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Neutron Sciences Directorate
Neutron Scattering Division

QUICK GUIDE FOR SNS-NSE REDUCTION SOFTWARE DRSPINE (DATA REDUCTION FOR SPIN ECHO)

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ABSTRACT

This is a general guide to quick access the most common commands for DrSpine (Data Reduction for Spin Echo) data reduction software of the SNS-NSE spectrometer. Over the length of the manuscript the symbol " **$** " represents the OS shell prompt, i.e., the beginning of a command line in a shell terminal, while the symbol "**-->**" represents the beginning of a command line in the DrSpine reduction software, after the activation of the reduction environment.

1. INTRODUCTION

Neutron Spin Echo spectrometer SNS-NSE operating at the Spallation Neutron Source, Oak Ridge National Laboratory is a high-resolution time-of-flight spectrometer particularly suitable for the investigation of slow dynamical processes[1]. The spectrometer is used to unravel molecular motions at the nanoscopic and mesoscopic scale for research in a variety of fields including soft-matter research, condensed matter physics, materials science, complex fluids, biophysics, and medical science. The Neutron Spin Echo instrument at SNS (SNS-NSE, Figure 1) is the first spectrometer of its class by design, the first spin-echo spectrometer situated at a pulsed neutron source and one of the best spectrometers in both resolution and dynamical range[2]. By employing time-of-flight techniques the spectrometer can use broad wavelength band of neutrons. With only a few instrumental settings, it can cover, in a quasi-continuous way, a large range of wavevector, *q*, and Fourier time, *tau*, space.

Figure 1. The Neutron Spin Echo spectrometer at SNS, SNS-NSE

Extracting all the information contained in the raw data and mapping them to a suitable physical space in the most efficient way presented a challenge to the existing software reduction programs. Therefore, a new dedicated software reduction program called DrSpine (Data Reduction for Spin Echo) was developed and published in the Journal of Applied Crystallography (2019)[3]. The algorithms employed in DrSpine allow extraction of the intermediate scattering function S (Q, tau). In addition, the software can also reduce the data from NSE spectrometers installed at a continuous source, like J-NSE Phoenix at FRMII, Garching, Germany. The reduction software is available to users via the SNS analysis cluster with a quick guide, extended manual [4] and help implemented in the program. The software source code can be also downloaded from its GitLab repository[5]. Users need to build and install the program locally, which can be accomplished by following the steps described in INSTALL.md file[5].

2. QUICK CONNECTION PROTOCOL

2.1(a) Log in to Neutron Sciences Remote Analysis Cluster via web browser

- in a browser navigate to: *https://analysis.sns.gov/*
- press Launch Session button
- use ORNL user credential details to login (XCAMS account)
- works on any operation software with any chosen web browser

Alternatively:

2.1(b) Log in to Neutron Sciences Remote Analysis Cluster via secure shell

- open a terminal in the user directory and type the following command:

```
$ ssh -Y analysis.sns.gov
```

- the system will prompt for user ID and password: use ORNL user credentials to login
- works on Linux and MAC-OS

2.2 NSE raw data (echoes) are uploaded and stored in the folder `/SNS/NSE/IPTS-NR`.

- **`IPTS-NR`.** represents the proposal number. No work should be done in this directory since every new data sync overwrites the contents of this folder
- this path will be used later in the data reading procedure

2.3 `/SNS/NSE/shared/` is a shared directory between user and Instrument Scientist

- a data reduction folder will be created in the shared directory and named with the appropriate IPTS number: **`ipts-<user-ipts>`**
- the Local Contact / Instrument Scientist will place the final data reduction and all the scripts and protocols needed for reduction in this directory

2.4 First time DrSpine users need to setup the DrSpine environment variables

- at the prompt type the following command (*this needs to be done before each new reduction*):

```
$ source /SNS/software/nse/etc/setup_nse.sh
```

- next type (*this will not be necessary on later reduction attempts*):

```
$ drspine_create_env.sh
```

- we recommend creating a local folder in the home user directory and transfer the reduction folder from shared directory, with all the scripts and protocols (paragraph 2.3), and work locally in the folder to avoid overwriting any previously reduced data. The **`ipts`** folder can be copied and later accessed by typing at the prompt the following commands (*to work it requires the DrSpine activation commands from above*):

```
$ nse_copy_ipts.sh <user-ipts>

$ cd ipts-<user-ipts>
```

- The DrSpine environment will stay active if the terminal window remains open. For a full list of commands with explanations, please see the extended DrSpine MANUAL[4] by typing at a terminal, after the activation of DrSpine environment, the command:

```
$ drspine_manual.sh
```

(Observation: if you are using PuTTY connection from a Windows OS machine you will need a X-server installed to allow graphical interface to Linux, see PuTTY User Manual: using X11 forwarding in ssh)

3. DATA REDUCTION MAJOR STEPS AND MOST USEFUL DRSPINE COMMANDS

3.1 Batch reduction using a template

Within the DrSpine environment the data reduction can be done using a compilation of commands in the form of a script or macro. To run a reduction macro, here named "**dr_macro_XYZ**", the user should type at the prompt:

```
$ drspine -x dr_macro_XYZ
```

Alternatively, the user can first start the reduction software by typing simply **drspine** at the shell prompt, followed by a second command that contains the name of the reduction macro (please observe the change in the prompt appearance that indicates the change from the shell to reduction environment prompt):

```
$ drspine
--> dr_macro_XYZ
```

A template example is provided at the end of the manuscript in APPENDIX A. The macro template will be provided to each user by the Instrument Scientist.

3.2 Step-by-step data reduction using DrSpine prompt commands

Within the DrSpine environment the data reduction can also be performed manually by typing individual commands at the prompt. In the following, the most important steps of the manual reduction process e.g., the most common DrSpine data reduction commands and additional explanations, are given. The individual reduction commands work only within the DrSpine environment after activation (*please follow previous point* 2.4)

- start DrSpine by opening a shell terminal and typing:

```
$ drspine
```

The above will start DrSpine and change your prompt to: **drspine -->**; you are now within the data reduction environment.

- set the initial data binning by typing at the DrSpine command prompt:

```
--> bins pix nbins 8
--> bins tof custom 4 10 16 23 30 38
```

In the first command above, the NSE signal is averaged over 8 detector pixels. In the second command, the NSE signal is averaged over time-of-flight, *tof*, acquired in 42-time channels spilt into several intervals, *i.e.*, *tof*4 *-to- tof*10; *tof*10 *-to- tof*16, etc. Channels from *tof*1-3 and *tof*38-42 are ignored due to bandwidth

contamination. This is just for reading data purposes. The software requires an initial *tof* binning of the data, but the user can re-bin later as needed.

- set the path to read the appropriate NSE data according to your IPTS number:

```
--> datapath /SNS/NSE/IPTS-NR.
```

- read the NSE echo files (raw data):

```
--> read sxxxx.echo sxxxx.echo sxxxx.echo as res                !8Å
--> read sxxxx.echo sxxxx.echo sxxxx.echo as sam tfac 0.92      !8Å
--> read sxxxx.echo sxxxx.echo sxxxx.echo as buf                !8Å
```

Here three (3) echo files are read in each line as an example and differentiated into resolution, sample, and buffer. The data are selected for wavelength 8Å. This is particularly important when buffer or background signal will be subtracted since transmission factor **`tfac`** is wavelength dependent. For all other cases is sufficient to specify the echo files and no particular order of the echoes is required. Here, **`tfac`** represents the transmission factor calculated by sample transmission divided by buffer transmission, usually < 1. The character "**`!`**" means *a comment will follow* and is not read by the software.

- process the NSE data by matching and fitting:

```
--> match all
--> fit all
```

DrSpine will match every wavelength and every scattering angle automatically, as well as different instrument modes (short and standard Fourier times). In most cases the automatic matching and fitting of the echoes (amplitude and phase) is sufficient. For additional, and more complex, matching and fitting commands please see the DrSpine MANUAL[4], ask the Instrument Scientist, or check the DrSpine HELP at the Drspine command prompt by typing:

```
--> help
```

- reduction output by automatic built-in histogram and collection:

```
--> set A 1E-10
--> set ns 1E-09
--> histo tau nbins 20 min 0.05*ns max 50*ns log
--> histo q   nbins 10 min 0.05/A max 0.2/A
--> collect
```

or

```
--> collect bgr 1 volfrac 0.9
```

Here, the user will specify the units of Angstrom and nanosecond since the native units are recorded as second (1ns = 1E-09 s), and meter (1Å = 1E-10 m). Users also specifies the numbers of Fourier times *tau* and the numbers of scattering vectors *q* desired to be collected, as well as the collection intervals for both. Basically, the user tells the program to split *tof* into a desired number of *q*'s each of them containing a desired number of *tau*'s. The collection of the data will be performed based on the acquired statistics. In the example above 20 *tau*'s between 0.05 ns (0.05E-09 s) and 50 ns (50E-09 s) are collected on a logarithmic scale for 10 *q*'s between 0.05Å^{-1} (0.05E-10 m) and 0.2Å^{-1} (0.2E-10 m). *q*'s and *tau*'s collection are done

automatically, with or without background subtraction and volume fraction weighing, as indicated by the **`collect`** command. **`bgr 1`** value activates the background subtraction. The default value is **`bgr 0`** which indicates that background subtraction will not be performed. Volume fraction represents the volume of the material of interest in a sample divided by the volume of the solute[6]. A histogram map is populated with all the *q*'s and *tau*'s collected values and the number of echoes contributing to each Fourier time, as shown in Figure 2. For detailed explanation on how the *tof* is sliced and grouped in intervals, and how the raw echoes are fitted and collected to contribute to each *q* and *tau* please consult our software reference article[3].

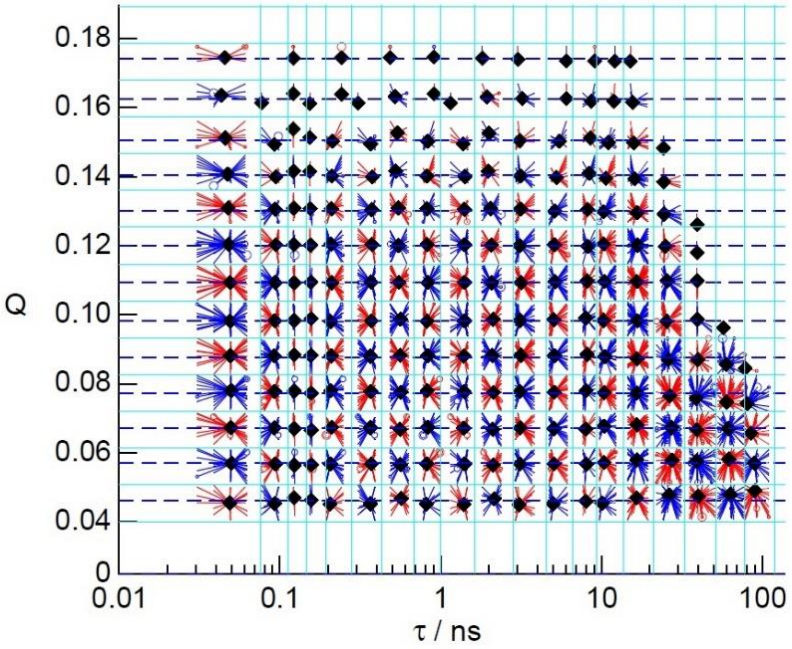


Figure 2. S (q, tau) histogram map: each line represents a *q* value, with the Fourier times *tau* represented by black diamonds. Each *tau* is obtained by the contribution of a different number of raw echoes (red and blue circles) as sliced by the *tof* grouping and collection.

As an alternative to the automatic built-in histogram and collection, the NSE users can, of-course histogram custom *tau*'s and custom *q*'s as desired, followed by the same collection protocol.

- reduction output by user customized mode**:**

```
--> histo tau custom 0.05*ns 0.1*ns 0.2*ns 0.4*ns … 50.0*ns
--> histo   q custom 0.045/A 0.055/A 0.065/A 0.075/A … 0.205/A
```

In this example the data collection is customized to provide the user requested values for *q* and *tau*. The results will be the average values withing each interval provided, *i.e.*, interval 0.045*/A* 0.055*/A* will provide the $q = 0.05 Å^{-1}$.

- name and save the reduced data:

User reduced data are saved temporarily in the file "**`last_sqt.dat`**". This file is overwritten by each new collection protocol. To save the data permanently under a desired title, at the DrSpine prompt type:

```
--> cp last_sqt.dat SampleXY_sqt.dat
```

The reduced data will be saved under the given "**SampleXY_sqt**" name and are also saved automatically in a file named "**reportXY.dtr**".

3.3 Generating a comprehensive report of the data reduction process

A reporting of the performed data reduction can be generated within the DrSpine environment. If the report comes out blank, containing no information, then reduction was problematic. Otherwise, a series of pdf reports will be created containing detailed information on the reduction and extensive graphics of all the echoes. In the following example of commands such a report is generated, and the S (q, tau) data are plotted and fitted by a stretched exponential with exponent 0.6 (for more functions to fit please see DrSpine HELP). The reduced data are saved automatically in file "**reportXY.dtr**" (this is a permanent file) and in the "**last_sqt.dat**" (this is a temporary file overwritten by any new collection protocol) as stated above.

```
--> report start dir
--> report details more
--> report sqtplot fix_beta 0.6
--> report end
```

3.4 Read, plot and fit output data, *i.e.*, S (q, tau) data from a file

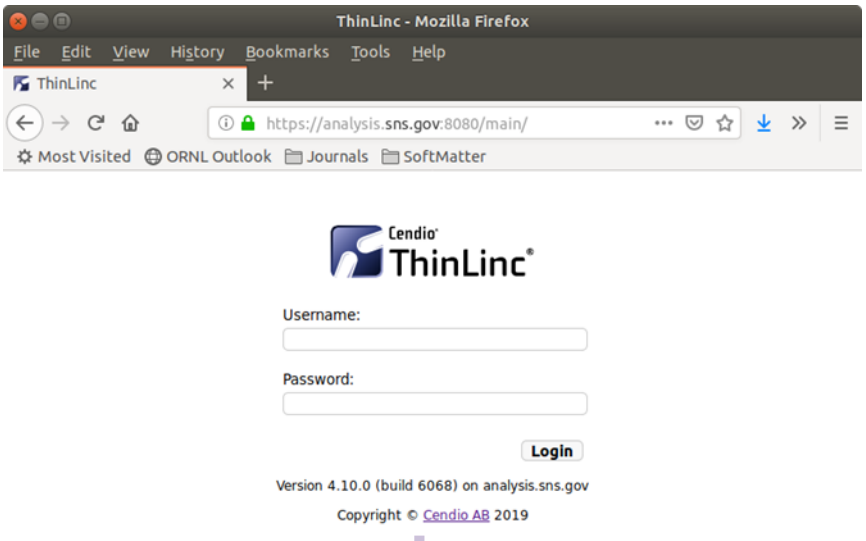
The NSE final reduced data, S(*q*, *tau*), are in ASCII format and can be easily accessed for further analysis by a variety of software (OriginPro, Igor, MATLAB, Python, IDL, Excel, etc.), as preferred by users. As an "*in house*" alternative, a python script has been developed to load, read, plot, and fit the reduced NSE data using the following command, directly from the shell terminal:

```
$ python ./stapler-DrSpine.py
```

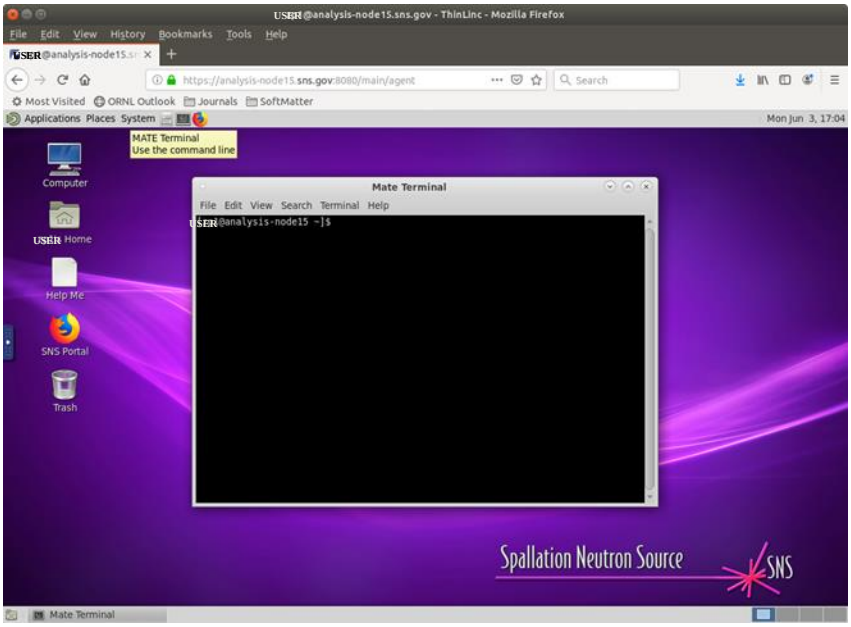
"**stapler-DrSpine.py**" is the name of the python script and needs to be modified accordingly with the correct data file names and the fitting function. The usage of the python script requires the activation of the DrSpine environment (see point 2.4) but works outside of the DrSpine, directly from the shell terminal. The package for visualization and analysis in the script uses Matplotlib for plotting and Scipy library function for fitting. The fitting routine includes the most commonly used model functions for analyzing NSE data from soft materials (KWW - Kohlrausch-Williams-Watts relaxation, ZG - Zilman-Granek relaxation, Diffusion, Power law, linear, exponential, cumulant fit …etc.). The usage of python and python script for the analysis of the data is entirely independent of the reduction software DrSpine and will not be detailed here.

4. VISUAL CONNECTION GUIDE

The ThinLinc web connection interface



Open a terminal window



Start by typing the commands at point 2.4 in the section Quick Connection Protocol

5. REFERENCES

1. sns-nse web page. https://neutrons.ornl.gov/nse.
2. Ohl, M. *et al.* The spin-echo spectrometer at the Spallation Neutron Source (SNS). *Nucl. Instruments Methods Phys. Res. Sect. A Accel. Spectrometers, Detect. Assoc. Equip.* **696**, 85–99 (2012).
3. Zolnierczuk, P. A. *et al.* Efficient data extraction from neutron time-of-flight spin-echo raw data. *J. Appl. Crystallogr.* **52**, 1022–1034 (2019).
4. DrSpine Manual. https://jugit.fz-juelich.de/nse/DRSPINE-MANUAL https://jugit.fz-juelich.de/nse/DRSPINE-MANUAL.
5. DrSpine hub. https://jugit.fz-juelich.de/nse/drspine.
6. https://en.wikipedia.org/wiki/Volume_fraction. https://en.wikipedia.org/wiki/Volume_fraction.

6. ACKNOWLEDGMENTS

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APPENDIX A. DATA REDUCTION MACRO TEMPLATE

APPENDIX A.

DATA REDUCTION MACRO TEMPLATE WITH COMMENTS

```
macro
clear all

c ==== set binning
bins pix nbins 8
bins tof custom 4 10 16 22 30 38
set bgr 1  !bgr value = 1/0 activates/deactivates background subtraction

c ==== set the paths toward the resolution, sample, and buffer raw data
datapath /SNS/NSE/IPTS-XXyyy

c ==== reading raw echoes protocol
! read resolution data
clear res
read s933x.echo s933x.echo as res            !8A
read s933x.echo            as res            !9A
read s933x.echo s933x.echo as res            !11A

! read sample data
clear sam
read s934x.echo s934x.echo as sam tfac 0.95  !8A with a transmission factor of 0.95
read s934x.echo            as sam tfac 0.94  !9A with a transmission factor of 0.94
read s934x.echo s934x.echo as sam tfac 0.90  !11A with a transmission factor of 0.90

! read buffer/background data
clear bgr
read s935x.echo s935x.echo as bgr            !8A
read s935x.echo            as bgr            !9A
read s935x.echo s935x.echo as bgr            !11A

c === process data
match all
fit all
collect

c === output
set A 1e-10
set ns 1e-09

c === populate histogram map
histo tau nbins 30 min 0.1*ns max 130*ns log
histo q   nbins 20 min 0.05/A max 0.25/A

c === collection protocol
collect bgr 1 volfrac 0.95

c === rename and save sqt data
cp last_sqt.dat SAMPLE1_sqt.dat

c === plot and fit sqt data
plot sqt model Diffusion   !here a diffusion model is used for fitting

c === create a comprehensive report of the reduction process
report start dir
report details more
report sqtplot fix_beta 1.0
report end
```