TAS Workshop

Report of Contributions

https://indico.frm2.tum.de/e/tripres

Contribution ID: **0** Type: **not specified**

Comparison of different analytical codes, visualization

Monday, 3 April 2017 13:10 (40 minutes)

The triple-axis resolution function is generally approximated as a four-dimensional ellipsoid in three momentum (Q) and the energy (E) dimensions. The ellipsoid denotes the probability of finding neutrons at specific Q and E coordinates in reciprocal space. In this talk, we present the formalism behind the calculation and visualisation of the resolution function in a general mathematical way. We furthermore discuss the classical methods by Cooper/Nathans [1] and Popovici [2] and compare their results to the new method by Eckold and Sobolev [3]. The latter method will also be discussed in further detail in a following talk of this workshop.

[1] M. J. Cooper and R. Nathans, Acta Crystallogr. 23, pp. 357-367 (1967).
[2] M. Popovici, Acta Crystallogr. Sect. A, 31, pp. 507-513 (1975).
[3] G. Eckold and O. Sobolev, Nucl. Instr. Meth. Phys. Res. A 752, pp. 54-64 (2014).

Presenter: Dr WEBER, Tobias (E21)

Session Classification: Resolution in general

Contribution ID: **1** Type: **not specified**

Resolution and multiplexing

Monday, 3 April 2017 14:30 (40 minutes)

An analytical approach for the calculation of the 4D-resolution function of a three-axes spectrometer is presented that takes into account all essential features of state-of-the art instruments. In particular, the performance of focusing techniques in direct and reciprocal space is considered in detail. Complementary to existing numerical simulation methods, the analytical treatment provides neutron users with almost instantaneous information about resolution effects of ongoing experiments. Moreover, it can be used as an efficient tool for the quantitative interpretation of experimental results. Several examples are shown which demonstrate the performance and the accuracy of the present approach.
The analytical algorithm is also incorporated in the software system MAX1 which allows the efficient use of the unique multi-analyser system at the thermal three-axes spectrometer PUMA@FRM II. It assists the user with the selection of the most appropriate spectrometerconfiguration for a particular experimental problem thereby avoiding to deal with details of the sophisticated mechanical set-up.

Presenter: Prof. ECKOLD, Götz (Georg-August University of Göttingen)

Session Classification: Resolution in general

Contribution ID: **2** Type: **not specified**

Using TAS resolution calculations to prepare experiments

Monday, 3 April 2017 13:50 (40 minutes)

The flexibility of the TAS instrument together with the selective nature of the corresponding experiments (as opposed to a global data collection by the TOF methods) calls for a certain refinement of the experiment strategy prior to the start of the measurements. In particular for the less experienced users, to assess the advantages and disadvatages of diverse optional instrument setups and to choose the right one may be a formidable task. Software permitting to visualize the diverse possible configurations in the real and reciprocal space (eg. vTAS) and to calculate the corresponding resolution (eg. Restrax) can provide help to deal with this task.

Presenter: Dr KULDA, Jiri (Institut Laue-Langevin)

Session Classification: Resolution in general

Contribution ID: **3** Type: **not specified**

Triple axis Tools (TASTools)

Contribution ID: **4** Type: **not specified**

RESTRAX

Monday, 3 April 2017 16:00 (45 minutes)

The software package RESTRAX includes both a high-speed analytical (Gaussian) convolution algorithm and a Monte Carlo ray-tracing code providing enhanced accuracy in description of most of the spectrometer components. The program is built up for a three-axis spectrometer layout, comprising a complete set of usual neutron optical devices. Their representation in the ray-tracing part includes all the present knowledge available both with respect to the laws of neutron optics and to the design parameters of the instrument. The results of the simmulation can be used to optimize the experimental setup prior to data acquisition as well as to evaluate the measured data by profile fitting of a a 4D convolution of the simmulated TAS resolution function with an S(Q,w) model.

Presenter: Dr KULDA, Jiri (Institut Laue-Langevin)

Session Classification: Software for resolution convolution

Contribution ID: **5** Type: **not specified**

Takin

Monday, 3 April 2017 16:45 (45 minutes)

We present the free and open-source software Takin [1], which aims to ease many of the tasks encountered during the planning phase and in the conduction of experiments performed at neutron triple-axis spectrometers. The software features an easy-to-use graphical user interface for live visualizations of reciprocal space, the corresponding instrument configuration, and the resolution function. Furthermore, resolution convolution simulations can be performed on-the-fly to assess the best scattering positions.

The software is currently in regular use at the MLZ in Garching, Germany, and – due to the program's modular nature – can be easily extended to work with many other instruments, network instrument control systems and data formats. Takin includes an implementation of the novel Eckold-Sobolev [2] approach to the triple-axis resolution function. This new method gives more accurate results for instrument configurations using monochromator or analyser focusing than the standard Popovici [3] method.

[1] T. Weber, R. Georgii, and P. Böni, SoftwareX 5, pp. 121-126 (2016).
[2] G. Eckold and O. Sobolev, Nucl. Instr. Meth. Phys. Res. A 752, pp. 54-64 (2014).
[3] M. Popovici, Acta Crystallogr. Sect. A, 31, pp. 507-513 (1975).

Presenter: WEBER, Tobias

Session Classification: Software for resolution convolution

Contribution ID: **6** Type: **not specified**

UFit

Monday, 3 April 2017 17:30 (30 minutes)

For neutron scattering experiments, two kinds of data analysis tool are needed, which are often implemented separately: quick and easy evaluation of scans during and immediately after the experiment, and in-depth processing for fitting arbitrary models to the data. Ufit is a tool tailored to the evaluation of neutron scan data that tries to provide the user with both. Here we will introduce its scripting interface using the full power of Python, as well as its graphical user interface that provides much of the same functionality as an optional frontend.

Presenter: BRANDL, Georg

Session Classification: Software for resolution convolution

Contribution ID: **7** Type: **not specified**

Data evaluation with python

Tuesday, 4 April 2017 09:00 (1h 30m)

We will use ufit as a library to read, visualize, treat and fit measured data.

Presenters: BRANDL, Georg; CERMAK, Petr; WEBER, Tobias

Session Classification: Hands-on Session

Contribution ID: **8** Type: **not specified**

Convolution and fitting –

Tuesday, 4 April 2017 11:00 (1h 30m)

We will use takin to convolute our model with instrument resolution and fit the experimental data.

Presenters: BRANDL, Georg; CERMAK, Petr (MLZ); WEBER, Tobias

Session Classification: Hands-on Session

Contribution ID: **9** Type: **not specified**

Spurions in TAS: how to predict, avoid

Tuesday, 4 April 2017 14:00 (20 minutes)

The proper interpretation of spurious signal (spurions) in the measured TAS data is a key aspect of every experiment. We will go through several possible types of spurions: Bragg peaks from Aluminium or Copper, Harmonic wavelengths in ki and kf, Currat-Axe spurions, Bragg tail contamination. We will show how to visualize and avoid them.

Presenter: SCHNEIDEWIND, Astrid

Session Classification: Good practices in TAS

Contribution ID: **10** Type: **not specified**

Good practices in TAS

Tuesday, 4 April 2017 14:20 (20 minutes)

This lecture will focus on several aspects of the TAS spectroscopy. In the first part we will focus on the ways how to enhance resolution and reduce background of the instrument. We will also show some benchmarking results of the top leading spectrometers.

Presenter: CERMAK, Petr

Session Classification: Good practices in TAS

Contribution ID: **12** Type: **not specified**

Discussion about future developments

Tuesday, 4 April 2017 15:30 (30 minutes)

Session Classification: Good practices in TAS

Contribution ID: **13** Type: **not specified**

Data publishing

Tuesday, 4 April 2017 14:40 (20 minutes)

Last lecture of the workshop will go little bit beyond the spectroscopy. In the academic community there is an increasing pressure on researchers to share, archive and cite measured data. Also more and more funding agencies is mandating data publication. This approach is still new to a lot of scientists, publishing data sets can be problematic and time consuming. Some large scale facilities started to offer data publication automatically [1,2] and others will follow. Using modern tools as iPython notebooks or data sharing services like figshare [3] will help scientists to automatize process of data publishing and increase the impact of their research.
[1] https://www.ill.eu/users/ill-data-policy/
[2] https://icatproject.org/collaboration/facilities/
[3] https://figshare.com/

Presenter: CERMAK, Petr (MLZ)

Session Classification: Good practices in TAS