**Polarised SANS NXcanSAS Metadata**

**NXcanSAS proposal:** <https://wiki.cansas.org/index.php?title=NXcanSAS_v1.1>

**General questions:**

* 1. How do we identify if the dataset is polarized?

*We agreed that it would be most reliable for this to be specified rather than determined automatically. Passing in a spin state order or names of relevant components could potentially indicate that the data is polarized.*

Additionally, for some of the recommended metadata we'll need to know whether a hyperpolarization polarizer and/or analyzer has been used - how can we tell this?

*This is not possible to determine automatically from the data, so may need to be specified in another way. Whether an instrument uses a hyperpolarization polarizer and/or analyzer is not likely to change frequently (i.e. not per experiment or even per cycle) and so would be well-suited to storing in the IDF and/or a parameter file. This is also the same for the number of flippers that are in use on the instrument. On LARMOR there are two polarizers – “short” and “long” polarizers that are used with different wavelengths. Either of these could be used for any given experiment, although only one is used at a time for any given measurement. Only one analyzer is used for any given measurement, but different analysers may be available for a given instrument. Occasionally users have also brought their own analyzer for their experiment.*

* 1. Do we have any use cases for a hyperpolarization polarizer at the moment?

*Skipped this question, wasn’t necessary to discuss.*

1.3) For the recommended transmission run and efficiency metadata, there are alternative ways of presenting it in the file depending on whether it’s wavelength dependant or fixed wavelength. Is the fixed wavelength version not relevant for ISIS but would be for a facility such as ILL?

*ISIS data will always be wavelength dependent.*

1.4) Are you ultimately aiming to include all the recommended metadata?

*For analysis at ISIS, the most important recommended metadata is the magnetic field strength and direction. This is required to set up the geometry for the analysis, so the first version of the polarised SANS NXcanSAS file will include all the mandatory information plus the magnetic field strength and direction. The rest of the recommended metadata that we’re aiming to include will be added gradually after that.*

**Mandatory metadata:**

*2.1) Add a name and type (i.e. supermirror, coil, etc.) for polarizer, flipper and analyzer.*

2.1.1: Are these names you will have chosen rather than names that should be auto-generated somehow?

*The names to use in the output metadata file should be provided rather than generated automatically by the save algorithm. This will ensure that the components that were used in the experiment can be identified correctly based on the names that scientists are using for them.*

*2.2) Record distance of polarizer, flipper and analyzer from sample.*

2.2.1: Only the sample location appears to be in the IDF at the moment, so where will these values come from? How often will they change?

*The location of the polarizer(s) and flipper are fixed, so these would be well-suited to being defined in the IDF. The helium analyzer moves per experiment. It was mentioned that SANS scientists are used to defining components in the IDF or parameter file and then moving them as required using the relevant Mantid algorithms, so they see this as a potential option for the analyzer.*

2.2.2: Units to use in the file?

*Meters*

*2.3) For polarized data, specify the polarization [Pin, Pout] as 1, -1 or 0 e.g. for PA SANS use [Pin, Pout], Polarizer Pol-SANS use [Pin, 0], Analyser Pol-SANS use [0, Pout].*

2.3.1: How to find out the polarization of each dataset?

*This should be provided in the same way that the spin state order is provided for the other polarized SANS algorithms.*

*2.4) All documentation must include the provided definition of polarization.*

2.4.1: For my understanding, when the proposal says that the definition inverts for the Southern hemisphere, do we mean the following:

Northern hemisphere:

non-spin-flip higher intensity = --

non-spin-flip lower intensity = ++

Southern hemisphere:

non-spin-flip higher intensity = ++

non-spin-flip lower intensity = --

So that someone trying to save southern hemisphere data would end up with the wrong polarization [Pin, Pout] metadata?

*Users of the SaveNXcanSAS algorithm will be expected to take any necessary steps to ensure their data will be labelled correctly in the output file. We do not need to provide a specific explanation to warn about this in the algorithm documentation.*

**Recommended metadata:**

*3.1) Include transmission run data and errors for polarizer, flipper and analyzer.*

3.1.1: I'm expecting this will be provided by passing in the relevant transmission workspaces, as the algorithm doesn't currently load any data.

*3.2) For a hyperpolarization polarizer and/or analyzer, include the empty cell transmission (and errors?).*

3.2.1: I'm expecting this will be provided by passing in the relevant empty cell transmission workspace(s), as the algorithm doesn't currently load any data.

*3.3) Include efficiencies and errors for polarizer, flipper and analyzer.*

3.3.1: I'm expecting this will be provided by passing in the relevant efficiency workspaces, as the algorithm doesn't currently load any data.

*3.4) Add magnetic field strength and direction across the sample, polarizer, flipper and analyzer.*

3.4.1: How to get these values and directions?

*We will only record the magnetic field strength and direction for the sample. We will not record these for the polarizer, flipper and analyzer.*

*For the sample, the magnetic field strength changes per measurement and is recorded in a sample log on the workspace. The log name varies and can be anything, although the instrument scientist will know what it is.*

3.4.2: What value will be entered into the @direction or @direction-spherical fields? Will it be a string value that can simply be read from the IDF/parameter file (i.e. “x”, “y”, “theta, psi”)?

*We should use the @direction-spherical field for this. The information will need to be provided by the scientist, it is not available on the workspace. Dirk will supply an example of what they would expect to see if they were looking at the @direction-spherical metadata in a saved NXcanSAS file.*

*Orientation should follow the Busing-Levy convention. The unit for angles should be degrees.*

* *You first apply azimuthal\_angle as a rotation around z. This rotates the whole coordinate out of the plane.*
* *Then you apply polar\_angle as a rotation around y in the tilted coordinate system.*
* *Azimuthal\_angle = 0 corresponds to the horizontal scattering plane of the instrument (along x direction). In this case polar\_angle maps directly to the scattering angle commonly known as two theta. A positive rotation of Azimuthal\_angle turn clockwise. Azimuthal\_angle =+90 degrees is vertical upright.*

*The easiest and humanly readable solution would be to follow the ratified NXMonotas format for Monochromatic Neutron and X-ray Triple-Axis Spectrometer (*[*https://github.com/nexusformat/wiki/blob/da819ca58501ca0fa68ce255d1d064ebebb761c4/content/NXmonotas\_example-NIAC2006.md?plain=1#L75*](https://github.com/nexusformat/wiki/blob/da819ca58501ca0fa68ce255d1d064ebebb761c4/content/NXmonotas_example-NIAC2006.md?plain=1#L75)*) and add the following parameters to [nxsample]*

*<polar\_angle units="degrees" type="NX\_FLOAT[np]">*

*{Polar angle of the sample with respect to the beam incident beam}*

*</polar\_angle>*

*<azimuthal\_angle units="degress" type="NX\_FLOAT[np]">*

*{Azimuthal angle of the sample with respect to the beam}*

*</azimuthal\_angle>*

*Note that the format also allows an additional rotation angle of the sample, which we did not proposed. This angle is not further specified to some absolute reference position, which makes it arbitrary.*

*<rotation\_angle units="degrees" type="NX\_FLOAT[np]">*

*{Rotation angle of the sample}*

*</rotation\_angle>*

*For a single crystal, it would be advisable to use rather an orientation matrix with respect to defined crystallographic orientations of the aligned crystal.*

*3.5) Add electric field strength and direction across the sample.*

3.5.1: How to get this value and direction?

*If this information is present in a workspace than it will be in the sample log – same as for magnetic field information. Diego has a PA example that shows this, but it’s not currently included in most workspaces.*

3.5.2: What value will be entered into the @direction or @direction-spherical fields? Will it be a string value that can simply be read from the IDF/parameter file (i.e. “x”, “y”, “theta, psi”)?

*Same as for magnetic field direction.*

*3.6) Add initial polarization plus errors for hyperpolarization polarizer/analyzer.*

3.6.1: How to find this value? Can we just calculate this from the initial efficiency using: polarization = (2 \* efficiency) – 1? Presumably this is wavelength dependent?

*This is a single value and is the polarization of the He3 analyzer rather than the neutrons. This will be the output fit parameter (phe and the error on phe) from the HeliumAnalyserEfficiency algorithm.*

3.6.2: Units should be "none" for this?

*Follow the standard. The unit for fields, where the units cancel out, like efficiencies, should be NX\_DIMENSIONLESS (NOTE: not the same as NX\_UNITLESS).*

*3.7) Add decay time plus errors for hyperpolarization polarizer/analyzer.*

3.7.1: How to find this value?

*This will be discussed and added later in the project when we have started looking at decay time.*

*3.8) Add gas pressure for hyperpolarization polarizer/analyzer.*

3.8.1: How to find this value?

*Is a known value and will be provided. We use a fitted value for the calculations, but we assume that the known value will be in the same ballpark. This one presumably may change when a cell is re-filled ~once a day.*

3.8.2: Relevant units?

*As per the standard, the units of pressure is Pa.*

*3.9) Add exchange distance (cell length?) for hyperpolarization polarizer/analyzer.*

3.9.1: How to find this value?

*Is a known value and will be provided. We use a fitted value for the calculations, but we assume that the known value will be in the same ballpark. This one is a characteristic of the cell that won’t change?*

3.9.2: Relevant units?

*As per the standard, unit should be meters.*