DrSPINE: Data Reduction for SPIN Echo experiments

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Abstract. High resolution neutron spin echo (NSE) spectroscopy is one of the most powerful techniques to study the dynamics of soft matter. For NSE spectroscopy at a pulsed source, the data reduction and analysis present new challenges and opportunities as compared to a steady (reactor) source experiment. We present a data reduction framework which extracts information of all time channels and detector images, grouping the results into $S(q,t)$ for a series of $q$ and $t$, also across different instrument settings (different $q$). This strategy helps to get the most out of an experiment (a set of scans at different diffraction angles) and also provides appropriate reporting on the quality of the evaluation. The same software is also capable of dealing with reactor source data, where no time-of-flight information is present.

INTRODUCTION

The highest energy resolution in neutron spectroscopy can be achieved with neutron spin echo spectrometers\cite{1}. It has been a powerful tool over the last decades to study thermal fluctuations in soft matter, such as for example polymer chain dynamics or membrane fluctuations in microemulsions and vesicles\cite{2-4}. An easy and reliable data reduction is key to an efficient usage of neutron spin echo spectrometers. The strategy for data reduction for the two spectrometers SNS-NSE at a pulsed (spallation) source\cite{5} and J-NSE at a steady (reactor) source\cite{6} has always been to apply a mostly automated algorithm with as little user interaction and necessary user decisions as possible. Up to now the data have been processed serially for each scattering angle, resulting in a $S(q,t)/S(q,0)$ vs $t$ curve for each angle setting (corresponding to a $q$-setting in reciprocal space for a single wavelength experiment at the reactor). For pulsed sources, the additional complication is to treat the time of flight data in the much broader wavelength frame properly, with a variation of $q$ and $t$ at the same time. For the evaluation of a single setting the strategy adapted from the reactor source experiments was to "flatten" the data structure by summing up a range of time frames and treating it in the same way as for a reactor based instrument. The goal of the new software DrSPINE, first introduced in Ref.\cite{7}, is provide a robust data treatment framework, where data from all instrument settings of one experiment (one sample, one temperature, etc.) are treated simultaneously and sufficient data evaluation reporting is automatically generated. Here we update on the progress of the DrSPINE software package and its advantages for both, reactor based (J-NSE-type) and spallation source (SNS-NSE-type) instruments.

SOFTWARE DESIGN

The DrSPINE software is designed for an easy workflow from experimental time of flight spin echo data to the intermediate scattering function, making use of all information available in the data. The existing software limited the user to select only a certain group of time-of-flight channels and discarding some of the available and useful time
channels, since grouping across time frames was difficult. In DrSPINE fitting is done for each setting for some regions in $dq_x$ and $dq_y$ (the detector plane) and $dt$ (time-of-flight channels) for all scattering angles of an experiment. Afterwards, it is possible to decide on the number of $q$-values and Fourier times and group all available data accordingly. Figure 1 shows the typical $q$ and time space available at the SNS-NSE for a standard soft matter experiment.

**FIGURE 1.** Typical available $q$-t-space for a series of scattering angle (5 different scattering angles from bottom to top).

The evaluation takes care of the symmetry phase determination, which works very reliably without any user interaction in order to obtain reliable intermediate scattering functions. The symmetry phase for the SNS-NSE data is obtained from the reference sample data by summing up all time channels and reducing therefore the width of the envelope of the echo group thus making the fit very reliable. At the J-NSE the selector provides a fixed width of the envelope due to its wavelength spread $\lambda_{max}/\lambda = 10\%$. Figure 2 shows the fitting procedure for the more difficult case of an incoherent scattering signal from the SNS-NSE, with a zoom to the symmetry point and an estimate of the uncertainty of the phase determination (the green vertical lines in both plots).
FIGURE 2. Phase fitting of the echo curve of an incoherent scatterer. The symmetry phase is determined by taking a broad wavelength band for the SNS-NSE. Top: whole echo curve fitted. Bottom: zoom into the region of the symmetry point.

RESULTS
First data evaluation has been done with reference samples from SNS-NSE and J-NSE. A typical work flow of the data evaluation routine is depicted in Fig. 3. The console based user interface allows to pack the data evaluation into a macro file (Fig. 3). It may be executed by invoking the program and executing the macro from its prompt or by calling the software with the macro as an parameter (e.g. $drspine --x macroname$), which produces a text data file with the intermediate scattering function for one or several desired q-values and Fourier times binning schemes (within typically 1 to 3 minutes on a standard laptop computer). It contains human readable tables of the normalized intermediate scattering functions, which also can be treated with any further evaluation tool or the Python scripts provided for direct plotting from DrSPINE. As shown in Fig. 3, the data collection can be repeated with different binning leading just to a number of output files which allow the user easily to choose the best binning for the present purpose without re-evaluation. For any "typical" experiment a macro just requires to specify an arbitrary sequence of all run numbers pertaining to the experiment with the respective tags "resolution", "background", "sample".
FIGURE 3.
Typical macro of the DrSPINE program which reads in a series of scattering angle settings for sample, reference and background measurement and evaluates the data summing up all q,τ-pairs with desired steps in q and τ.

```
makro
! example macro for DrSPINE

! ===== set paths
datapath ./nse_data
savepath ./drspine

! ===== set binning
bins pix nbins 8
bins tof custom 2 13 26 39

! ===== read data
read s7360.echo s7361.echo s7362.echo s7363.echo s7364.echo s7365.echo as resolution
read s7375.echo s7376.echo s7377.echo s7378.echo s7379.echo s7380.echo as sample
read s7396.echo s7397.echo s7398.echo s7399.echo s7394.echo s7395.echo as background

! ===== process
match all
fit all

! ===== output
histo tau nbins 20 min 0.002E-9 max 30E-9 log
histo q nbins 8 min 0.050E10 max 0.16E10
collect bgr 0 tfac 1/1.043
report start
report sqrtplot

histo tau nbins 10 min 0.002E-9 max 30E-9 log
histo q nbins 12 min 0.050E10 max 0.16E10
collect bgr 0 tfac 1/1.043
report sqrtplot

histo tau nbins 30 min 0.002E-9 max 60E-9 log
histo q nbins 4 min 0.050E10 max 0.16E10
collect bgr 0 tfac 1/1.043
report sqrtplot

report end
```

Background of buffer
CONCLUSION AND OUTLOOK

DrSPINE is now in a state where data from the SNS-NSE and J-NSE can be evaluated with a reliable fitting procedure for the symmetry phase determination and echo group and produces the intermediate scattering function using all available data of an experiment. It is a console based Fortran 2008 program with no external dependencies that can be installed on a user’s computer with any modern operating system. If LaTeX and/or Matplotlib/Python is installed further reporting and plotting functionality is immediately available. Reporting functions yield an immediate overview of the evaluation process and its outcome, which allows an easy detection of possible experimental problems or inconsistencies and the basic properties of the scattering function. The program code is documented and available via a git repository. Further development is ongoing to optimize the background subtraction procedures and to yield the scattering function in terms of S(Q,t) on an absolute scale in addition to the usual normalized S(Q,t)/S(Q) using the resolution runs also as intensity calibration.

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We routinely test the software on Debian Linux, Red Hat Enterprise Linux and Mac OSX.