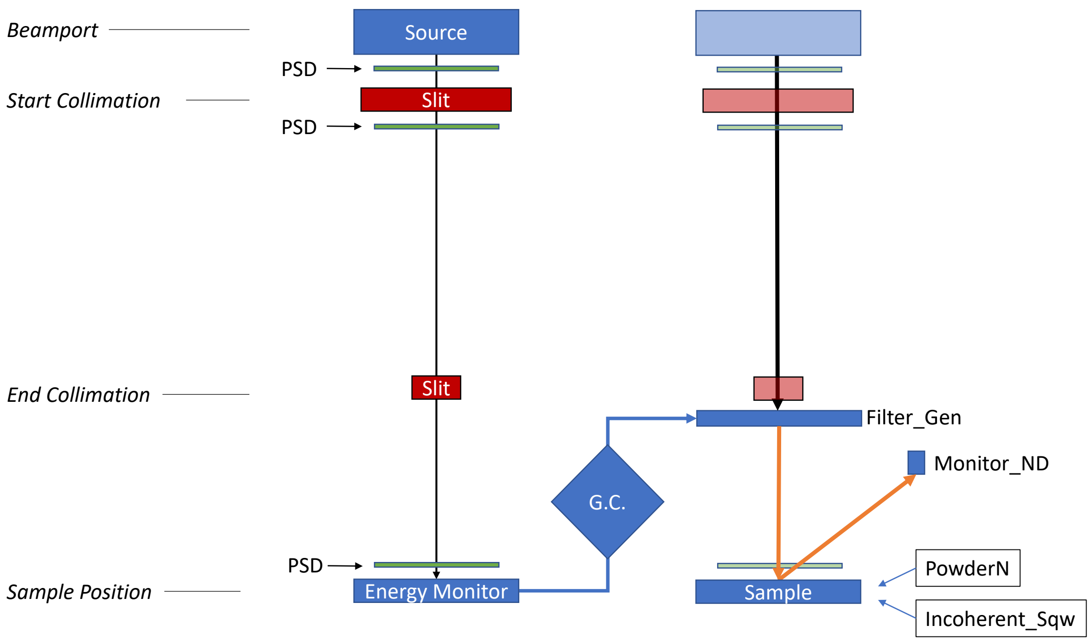

Figure 1. Simulation setup for collimation analysis (left) and backscattering analysis (right) after the inclusion of the "generating correction" (GC) component, "Filter_Gen".

3. Results and Discussion

Inspection of Figure 2 shows how the collimation stages modify the shape of the beam from a large square of about 8 cm side to a circle of diameter about 4 cm. The sole reduction of the size of the beam corresponds to a decrease of about one order of magnitude in the beam intensity at the sample position compared to that before the collimation. Indeed, the ratio of simulated beam fluxes at the two positions is found constant, with no visible dependence upon the incident neutron energy. Moreover, the original beam, homogeneous in the (x, y) plane transverse to the sample-moderator direction, is modified into a Gaussian-like profile. The file representing the brightness of the upstream water moderator was provided by the ISIS Neutronics Group and was created using current MCNP-X model of ISIS Target Station 1 [2].

The simulated results for the energy spectrum and the beam profile of incident neutrons at the sample position were compared with recent experimental measurements [5]. As the result from the simulation are expressed for unit proton current, the simulated spectra were multiplied by the actual proton current ca. 155 μA to TS1 during the measurement. The experiment was performed with the detector and about 1.5 m of the beamline in air, causing an attenuation of the neutron beam of about 0.895 with respect to standard measurement in vacuum. Moreover, the neutron beam needs to cross about 1.5 cm of Al windows between the moderator and the

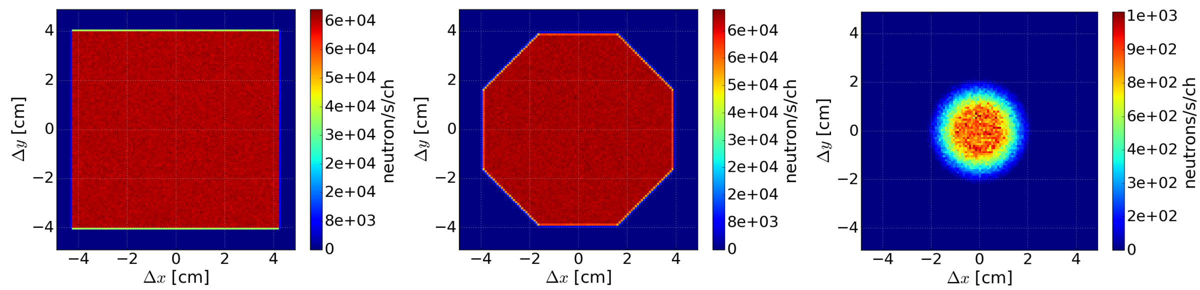

Figure 2. Transverse shape of the neutron beam before (left) and after (center) the beam port slit. (right) Shape for the neutron beam at sample position. The PSDs consist on a 120x120 pixel square matrix with 10 cm side length.

detector, therefore requiring an additional attenuation factor of about 0.855. Figure 3 shows how the present model gives an absolute intensity of the neutron beam between 1.5 and 3 times larger than the experimental data [5]. The agreement between experiment and simulation improves as the incident neutron energy approaches the epithermal region. Similar discrepancies have been previously discussed in Ref[22] about the modelling of the TOSCA spectrometer, where a ratio of simulated-to-experimental intensities ca. 1.77 was reported between 0.28 $\AA$ and 4.65 $\AA$, that favourably compares to the factor 2.39 in our case and in the same energy window.

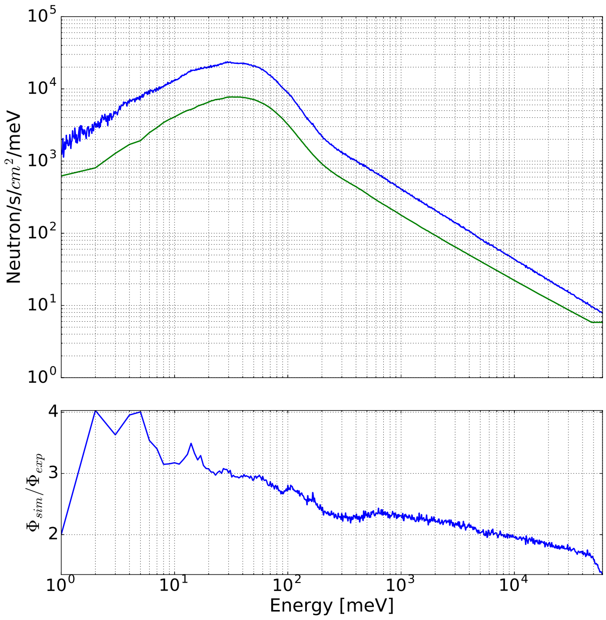

Figure 3. Simulated (blue) and experimental (green) fluxes at the sample position, and the simulated-to-experimental ratio in the bottom panel.

In particular, the flux in the epithermal region is expected to behave as $\propto E^{\alpha-1}$ for real moderators with α leakage exponent. By fitting this model to the experimental and simulated data, we obtained $\alpha = 0.04$ and $\alpha = 0.08$ for simulation and experiment, respectively. Such a small discrepancy could be related to the uncertainties present in the MCNP model which the table of emission TS1_S02_Vesuvio.mcstas that describes the moderator in McStas is based on. It is interesting to notice how, despite the discrepancy in the absolute value of the flux intensity, the simulated shape of the beam compares very favourably to the experimental results. The slightly wider experimental profile, shown in Figure 4, can be partially explained by the broadening due to the spatial resolution component from the nGEM detector used in Ref. [5].

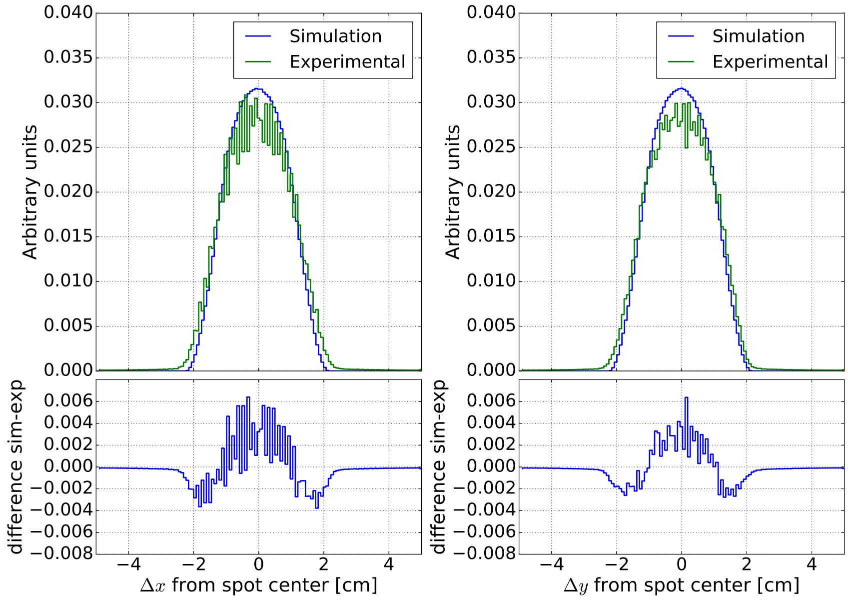

Figure 4. Simulated (blue) and experimental (green) along the two directions in the transverse plane, as well as their difference in the bottom panel. The experimental beam profiles from Ref. [5] have been shifted in order to share the same axis as in the simulation. Data is normalized to unit area.

Finally, the simulation of the backscattering from a 2-mm-thick lead foil was attempted, to be compared to the standard sample available on VESUVIO. Backscattering detectors on the instrument have distances from the sample between 0.45 m and 0.70 m, dimensions of $4\times2\times0.6$ cm^3, and they cover a range of scattering angles between 130 degrees and 163 degrees. Comparisons were drawn with the detector S44 at the Cartesian coordinates $(x, y, z) = (-0.158 \text{ m}, -0.048 \text{ m}, 0.460 \text{ m})$ [24], with the origin at the sample position, the direction z along the incident neutron beam pointing from the sample to the moderator, and the directions (x, y) in the transverse plane. A table with positions of the detectors is available within the MANTID software [25, 26, 27]. In order to properly compare the spectra from the simulation and the experiment, a series of normalisations and corrections were applied. First, the output of the McStas simulation expressed as a count rate in neutrons per second was converted into neutrons per microsecond, generally provided within MANTID. Then, the simulation spectra were multiplied by detector efficiency described in Equation 1. Simulation results generated for a proton beam current of 1 μA were normalised to the nominal current of ca. 160 μA in TS1, and finally multiplied by the duration of the measurements expressed in seconds. In order to reproduce the experimental time-of-flight spectra, we used both a "PowderN" virtual sample, and an "Incoherent_SQW" virtual sample. The former component uses the "Pb.laz" file where the scattering properties of the sample are stored, including the information about Bragg peaks. Additionally, the incoherent cross section was manually set to 11.118 barn [28]. In the case of the "Incoherent_SQW" component, a table was generated including the scattering law as predicted in the framework of the impulse approximation [29]. Figure 5 shows the comparison between simulation and experimental data in the case of detector S44, after the correction by the "Filter_gen" component. The shape and intensity of the spectra in the energy region of epithermal neutrons, for time-of-flight values lower than 2000 μs, are in satisfactorily agreement between the experiment and the simulation. Moreover, in the case of cold and thermal neutrons, the position of the Bragg peaks is very well reproduced by the simulation. Discrepancies in the intensity of the Bragg peaks, in particular the excess intensity in the case of the simulated peak, is completely ascribed to the fact that the actual sample was a foil rather than a powder, and lacking of the correction by the Debye-Waller factor in the simulation.

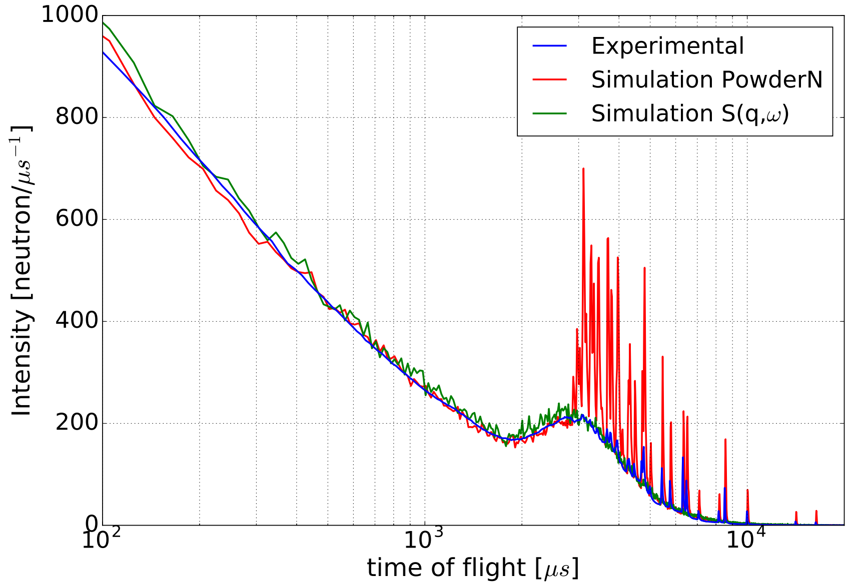

Figure 5. Raw experimental data (blue) for detector S44 and simulation results with PowderN component (green) and custom S(q,ω) from Pb (red). Data are normalized to $1\mu Ah$

4. Outlook and Conclusions

We presented preliminary results of the modelling VESUVIO spectrometer using McStas. Due to the geometry of the instrument, a broad-range white neutron beam flows in both the primary and secondary paths, making the modelling of VESUVIO challenging with respect to other instruments using cold and thermal neutrons. We have shown how the incident neutron beam intensity and shape are overall satisfactorily reproduced by the simulation, and that the backscattering time-of-flight data can be reproduced for cold-to-epithermal neutron energies. Having assessed the capabilities of McStas to cope with the broad energy band of VESUVIO, this work paves the way for the simulation of electron-Volt spectrometers and deep-inelastic-neutron-scattering virtual-experiments.

Acknowledgement

This work was partially supported within the CNR-STFC Agreement (2014-2020) concerning collaboration in scientific research at the ISIS pulsed neutron and muon source. The authors gratefully acknowledge the UK Science & Technology Facilities Council for financial support and access to beam time at the ISIS Facility. Computing resources were provided by the STFC Scientific Computing Department's SCARF cluster. Finally, we thank Dr G Škoro for useful and constructive discussions.

References

[1] Pinna, Roberto S, RudiÄĞ, Svemir, Parker, Stewart F, Gorini, Giuseppe and Fernandez-Alonso, Felix 2015 *EPJ Web of Conferences* **83** 03013 URL `https://doi.org/10.1051/epjconf/20158303013`

[2] Škoro G, Lilley S and Bewley R 2017 *Physica B: Condensed Matter* URL `https://doi.org/10.1016/j.physb.2017.12.060`

[3] Lefmann K and Nielsen K 1999 *Neutron News* **10** 20–23

[4] Last accessed on September 2017 Vesuvio URL `http://www.isis.stfc.ac.uk/Pages/VESUVIO.aspx`

[5] Romanelli G, Krzystyniak M, Senesi R, Raspino D, Boxall J, Pooley D, Moorby S, Schooneveld E, Rhodes N J, Andreani C and Fernandez-Alonso F 2017 *Measurement Science and Technology* **28** 095501 URL `http://stacks.iop.org/0957-0233/28/i=9/a=095501`

[6] Last accessed on November 2017 Iris webpage URL `http://www.isis.stfc.ac.uk/Pages/IRIS.aspx`

[7] Andreani C, Krzystyniak M, Romanelli G, Senesi R and Fernandez-Alonso F 2017 *Advances in Physics* **66** 1–73 URL `http://dx.doi.org/10.1080/00018732.2017.1317963`

[8] Krzystyniak M and *et al* in press *Journal of Physics Conference Series*

[9] Romanelli G, Liscio A, Senesi R, Zamboni R, Treossi E, Liscio F, Giambastiani G, Palermo V, Fernandez-Alonso F and Andreani C 2016 *Carbon* **108** 199–203
[10] Syrykh G F, Stolyarov A A, Krzystyniak M, Romanelli G and Sadykov R A 2017 *JETP Letters* **105** 591–594 URL https://doi.org/10.1134/S0021364017090041
[11] Andreani C, Romanelli G and Senesi R 2016 *The Journal of Physical Chemistry Letters* **7** 2216–2220
[12] Krzystyniak M, Druzbicki K, Romanelli G, Gutmann M J, Rudic S, Imberti S and Fernandez-Alonso F 2017 *Physical Chemistry Chemical Physics* **19**(13) 9064–9074 URL http://dx.doi.org/10.1039/C7CP00997F
[13] Rodríguez Palomino L A, Dawidowski J, Márquez Damián J I, Cuello G J, Romanelli G and Krzystyniak M 2017 *Nuclear Instruments and Methods in Physics Research Section A* **870** 84 – 89 ISSN 0168-9002 URL http://www.sciencedirect.com/science/article/pii/S0168900217307696
[14] Romanelli G, Rudic S, Zanetti M, Andreani C, Fernandex-Alonso F, Gorini G, Krzystyniak M and Skoro G 2018 *Nuclear Instruments and Methods in Physics Research Section A* **in press**
[15] G Romanelli *et al* in press *Journal of Physics Conference Series*
[16] Last accessed on February 2018 Mcstas homepage URL http://mcstas.org/
[17] Last accessed on February 2018 Scarf homepage URL http://www.scarf.rl.ac.uk/
[18] Last accessed on April 2018 URL https://isisneutronmuon.github.io/mcstas/How-to-Use-the-ISIS-moderator-component
[19] Ansell S S G 2015 The viewmodisis component, mcstas simulation package (accessed on the 11 january 2018). URL http://www.mcstas.org/download/components/contrib/ViewModISIS.pure.html
[20] Willendrup P, Filges U, Keller L, Farhi E and Lefmann K 2006 *Physica B: Condensed Matter* **385** 1032–1034
[21] Farhi E, Hugouvieux V, Johnson M and Kob W 2009 *Journal of Computational Physics* **228** 5251–5261
[22] Pinna R S, Rudić S, Capstick M J, McPhail D J, Pooley D E, Howells G D, Gorini G and Fernandez-Alonso F 2017 *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **870** 79–83
[23] Bewley R I Ansell S S G 2016 *Proc. of the 21st Meeting of the International Collaboration on Advanced Neutron Sources ICANS XXI*
[24] Mayers J and Adams M A 2011 *Nuclear Instruments and Methods in Physics Research Section A* **625** 47–56
[25] Arnold O, Bilheux J, Borreguero J, Buts A, Campbell S, Chapon L, Doucet M, Draper N, Leal R F, Gigg M, Lynch V, Markvardsen A, Mikkelson D, Mikkelson R, Miller R, Palmen K, Parker P, Passos G, Perring T, Peterson P, Ren S, Reuter M, Savici A, Taylor J, Taylor R, Tolchenov R, Zhou W and Zikovsky J 2014 *Nuclear Instruments and Methods in Physics Research Section A* **764** 156 – 166 ISSN 0168-9002 URL http://www.sciencedirect.com/science/article/pii/S0168900214008729
[26] Jackson S, Krzystyniak M, Seel A G, Gigg M, Richards S E and Fernandez-Alonso F 2014 *Journal of Physics: Conference Series* **571** 012009 URL http://stacks.iop.org/1742-6596/571/i=1/a=012009
[27] Last accessed on September 2017 Mantid website URL http://download.mantidproject.org/
[28] Sears V F 1992 *Neutron News* **3** 26–37 (*Preprint* http://dx.doi.org/10.1080/10448639208218770) URL http://dx.doi.org/10.1080/10448639208218770
[29] Ivanov G K and Sayasov Y S 1964 *Soviet Physics Doklady* **9** 171