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PySEN: A Python Package for Aiding Experiments at the SNS Neutron Spin Echo Spectrometer

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PYSEN: A PYTHON PACKAGE FOR AIDING EXPERIMENTS AT THE SNS NEUTRON SPIN ECHO SPECTROMETER

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ABBRIEVIATIONS

ORNL	Oak Ridge National Laboratory
SNS	Spallation Neutron Source
NSE	Neutron Spin Echo
SNS-NSE	Neutron Spin Echo spectrometer at the Spallation Neutron Source

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ABSTRACT

PySEN is a Python package that aids experiment planning, data collection, reduction, and analysis at the Neutron Spin Echo instrument (SNS-NSE) located at Beam Line 15 of the First Target Station at the Spallation Neutron Source.

1. INTRODUCTION

Neutron Spin Echo (NSE) spectroscopy is the highest resolution neutron scattering technique available today. The SNS-NSE spectrometer shown in Figure 1 is located at the BL-15 of the Spallation Neutron Source, Oak Ridge National Laboratory (see also Refs. [1.] and [2.]). It is the first, and to date, the only one "classic" NSE spectrometer installed at a pulsed neutron source.

Typical applications of the SNS-NSE spectrometer are studies of molecular motions at the nano- and mesoscopic scale and include soft matter science, condensed matter physics, materials science, complex fluids, and biophysics.

Figure 1. SNS-NSE spectrometer operating at Beam Line 15 of the Spallation Neutron Source, Oak Ridge National Laboratory. Image credit: G. Martin, ORNL.

2. OVERVIEW AND QUICK GUIDE

The PySEN software package is written in Python[1]. It grew out of scripts that were written to aid instrument staff in planning, executing, and evaluating experiments performed at SNS-NSE spectrometer, Oak Ridge National Laboratory, but hopefully will be useful for all NSE users. The source code for the programs described in this Technical Note is available at the ORNL git repository https://code.ornl.gov/zp1/pysen.

2.1 LOGIN TO ANALYSIS CLUSTER

The programs described here are typically launched from the Neutron Sciences Remote Analysis Service analysis cluster. For more information about this service, please refer to Ref. [3.].
In order to use the Neutron Sciences Remote Analysis Cluster, one needs to obtain an XCAMS account credentials, see Ref. [4.] for details.

Two methods of logging into the analysis cluster exist:

1. Using a web browser, this is operating system agnostic, see below.
2. Using a secure shell (SSH) client. It is somewhat a more "advanced" method and works on Linux and macOS computers, for details see APPENDIX C.

Log in using a web browser:

- Point your web browser to https://analysis.sns.gov
- Click the Launch Session button.
- Provide your XCAMS credentials.
- Once logged in, open a terminal window

2.2 SET-UP AND ACTIVATE THE ENVIRONMENT

After successful login, one must activate the NSE reduction and analysis environment, see Figure 2 (top):

1. Click menu **`Applications`** in the top left corner of the desktop.
2. Select **`Analysis`** group.
3. Scroll down to **`NSE`** menu item and click it.

It will open an NSE Terminal Window like the one shown in Figure 2. All the commands will be typed in the NSE Terminal Window.

---

[1] PySEN requires Python interpreter 3.7 or newer.

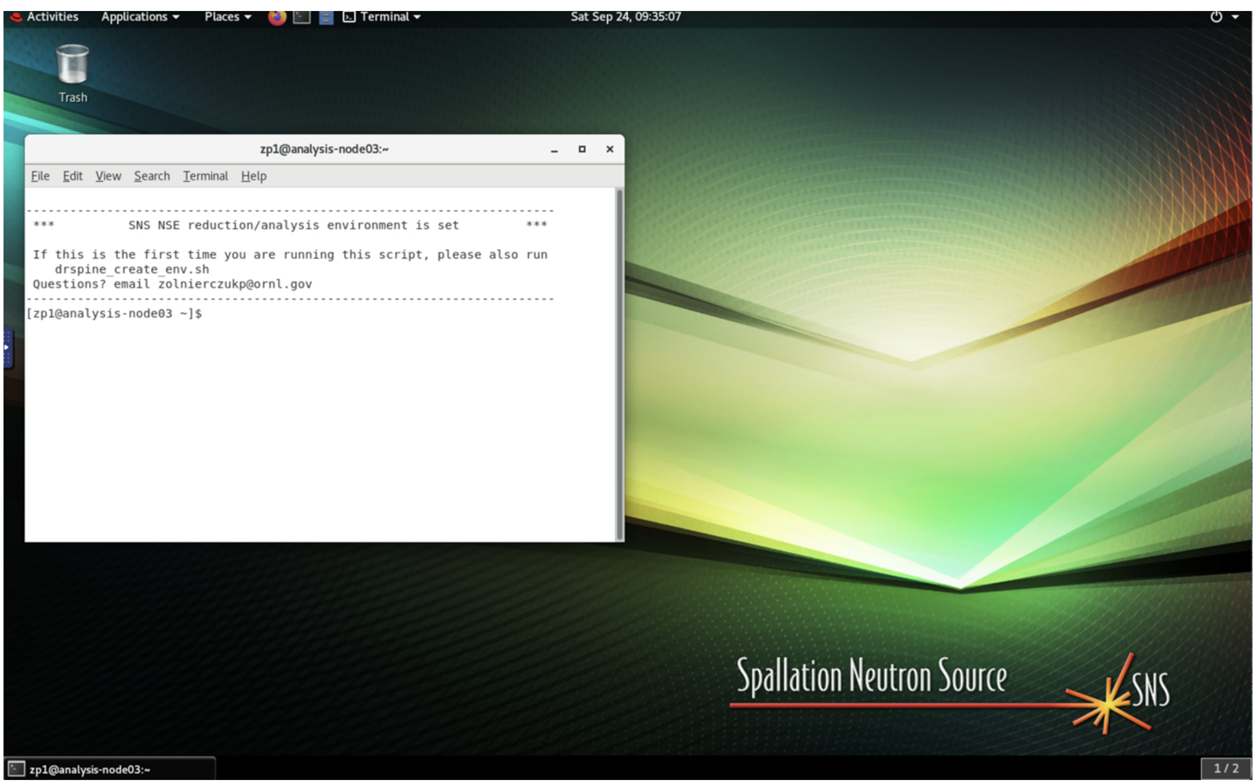

Figure 2 Top: Launch the NSE environment, bottom: the NSE Terminal Window

2.3 QUICK USAGE

The main text user interface (TUI) to the PySEN package is the **`nseplot`** command.

A typical usage is illustrated below, where we create a summary plot, including the so-called "atari plot" in the upper right corner, for the third echo (tau) in run s10938, that in turn belongs to SNS-NSE instrument calibration proposal IPTS-4531.

```
$ nseplot atari /SNS/NSE/IPTS-4531/s10938.echo --tau 3
```

The result is shown in Figure 3.

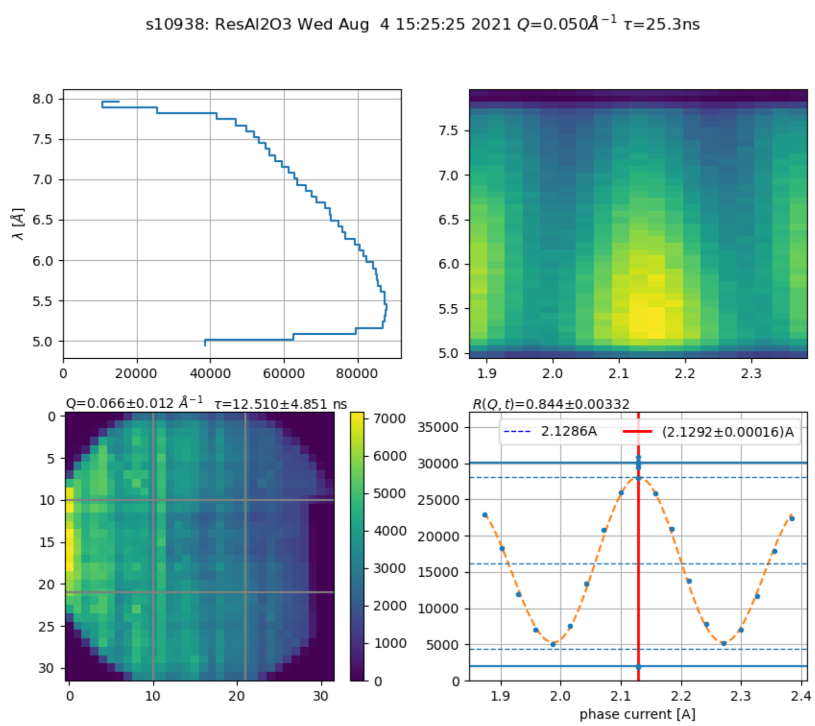

Figure 3 Example of the so-called "Atari" plot for a single Fourier time tau=25ns. Upper left: neutron wavelength spectrum, upper right neutron intensity vs wavelength and phase current. Lower left: neutron intensity on the detector, lower right: echo plot with the echo group fit. The upper right plot loosely resembles the Atari® computers logo.

3. THE NSEPLOT OVERVIEW

The nseplot command allows to plot, preliminarily reduce, and analyze the data generated by the SNS-NSE spectrometer. It is not meant as a substitute for a comprehensive data reduction program such as DrSPINE, see Ref. [5.].

Each nseplot command has the following general syntax:

```
$ nseplot <command> [<filename(s)>] [options]
```

where:

- `<command>` is a directive (command) to the nseplot telling it what to plot.
- `<filenames(s)>` is a list of files to process (plot), if any.
- `[options]` is a (optional) list of modifiers that change the presentation output.

In the case of the example given in Section 2.3, the command was `atari` and the optional modifier was `--tau 3` telling the nseplot to only plot the third echo (third 'tau') of the `/SNS/NSE/IPTS-4531/s10938.echo` file. Table 1 shows currently supported commands.

*Table 1 Currently supported **`nseplot`** commands*

Command	Alias	Short description
echo	**ec**	Plot and fit NSE echo data
atari	**at**	Create so-called atari plot
xyz		Perform XYZ analysis (paramagnetic echo mode)
diffrun	**df**	Plot diffraction scan data
transmission	**tr**	Plot transmission data
bfield	**bf**	Plot magnetic fields recorded during the measurements
qtau	**qt**	Create q-tau coverage map. Useful for experiment planning
phase_table	**pt**	Create phase table

All commands (except xyz) have an "alias" i.e., shorthand notation for a given command. For example,

```
$ nseplot df mydata.dat
```

is equivalent to

```
$ nseplot diffrun mydata.dat
```

Each command has a comprehensive help which can be invoked using `--help` option. For example, the help output for the echo command is produced as follows (also shown in Table 2):

```
$ nseplot echo --help
```

Table 2 Example of nseplot help for the echo command.

```
usage: nseplot echo [-h] [--version]
                    [--save-figure file] [--save-file file]
                    [--verbose | --quiet] [--t1 TBIN1] [--t2 TBIN2]
                    [--x1 XPIX1] [--x2 XPIX2] [--y1 YPIX1] [--y2 YPIX2]
                    [--whole-detector] [--tau [tau ...]] [--center-only]
                    [--only-echo] [--incoherent] [--absolute-y V]
                    [--num-pix N] [--resolution]
                    filename [filename ...]

create echo plot(s)

positional arguments:
  filename              file to process

optional arguments:
  -h, --help            show this help message and exit
  --version, -V         show program's version number and exit
  --output-file FILE, -o FILE
                        save resulting data (if any) to a FILE.
  --save-figure FILE, -S FILE
                        save the output figure to a FILE
                        and do not show it.
  --verbose, -v         verbose output
  --quiet, -q           suppress output
  --tau [tau ...]       select list of taus
  --center-only, -C     show only center patch
  --only-echo           show only echo (no “up/down”)
  --incoherent, -I      treat data as from incoherent scatterer
  --absolute-y V, -Y V  use the same vertical scale for all pixels
  --num-pix N, -N N     set pixel binning (default=4)
  --resolution, -R      plot resolution vs tau

options to select TOF bins:
  --t1 TBIN1, -b TBIN1  set min TOF bin (default=0)
  --t2 TBIN2, -B TBIN2  set max TOF bin (default=None)

options to select pixels:
  --x1 XPIX1            set min X pix (default=10)
  --x2 XPIX2            set max X pix (default=-10)
  --y1 YPIX1            set min Y pix (default=10)
  --y2 YPIX2            set max Y pix (default=-10)
  --whole-detector, -W  show sum over entire detector area
```

4. NSEPLOT COMMANDS

This section describes the nseplot commands. First, we list options common for all or some commands, and then we go over every command in more detail.

4.1 THE COMMON OPTIONS

Each nseplot command accepts general options as listed in Table 3.

Table 3 Common program options.

Long option	Short option (if available)	Description
`--version`	`-V`	Print program version and exit.
`--output-file FILE`	`-o FILE`	Save resulting data (if any) to a file.
`--save-figure FILE`	`-S FILE`	Save the output figure to a file. The figure is not shown on the display.
`--verbose`	`-v`	Be verbose when processing a command. Can be combined, e.g. `-vvv` to increase verbosity level. Mostly useful for debugging.
`--quiet`	`-q`	The opposite of `-v`. Silence any output messages the program may produce, except the errors.

4.1.1 The TOF and pixel selection options

Most commands (echo, atari, diffrun, transmission, xyz and phase_table) support time-of-flight (TOF) selection. In addition, the echo, atari, xyz and phase_table commands allow for the detector pixel selection. These options, shown in Table 4, make it possible to limit processing data to a given TOF bin range and/or to specified rectangular area of the detector.

Note that, at SNS-NSE, the standard number of TOF bins is 42 and the detector has 32x32 pixels. For example, the “center” of the SNS-NSE detector is usually defined as square with pixels between 10 and 22 (in both horizontal and vertical direction). See APPENDIX A for more detailed explanation.

Table 4 TOF and pixel selection options.

Long option	**Short option (if available)**	**Description**
TOF (neutron wavelength) selection options		
`--t1 TBIN1`	`-b TBIN1`	Set minimum TOF bin.
`--t2 TBIN2`	`-B TBIN2`	Set maximum TOF bin.
Detector pixel selection options		
`--x1 XPIX1`		Set minimum x (horizontal) pixel. The default is 10
`--x2 XPIX2`		Set maximum x (horizontal) pixel. [2] The default is -10
`--y1 YPIX1`		Set minimum y (vertical) pixel.
`--y2 YPIX2`		Set maximum x (horizontal) pixel. [3] The default is -10
`--whole-detector`	`-W`	Select the entire detector. A shorthand for: `--x1 0 --x2 32 --y1 0 --x2 32`

4.1.2 The vertical axis control options

Two commands (atari and xyz) allow the user to control the presentation on the vertical axis, see Table 5.

Table 5 Vertical axis options.

Long option	**Short option (if available)**	**Description**
`--vmin VMIN`		Set minimum vertical scale to `VMIN`.
`--vmax VMAX`		Set maximum vertical scale to `VMAX`.
`--logz`		Plot vertical scale as logarithmic.
`--normalize`	`-n`	Normalize resulting vertical scale.[4]

4.2 THE SPECTROMETER COVERAGE PLOT

The qtau spectrometer coverage command is used for experiment planning. It allows one to verify e.g., whether the required Q and τ range (coverage) is accessible or how many instrument settings are required to cover the desired Q and τ space.

[2] Negative numbers mean count from the end: for example --x2 -10 is equivalent to --x2 22 as 22=32-10
[3] Negative numbers mean count from the end: for example --y2 -10 is equivalent to --y2 22 as 22=32-10
[4] The actual normalization process varies for different commands.

4.2.1 Simple q-tau coverage plot

Here's an example of how to plot the NSE coverage for a single spectrometer setting: position p2 (21.3m), Q_{min}=0.05Å^{-1} and λ_{max}=11Å.

```
$ nseplot qtau -l 11 -Q 0.05 –pos p2
```

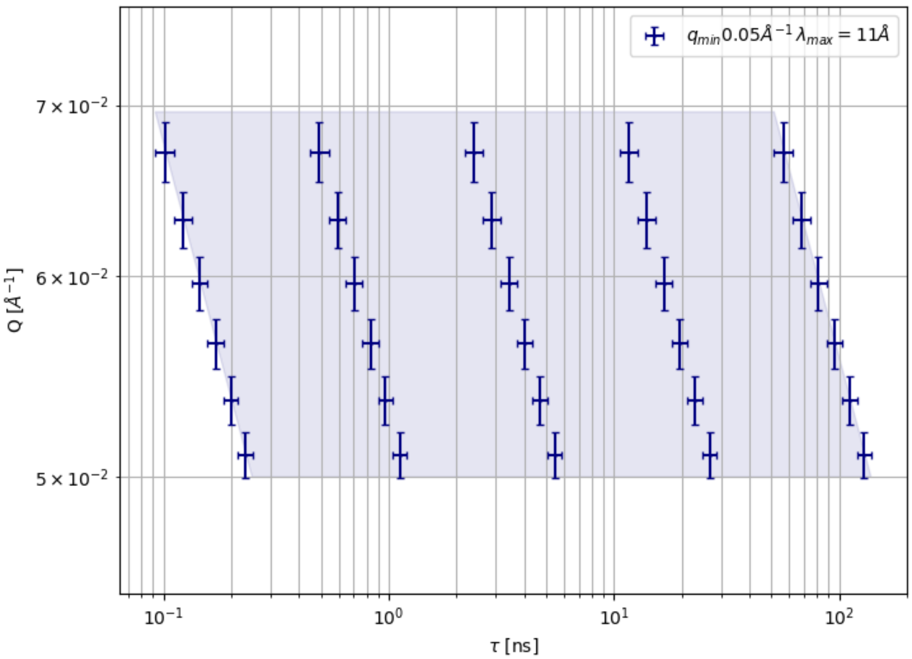

Figure 4 A simple Q-tau coverage for a single spectrometer setting at position p2, scattering angle2θ=5º, and neutron wavelength band of λ=8-11Å.

Position p2 corresponds to neutron wavelength band Δλ=3Å (or λ=8-11Å) and the chosen Q_{min} and λ_{max} correspond to the scattering angle 2θ=5º.

4.2.2 Complex q-tau coverage, using input file

More complex, q-tau coverage plots can be accomplished with a help of an input file.

```
$ nseplot qtau qtau_inp.py
```

where the coverage input file is called qtau_inp.py. An example of the coverage file is shown in Table 6. A template for the input file can be generated with

```
$ nseplot qtau --show-template
```

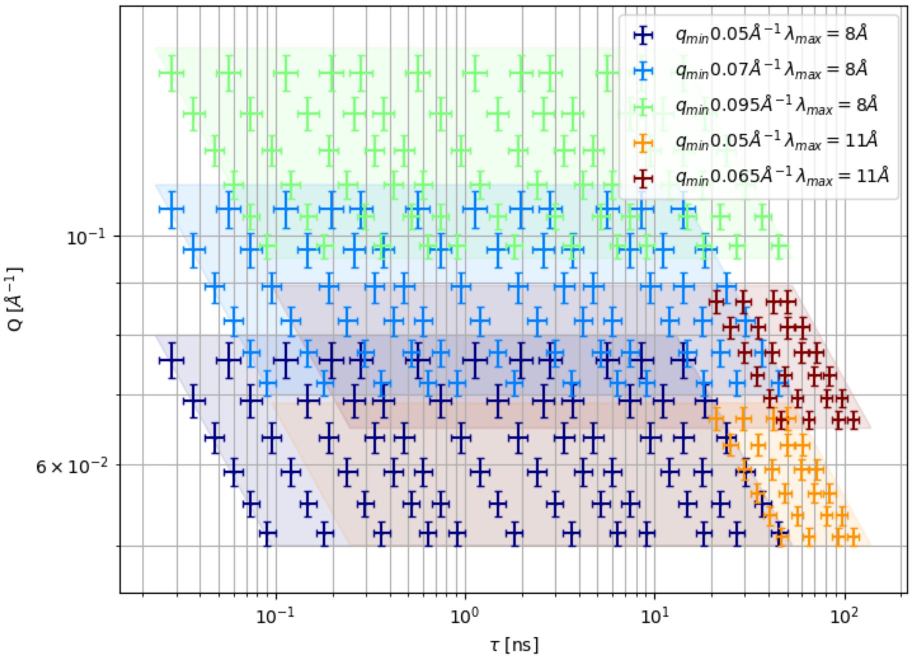

Figure 5 A more complex experiment coverage example. It was generated with an input file given in Table 6.

Table 6 An example of qtau input file

```
# -*- python -*-
# list of taus for 8A
taus_8A  = [0.1,0.2,0.4,0.7,1,2,4,7,10,20,30,50]
# list of taus for 11A
taus_11A = [50,70,100,120]

# coverage data, a list of coverage statements
data = [
    # 8A coverage
    coverage(8.0,  qmin=0.050, pos='p2', taus=taus_8A ),
    coverage(8.0,  qmin=0.070, pos='p2', taus=taus_8A ),
    coverage(8.0,  qmin=0.095, pos='p2', taus=taus_8A ),
    # 11A coverage
    coverage(11.0, qmin=0.050, pos='p2', taus=taus_11A),
    coverage(11.0, qmin=0.065, pos='p2', taus=taus_11A),
]
```

Table 7 Spectrometer coverage options

Long option	Short option (if available)	Description
`--lmax LMAX`	`-l LMAX`	Set the maximum neutron wavelength λ_{max} in [Å].
`--qmin QMIN`	`-Q QMIN`	Set the minimum scattering vector Q_{min} in [$Å^{-1}$].
`--pos POS`	`-p POS`	Set the instrument position: p1, p2, p3 or p4. The default is p2. See APPENDIX A for details.
`--mode MODE`	`-m MODE`	Set the instrument mode: standard or shorty_2. The default is mixed – meaning show the values for both standard and shorty_2.
`--tau [tau ...]`		Set a list of τ values in [ns] to plot. For example: `--tau 0.1 1.0 10.0` selects τ values of 0.1, 1 and 10 ns. It is safe to leave this option as the program will infer the tau range based on the instrument settings.
`--tbin [tbin ...]`		Set a list of TOF binning. This is an advanced option, and it is safe to leave this out.
`--show-template`		Print q-tau input file template.
Presentation options		
`--title TITLE`		Set the title for the q-tau plot
`--full`	`-F`	Full detector coverage. By default, the coverage is calculated only for the center of the detector. Note: experimental option.
`--no-errors`	`-E`	Do not plot error bars on the q/tau averages. Note: experimental option.
`--color-map CMAP`	`-C cmap`	Select matplotlib colormap if one does not like jet, see Ref [9.] for details on available matplotlib color maps.

4.3 THE ECHO PLOT

This command is used to plot (and fit) data from echo files. In addition to TOF and pixel selection options (see Table 4), one can specify which taus to plot (`--tau` option) or whether to plot a summary or a detailed echo portrait, see Figure 6. For a complete list of options that the echo command supports, please refer to Table 8.

4.3.1 Echo summary plot

This is one of the most useful and commonly used commands. It gives a quick preview of the data. An example how to invoke the summary (center-only) plot is given below and the result is shown in Figure 6 (right).

```
$ nseplot echo /SNS/NSE/IPTS-4531/s10938.echo -C
```

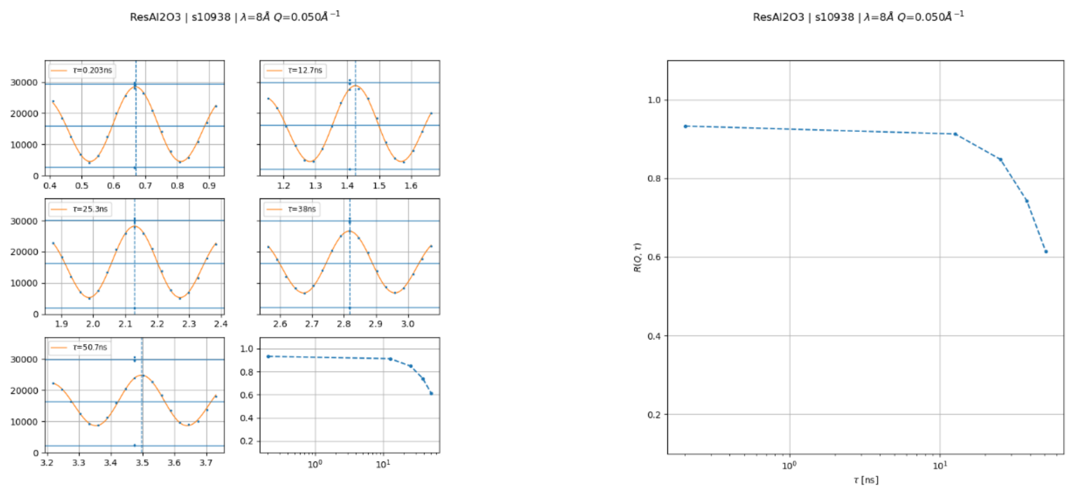

Figure 6 Echo summary and resolution plots.
Left plot: each subpanel shows an echo for the center of the detector and the last one shows the R(Q,t) as function of t. Note that the R(Q,t) data are not corrected for instrument resolution.
Right: same data plotted with an -R option show only the R(Q,t) plot.

4.3.2 Resolution plot

This command produces a single figure of $R(Q,\tau)$ as a function of Fourier time τ, see Figure 6 (left).

```
$ nseplot echo /SNS/NSE/IPTS-4531/s10938.echo -R
```

See APPENDIX B for more details.

4.3.3 Detailed echo portrait

A detailed echo portrait can be generated for each individual echo (tau) as given in the following example, see Figure 7:

```
$ nseplot echo /SNS/NSE/IPTS-4531/s10938.echo --tau 2
```

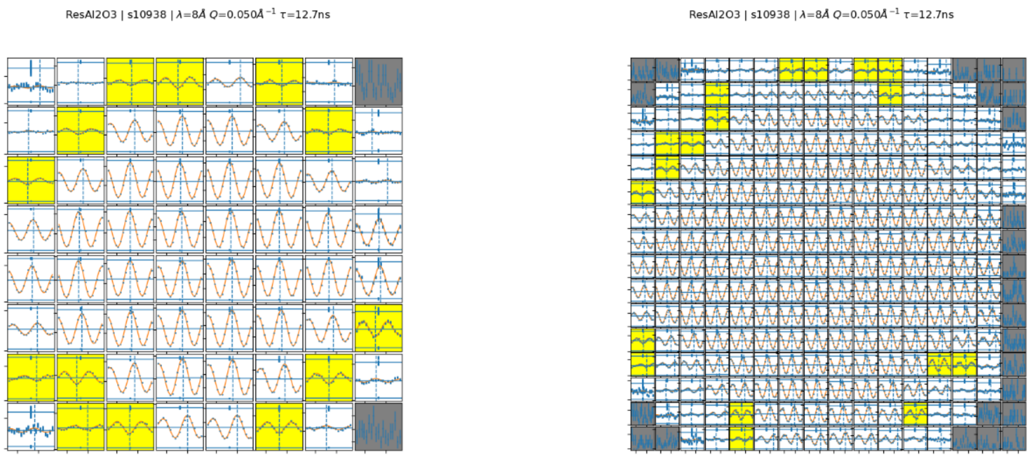

Figure 7 The echo portraits for the same data as in Figure 6.. Left the default detector pixel binning (4x4), right – 2x2 detector pixel binning selected by option -N 2. For pixel color coding see text.

The color coding in the above plots is as follows:

- Yellow means that the echo group is shifted and the fit results in a negative amplitude.
- Gray means that there's insufficient statistics to perform an echo group fit.

Note that DrSPINE (Ref. [5.]) can cope with such "difficulties" quite easily.

Table 8 Echo plot command options.

Long option	**Short option (if available)**	**Description**
`--tau [tau ...]`		Select a list of echoes (tau) to plot. For example: `--tau 2 4 5` to plot 2nd, 4th and 5th echo.
`--center-only`	`-C`	Plot echo summary for the center of the detector, see Figure 6. By default, the echo command plots echo portraits for each tau in a separate figure. This option produces one "summary" plot for the center part of the detector – pixels [10-22, 10-22].
`--only-echo`		Ignore the 'up' and 'down' data and plot only echo group.
`--incoherent`	`-I`	Pick a minimum for the echo symmetry phase instead of maximum. Useful for incoherent data.
`--absolute-y VAL`	`-Y VAL`	By default, each echo is auto scaled to its own maximum value. This option allows to set a common scale for all echoes.

`--num-pix N`	`-N N`	Change the standard pixel binning from 4x4 for echo portraits. The N must be a power 2 between 1 and 16 i.e., $N=2^k$, where k=0…4
`--resolution`	`-R`	Create resolution plot, see Figure 6.

4.4 THE ATARI PLOT

The atari plot supplements the echo plot, see Figure 3. It gives a quick overview of the neutron wavelength spectrum, detector image counts and the echo group.

In addition to common and TOF and pixel selection options (see Table 4) and vertical axis options (see Table 5), the atari command accepts the options given in Table 9.

Table 9 The atari plot command options.

Long option	Short option (if available)	Description
`--tau [tau ...]`		Select a list of echoes (tau) to plot. For example, use `--tau 2 5` to plot 2nd and 5th echo.
`--only-echo`		Ignore the ‘up’ and ‘down’ data and plot only echo part.
`--incoherent`	`-I`	Fit a minimum symmetry echo instead of maximum. Useful for incoherent data.
`--phase0 PHASE`		Set initial symmetry phase (as opposed to guessing by the program).

4.5 THE DIFFRACTION SCAN

The diffraction scan is a polarized scan of neutron count rates vs the scattering angle (or Q). It is a convenient experimental pre-check for the sample count rates and polarization (flipping ratio). It also allows for decomposition of coherent and/or incoherent contributions. For details, see Table 10 and APPENDIX B.

4.5.1 Count rate plot

Here’s an example of the counts rate plot, which plots the up and down count rates as a function of the scattering vector Q:

```
$ nseplot diffrun
/SNS/NSE/calib/diffrun_{Al2O3,Grafoil,Diamond}_16385.dat -l
```

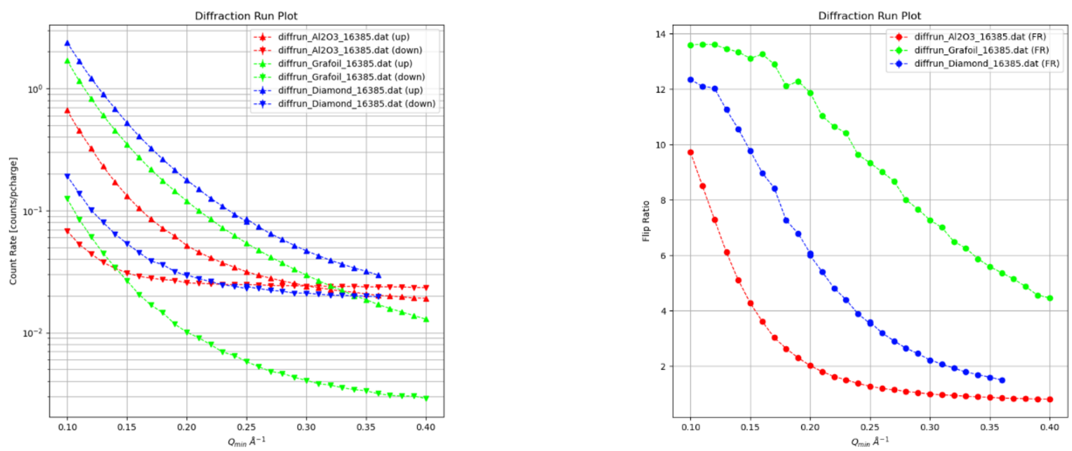

Figure 8 Diffraction scan data.
Left: Count rates plot for three different resolution samples: Al_2O_3 powder, graphite foil ("grafoil") and diamond powder. The "up" counts are labeled with ▲ symbol (triangle up) and the "down" counts are labeled with ▼symbol (triangle down).
Right: Flipping ratios (FR) plot for the same resolution samples.

4.5.2 Flipping ratio plot

The command below is an example of flipping ratio (FR=up/down) plot as a function of the scattering vector Q:

```
nsepl
$ nseplot diffrun
/SNS/NSE/calib/diffrun_{Al2O3,Grafoil,Diamond}_16385.dat  -r
```

The plot is a very good check whether the sample can produce a measurable signal in the NSE spectrometer. Samples and or Q's, where the FR<3 are, in general, very difficult or impossible to measure. The diffraction scan often puts a limit on a Q-range, where experiment is feasible.

Table 10 The diffraction scan options.

Long option	Short option (if available)	Description
`--up`	`-u`	Plot flippers 'up' counts
`--down`	`-d`	Plot flippers 'down' counts
`--coherent`	`-c`	Plot 'coherent' counts c=up-down/2
`--incoherent`	`-i`	Plot 'incoherent' counts i=3/2 down
`--ratio`	`-r`	Plot flipping ratio FR=up/down
`--average`	`-a`	Plot 'average' counts a=(up+down)/2
`--coherent-ratio`	`-C`	Plot coherent/incoherent ratio C=2/3(up/down-1)
`--logscale`	`-l`	Plot in semi-log scale

4.6 THE TRANSMISSION PLOT

The transmission plot is used to determine the relative transmission factor, T_{fac}, of a sample with respect to the background (buffer). The transmission factor is used when subtracting the background contribution from the sample signal, see also APPENDIX B.

A command below, shows an example how to produce a transmission plot. The first filename is typically the buffer and the subsequent are the samples.

```
$ nseplot transmission
/SNS/NSE/calib/transmission_16736_{Buffer1,Sample?}.dat
```

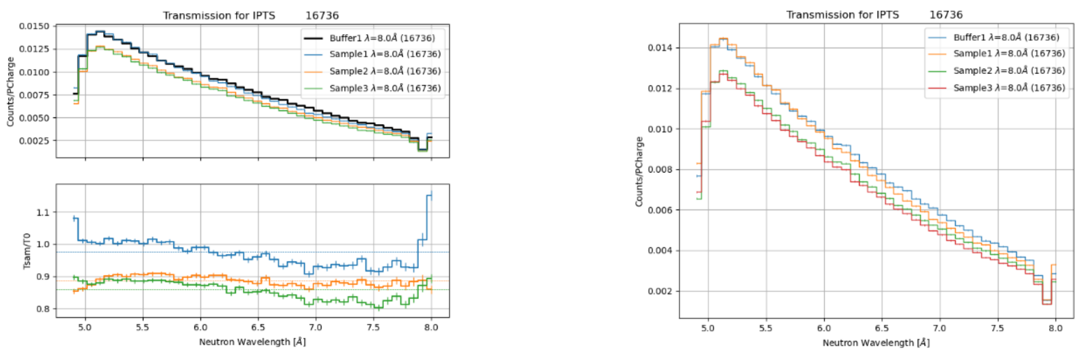

Figure 9 Transmission data plot.

The command also prints the average transmission factor as for example shown in Table 11.

Table 11 Transmission factor output example

```
#sample name          transmission factor
Sample1               0.9764 +/- 0.0417
Sample2               0.8867 +/- 0.0155
Sample3               0.8599 +/- 0.02729
```

Table 12 Transmission plot options.

Long option	Short option (if available)	Description
`--pos POS`	`-p POS`	Set the instrument position: p1, p2, p3, or p4. The default is p2. See APPENDIX A for details.
`--logscale`	`-l`	Plot in semi-log scale
`--spectrum-only`	`-w`	Plot neutron spectrum only, do not calculate/plot transmission.
`--poly-deg deg`	`-P deg`	Fit a polynomial to the transmission spectrum.

4.7 THE XYZ PLOT

The XYZ plot is used to aid the XYZ analysis used when performing paramagnetic echo measurement with addition of the so-called "Q-coils", see APPENDIX B for more details of the XYZ analysis. In addition to common and TOF and pixel selection options, see Table 4, and vertical axis options, see Table 5, the xyz command allows to control the range of scattering vectors accepted in the XYZ analysis, see Table 14.

Here's an example command to make XYZ analysis plot for an $Ho_2Ti_2O_7$ (HTO) sample measured at T=10K for all detector pixels:

```
$ nseplot xyz /SNS/NSE/calib/Res10K_17095_* -W
```

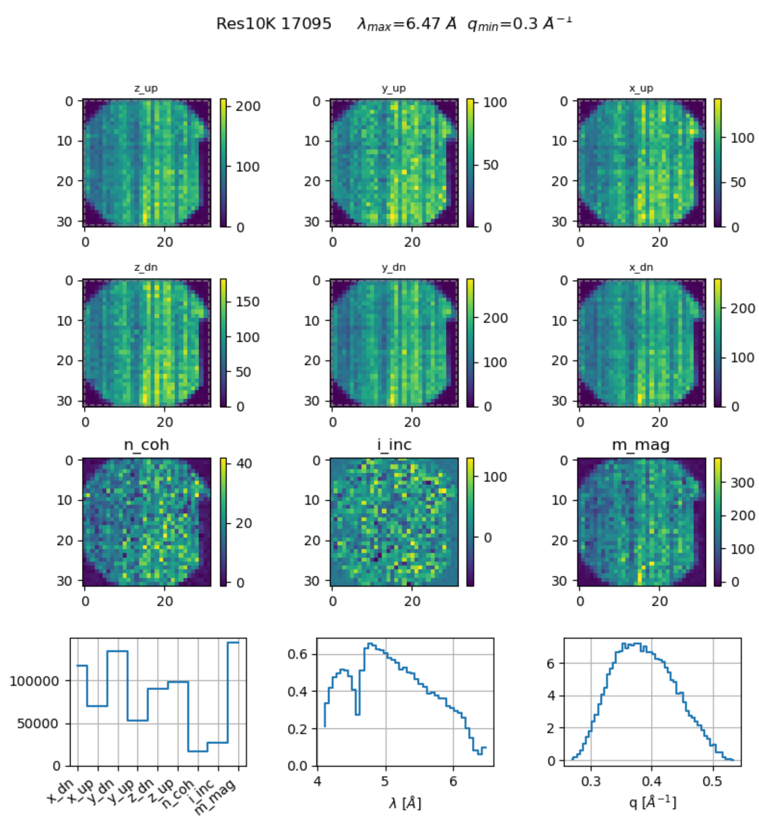

Figure 10. XYZ plot example as measured for an HTO ($Ho_2Ti_2O_7$) powder resolution sample for T=10K. The 1st (top) row shows "flipper up" detector image scattering pattern for x, y and z direction of the Q-coils. The 2nd row shows the "flipper down" scattering for the x, y and z directions of the Q-coils. The 3rd row shows the coherent (n_coh), incoherent (i_inc) and magnetic (m_mag) contributions. The bottom row: left – sum of counts and magnetic scattering for all six (up/down and xyz) combinations of Q-coils, middle - neutron wavelength spectrum, right - scattering vector spectrum.

The xyz command produces an output with intensity for each flipper/Q-coil configuration and calculates the magnetic strength, see Table 13.

Table 13 XYZ analysis output file. The columns are as follows: "label"- measurement type, "intensity" – count rates, "average q" – Q and σ_Q in $Å^{-1}$, "average wavelength" λ and σ_λ in Å.

```
#label   counts  average q  average wavelength
x_dn       117040.2   0.3869 0.0497     5.12   0.58
x_up        70063.0   0.3886 0.0506     5.10   0.59
y_dn       133794.5   0.3872 0.0497     5.12   0.58
y_up        52490.6   0.3885 0.0509     5.10   0.60
z_dn        90160.3   0.3874 0.0498     5.12   0.58
z_up        97796.8   0.3880 0.0501     5.11   0.59
#summary
n_coh       16617.6   n_coh/tot     8.881%
i_inc       26943.3   i_inc/tot    14.399%
m_mag      143554.2   m_mag/tot    76.720%
```

Table 14 The xyz plot options to control the Q-scattering vector selection

Long option	Short option (if available)	Description
`--qmin QMIN`		Minimum value of Q (in A) accepted in the XYZ analysis.
`--qmax QMAX`		Maximum value of Q (in A) accepted in the XYZ analysis.
`--delta-q DELTAQ`		Binning resolution of the Q-spectrum histogram.
`--details`		Print more detail information of the XYZ analysis.

4.8 THE PHASE TABLE PLOT

From time to time, it is necessary to create or verify the phase table i.e., the calibration file that maps the main superconducting coil i_{00} and the spectrometer scattering angle ϕ to the phase coil current i_5.

A typical measurement would comprise measuring 5 echos, for example τ=0.2ns,12.5ns, 25ns, 37.5ns and 50ns at a series of scattering vectors e.g., Q=0.05 $Å^{-1}$, ..., 0.4$Å^{-1}$. Consult with the NSE instrument staff on how to perform this measurement.

Then the phase table can be generated as in the example below:

```
$ nseplot phase_table /SNS/NSE/IPTS-4531/s1093[89].echo
/SNS/NSE/IPTS-4531/s1094[0-2,4].echo
```

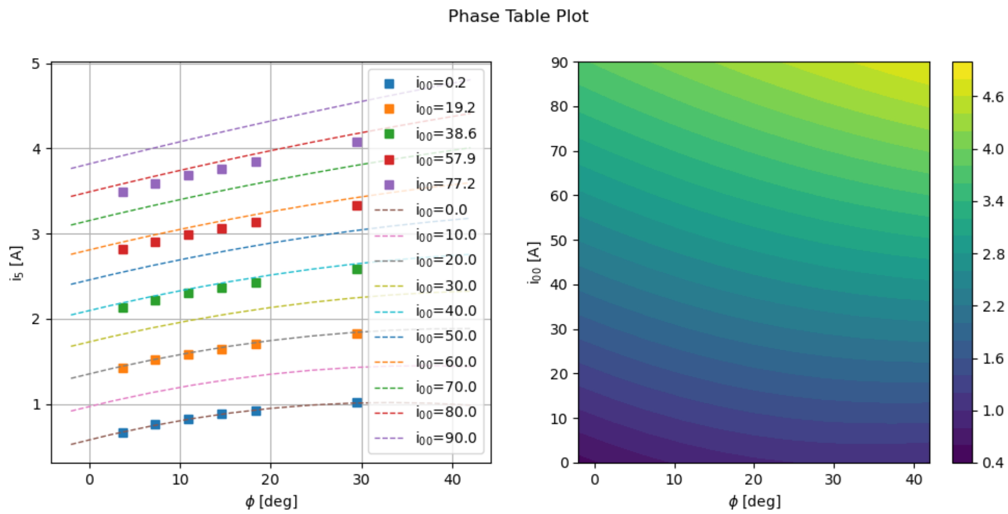

Figure 11 An example of phase table plot.

The resulting phase table, see Table 15, can be directly imported into the SNS-NSE control program.

Table 15 Phase Table

```
input phasetable
phasetable pos2 rebuild
c time:  Mon Aug 22 14:05:16 2022
c max interpolation error [0.0213A, 1.422%]
*          angles -2.0000  2.4000  6.8000 11.2000 15.6000 20.0000 24.4000 28.8000 33.2000 37.6000 42.0000
c amperes(main) --- phase current(i5)
*           0.000  0.5262  0.6417  0.7418  0.8264  0.8956  0.9494  0.9878  1.0107  1.0182  1.0103  0.9869
*          10.000  0.9180  1.0320  1.1322  1.2187  1.2915  1.3506  1.3959  1.4276  1.4455  1.4497  1.4402
*          20.000  1.3019  1.4147  1.5154  1.6041  1.6806  1.7451  1.7975  1.8378  1.8660  1.8822  1.8862
*          30.000  1.6777  1.7898  1.8914  1.9825  2.0630  2.1330  2.1925  2.2414  2.2798  2.3077  2.3250
*          40.000  2.0455  2.1574  2.2602  2.3540  2.4387  2.5144  2.5809  2.6384  2.6869  2.7262  2.7565
*          50.000  2.4053  2.5174  2.6218  2.7186  2.8077  2.8891  2.9628  3.0288  3.0872  3.1378  3.1808
*          60.000  2.7570  2.8698  2.9762  3.0763  3.1699  3.2572  3.3381  3.4126  3.4807  3.5425  3.5978
*          70.000  3.1007  3.2147  3.3234  3.4270  3.5254  3.6187  3.7068  3.7898  3.8675  3.9402  4.0076
*          80.000  3.4364  3.5519  3.6634  3.7708  3.8742  3.9736  4.0690  4.1603  4.2476  4.3309  4.4101
*          90.000  3.7641  3.8816  3.9962  4.1077  4.2163  4.3219  4.4246  4.5242  4.6209  4.7147  4.8054
eof
```

4.9 THE MAGNETIC FIELD PLOT

The SNS-NSE spectrometer has 5 external Hall probes i.e., outside the experimental cave, and 3 internal ones i.e., on the inside that monitor the magnetic field. The magnetic field plot is a diagnostic, showing the stability of the magnetic field during measurement.

An example command to produce the magnetic field plot is given below and the resulting plot is shown in Figure 12.

```
$ nseplot bfield /SNS/NSE/IPTS-4531/s10537.echo --tau 4
```

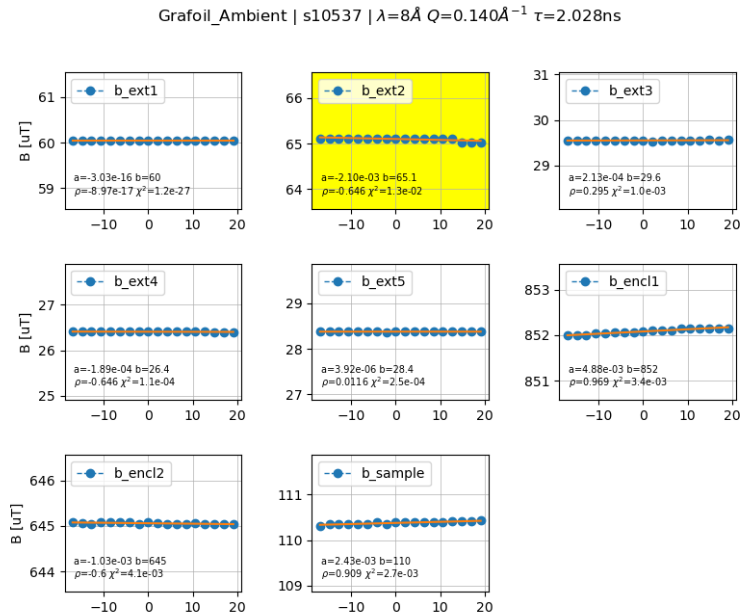

Figure 12 An example of magnetic field plot. Note that the external probe #2 recorded a small discontinuity in the magnetic field. The internal probes look very normal.

Table 16 Options for the bfield command

Long option	**Short option (if available)**	**Description**
`--tau [tau ...]`		Select a list of echos (tau) to plot. For example: `--tau 2 4 5` to plot 2nd, 4th and 5th echo.
`--max-chi2 CHI2`		Max χ^2 threshold. Warning is issued if χ^2 is exceeded (default is 10^{-2}).
`--axis AXIS`		Select magnetic field axis to plot: 0. |**B**| – absolute value of the magnetic field vector 1. $\mathbf{B}_x$ – horizontal component – along the neutron beam. 2. $\mathbf{B}_y$ – horizontal component – perpendicular to the neutron beam. 3. $\mathbf{B}_z$ – vertical component – perpendicular to the neutron beam.

5. REFERENCES:

[1.] SNS-NSE Spectrometer https://neutrons.ornl.gov/nse

[2.] M. Ohl *et al.,* Nucl. Inst. and Meth. in Phys. Res. **A696**, 85-99 (2012).

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[5.] P. Zolnierczuk *et al.*, J. Appl. Cryst **52,** 1022-1034 (2019).

[6.] G. Ehlers *et al.*, Rev. Sci. Inst. **84,** 093901 (2013).

[7.] Neutron Data Booklet, A-J Dianoux, G. Lander (eds), Institut Laue-Langevin (2003)

[8.] Neutron Spin Echo Spectroscopy, F. Mezei, C. Pappas and T. Gutberlet (eds), Springer (2003)

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APPENDIX A.

APPENDIX A. SNS-NSE INSTRUMENT OVERVIEW

The SNS-NSE instrument is described in more detail in Ref. [2.] and the standard data reduction procedures are given in Ref. [5.]. Here we repeat only main features that are relevant to the PySEN package.

Since the SNS-NSE instrument operates in a time-of flight (TOF) mode, raw data are typically binned into 42 TOF channels that correspond to a given wavelength band e.g., 5-8Å, and the area detector has coverage of 32x32 pixels.

The instrument can be "positioned" in one of the four different distances from the neutron source: p1, p2, p4 and p4, see Table 17. Only p2 ("standard") and p4 ("high-Q") are routinely used during the measurements.

Table 17 SNS-NSE instrument positions.

Instrument Position	Source to detector distance: L[m]	Neutron Wavelength Band: Δλ [Å]	Max. Scattering Angle: 2θ [deg]	Comments
p1	*18.3*	*3.6*	*29.0*	*not used*
p2	21.3	3.1	40.0	"standard"
p3	*24.3*	*2.7*	*56.0*	*not used*
p4	27.3	2.4	79.5	"high-Q"

Typically, the instrument operates in one of the three precession modes, see Figure 13 and Ref. [2.].

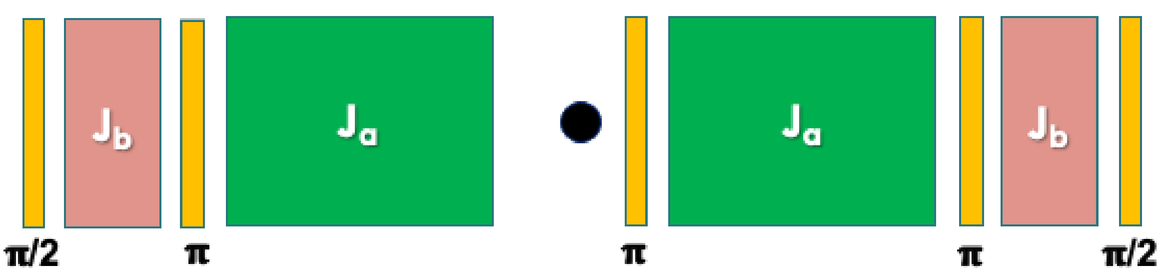

Figure 13 SNS-NSE standard vs shorty_2 modes. In standard mode only "green" precession zones (J_a) and one central π-flipper are on. In shorty_2 all π-flippers are on and both J_a and J_b precession zones are active. In both cases neutron precession is started and terminated with π/2-flippers.

Standard Mode:

In standard mode only "green" precession zones (J_a) and one central π-flipper are on and the field integral range $J=J_a=0.005\text{-}0.560$ Tm.

Small Echo Mode (a.k.a "shorty_2")

In shorty_2 mode, all π-flippers are on and both J_a and J_b precession zones are active and the field integral $J=J_a-J_b \cong 0 - 0.10$ Tm

Paramagnetic Mode:

In paramagnetic mode, the sample acts as a π-flipper and the echo normalization is achieved with addition of so-called Q-coils, see Ref. [6.].

APPENDIX B.

APPENDIX B. A QUICK GUIDE TO THE SNS-NSE MEASUREMENTS

This an extremely brief overview of the NSE measurements, for more details see e.g., Ref. [7.] and Ref. [8.].

The spin coherent scattering preserves the neutron polarization and the incoherent is 1/3 no spin-flip and 2/3 spin-flip. Therefore, with all the flippers off (also known as "flippers up") the intensity can be given as:

$$U = I_{coh} + \frac{I_{inc}}{3}$$

where I_{coh} and I_{inc} are spin coherent and spin incoherent intensities, respectively. The intensity with the main π-flipper on and all others off (also known as "flippers down") is similarly expressed as:

$$D = \frac{2}{3} I_{inc}$$

A useful thing is a quantity called flipping ratio, FR:

$$FR = \frac{U}{D}$$

And finally, the echo intensity if given as

$$E = I_{coh}\, f_{coh}(\tau) - \frac{1}{3} I_{inc}\, f_{inc}(\tau)$$

where $f_{coh}(\tau)$ and $f_{inc}(\tau)$ denote the "dynamics" of the coherent and incoherent scattering, respectively.

The Echo Measurement

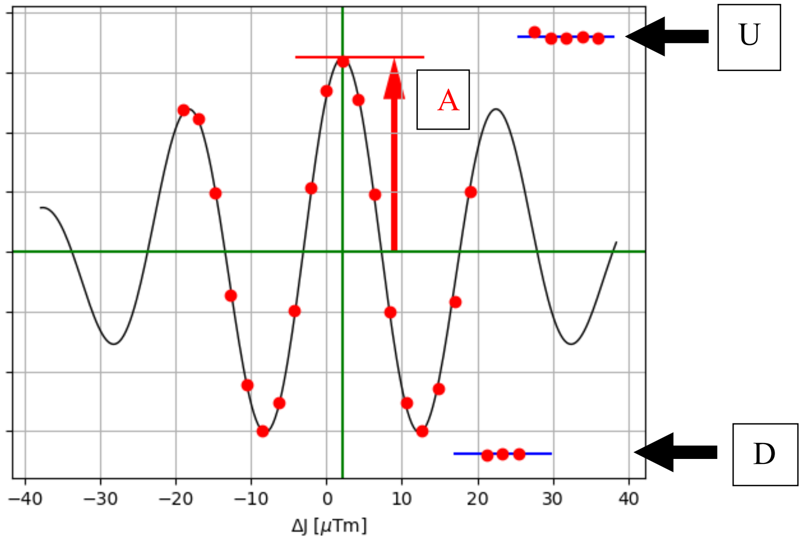

Figure 14 Echo group: A – echo amplitude, U – "up" counts, D – "down" counts.

In order to obtain the intermediate scattering function $S(Q,\tau)$ one needs first to measure the instrument resolution using e.g., graphite foil, or Al_2O_3 powder.

$$R(Q,\tau) = \frac{2A_{res}}{U_{res} - D_{res}}$$

The sample is similar:

$$F(Q,\tau) = \frac{2A_{sam}}{U_{sam} - D_{sam}}$$

And finally, we get the normalized intermediate function as:

$$\frac{S(Q,\tau)}{S(Q,0)} = \frac{F(Q,\tau)}{R(Q,\tau)}$$

For background (sometimes called "the buffer") correction, replace A_{sam} with the following expression:

$$A_{sam}^{corrected} = 2\,\frac{A_{sam} - (1-\varphi)T_{fac}A_{buf}}{(U_{sam} - D_{sam}) - (1-\varphi)T_{fac}\left(U_{buf} - D_{buf}\right)}$$

where "sam" and "buf" indices refer to sample and buffer, respectively; T_{fac} is the transmission factor (defined below) and φ is the sample volume fraction in the buffer.

The Transmission Measurement

The measurement is typically performed in a "straight" instrument configuration i.e., with scattering angle set to 0. One measures the count intensity of the sample and buffer. The result is the transmission factor, T_{fac}, defined as

$$T_{fac} = \frac{T_{sam}}{T_{buf}}$$

where T_{sam} and T_{buf} are the intensities for the sample and buffer, respectively. An example of a transmission measurement is given in Figure 9.

The Diffraction Scan

The diffraction scan is a quick way to establish viability of the NSE measurements. It is simply a measurement of flipper up (U) and flipper down (D) intensities as a function of Q.
An example of a diffraction scan is shown in Figure 8.

XYZ Analysis

The XYZ plot is used to aid the XYZ analysis used when performing paramagnetic echo measurement with addition of the so-called "Q-coils". The magnetic scattering "strength" is given by the following formula (see Ref. [6.]):

$$M = 2\left(N_z^+ - N_z^-\right) - \left(N_x^+ - N_x^-\right) - \left(N_y^+ - N_y^-\right)$$

where $N_{x,y,z}^{+,-}$ denote count rates with flippers "up" (+) and "down" (-) for the three directions of the Q-coils magnetic field.

APPENDIX C.

APPENDIX C. USING PYSEN WITH A SECURE SHELL (SSH)

This somewhat more advanced method of running PySEN commands using terminal and bypassing web login.

Log in using the SSH client:

- Open a terminal on your Linux or macOS computer.
- Type the following command:
  ```
  $ ssh -Y analysis.sns.gov
  ```
- Provide your XCAMS credentials.

After successful login, one must activate the NSE reduction and analysis environment, which is accomplished by typing the following command:

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

It is convenient to create a short "alias" command (instead of typing the above long line). The following command will create an **nse** alias command in one's OS shell startup file (typically ~/.bashrc):

```
$ /SNS/software/nse/etc/setup_nse.sh -i
```

And then simply setup the environment by typing the following command:

```
$ nse
```

before running the commands described in this Technical Note.

APPENDIX D.

APPENDIX D. INSTALLING PYSEN ON A PERSONAL COMPUTER

This appendix describes the installation of PySEN on a personal computer. PySEN requires Python 3.7 or newer. Table 18 shows Python packages that are required to run PySEN.

One of the simplest methods to install Python is to download Anaconda Python (anaconda.com).

Table 18. Prerequisites

Package	Minimal version
numpy	1.16
scipy	1.2
matplotlib	3.0
PyQt	5.0
pip	19.0

Installation

Download PySEN from https://code.ornl.gov/zp1/pysen

Open a terminal and navigate to the directory, where PySEN sources reside.

Type the following command:

```
pip install .
```

or for a "per-user" installation

```
pip install –user
```