3.3.2.3. NXcanSAS

Status:

application definition, extends NXobject, version 1.0

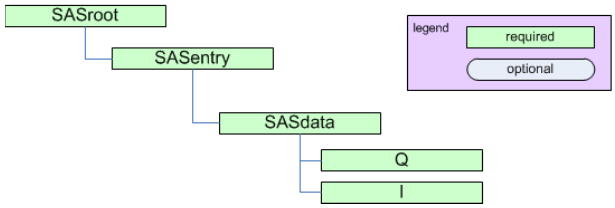
Description:

Implementation of the canSAS standard to store reduced small-angle scattering data of any dimension.

For more details, see:

- http://www.cansas.org/
- http://www.cansas.org/formats/canSAS1d/1.1/doc/
- http://cansas-org.github.io/canSAS2012/
- https://github.com/canSAS-org/NXcanSAS_examples

The minimum requirements for *reduced* small-angle scattering data as described by canSAS are summarized in the following figure:



The minimum requirements for *reduced* small-angle scattering data. (**full image**)

Implementation of canSAS standard in NeXus

This application definition is an implementation of the canSAS standard for storing both one-dimensional and multi-dimensional *reduced* small-angle scattering data.

- NXcanSAS is for reduced SAS data and metadata to be stored together in one file.
- *Reduced* SAS data consists of $I(\vec{Q})$ or $I(|\vec{Q}|)$
- External file links are not to be used for the reduced data.
- A good practice/practise is, at least, to include a reference to how the data was acquired and processed. Yet this is not a requirement.
- There is no need for NXcanSAS to refer to any raw data.

The canSAS data format has a structure similar to NeXus, not identical. To allow canSAS data to be expressed in NeXus, yet identifiable by the canSAS standard, an additional group attribute `canSAS_class` was introduced. Here is the mapping of some common groups.

group (*)	NX_class	canSAS_class
sasentry	NXentry	SASentry
sasdata	NXdata	SASdata
sasdetector	NXdetector	SASdetector
sasinstrument	NXinstrument	SASinstrument

group (*)	NX_class	canSAS_class
sasnote	NXnote	SASnote
sasprocess	NXprocess	SASprocess
sasprocessnote	NXcollection	SASprocessnote
sastransmission	NXdata	SAStransmission_spectrum
sassample	NXsample	SASsample
sassource	NXsource	SASsource

(*) The name of each group is a suggestion, not a fixed requirement and is chosen as fits each data file. See the section on defining NXDL group and field names.

Symbols:

No symbol table

Groups cited:

NXaperture, NXcollection, NXcollimator, NXdata, NXdetector, NXentry, NXinstrument, NXnote, NXprocess, NXsample, NXsource

Structure:

(entry): NXentry

Place the canSAS `SASentry` group as a child of a NeXus `NXentry` group (when data from multiple techniques are being stored) or as a replacement for the `NXentry` group.

Note: It is required for all numerical objects to provide a *units* attribute that describes the engineering units. Use the Unidata UDunits [1] specification as this is compatible with various community standards.

[1] The UDunits specification also includes instructions for derived units.

@default: NX_CHAR

Declares which NXdata group contains the data to be shown by default. It is needed to resolve ambiguity when more than one NXdata group exists. The value is the name of the default NXdata group. Usually, this will be the name of the first *SASdata* group.

@canSAS_class: NX_CHAR

Official canSAS group: **SASentry**

Obligatory value: `SASentry`

@version: NX_CHAR

Describes the version of the canSAS standard used to write this data. This must be a text (not numerical) representation. Such as:

```
@version="1.0"
```

Obligatory value: `1.0`

definition: NX_CHAR

Official NeXus NXDL schema to which this subentry conforms.

Obligatory value: `NXcanSAS`

title: NX_CHAR

Title of this *SASentry*.

run: NX_CHAR

Run identification for this *SASentry*. For many facilities, this is an integer. Use multiple instances of `run` as needed, keeping in mind that HDF5 requires unique names for all entities in a group.

@name: NX_CHAR

Optional string attribute to identify this particular *run*. Could use this to associate (correlate) multiple *SASdata* elements with *run* elements.

(data): NXdata

A *SASData* group contains reduced a single small-angle scattering data set that can be represented as $I(\vec{Q})$ or $I(|\vec{Q}|)$.

Q can be either a vector ($\vec{Q}$) or a vector magnitude ($|\vec{Q}|$)

The name of each *SASdata* group must be unique within a SASentry group. Suggest using names such as `sasdata01`.

NOTE: For the first *SASdata* group, be sure to write the chosen name into the *SASentry/@default* attribute, as in:

```
SASentry/@default="sasdata01"
```

A *SASdata* group has several attributes:

- I_axes
- Q_indices
- Mask_indices

To indicate the dependency relationships of other varied parameters, use attributes similar to `@Mask_indices` (such as `@Temperature_indices` or `@Pressure_indices`).

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SASdata

Obligatory value: `SASdata`

@signal: NX_CHAR

Name of the default data field.

Obligatory value:

- `I`: For canSAS **SASdata**, this is always “I”.

@I_axes: NX_CHAR

String array that defines the independent data fields used in the default plot for all of the dimensions of the *signal* field (the *signal* field is the field in this group that is named by the `signal` attribute of this group). One entry is provided for every dimension of the `I` data object. Such as:

```
@I_axes="Temperature", "Time", "Pressure", "Q", "Q"
```

Since there are five items in the list, the intensity field of this example `I` must be a five-dimensional array (rank=5).

@Q_indices: NX_INT

Integer or integer array that describes which indices (of the I data object) are used to reference the `Q` data object. The items in this array use zero-based indexing. Such as:

```
@Q_indices=1,3,4
```

which indicates that `Q` requires three indices from the I data object: one for time and two for Q position. Thus, in this example, the `Q` data is time-dependent: $\vec{Q}(t)$.

@Mask_indices: NX_CHAR

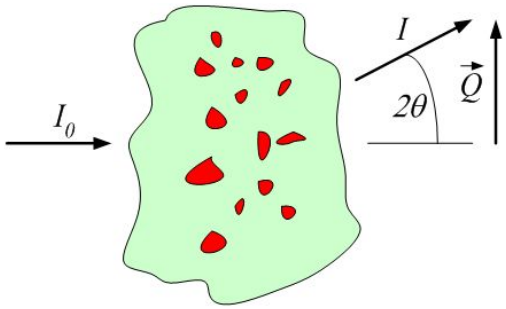
Integer or integer array that describes which indices (of the I data object) are used to reference the `Mask` data object. The items in this array use zero-based indexing. Such as:

```
@Mask_indices=3,4
```

which indicates that Q requires two indices from the I data object for Q position.

Q: NX_NUMBER {units=NX_PER_LENGTH}

Array of Q data to accompany I.



The $\vec{Q}$ geometry. (**full image**)

Q may be represented as either the three-dimensional scattering vector $\vec{Q}$ or the magnitude of the scattering vector, $|\vec{Q}|$.

$$|\vec{Q}| = (4\pi/\lambda)sin(\theta)$$

When we write Q, we may refer to either or both of $|\vec{Q}|$ or $\vec{Q}$, depending on the context.

@resolution: NX_CHAR

(optional) Generally, this is the principal resolution of each Q. Names the data object (in this SASdata group) that provides the Q resolution to be used for data analysis. Such as:

```
@resolution="Qdev"
```

This may be used to describe the slit-length at each datum. Use a subgroup to describe any supplementary resolution data.

To specify two-dimensional resolution, such as (*dQw*, *dQl*), use a string array, such as:

```
@resolution="dQw", "dQl"
```

The name of the dataset containing the Q resolution is flexible. The name must be unique in the *SASdata* group.

There may also be a subdirectory (optional) with constituent components.

This pattern will demonstrate how to introduce further as-yet unanticipated terms related to the data.

By default, the values of the resolution data object are assumed to be one standard deviation of any function used to approximate the resolution function. This equates to the width of the gaussian distribution if a Gaussian is chosen. See the `@resolution_description` attribute.

Note

To report uncertainty in reported Q values, use the `@uncertainties` attribute. It is possible for both `@resolution` and `uncertainties` to be reported.

@resolution_description: NX_CHAR

(optional) Generally, this describes the Q `@resolution` data object. By default, the value is assumed to be “Gaussian”. These are suggestions:

- Gaussian
- Lorentzian
- Square : note that the width of the square would be ~1.4 times the standard deviation specified in the vector
- Triangular
- Sawtooth-outward : vertical edge pointing to larger Q
- Sawtooth-inward vertical edge pointing to smaller Q
- Bin : range of values contributing (for example, when 2-D detector data have been reduced to a 1-D $I(|Q|)$ dataset)

For other meanings, it may be necessary to provide further details

such as the function used to assess the resolution. In such cases, use additional datasets or a NXnote subgroup to include that detail.

I: NX_NUMBER

Array of intensity (I) data.

The intensity may be represented in one of these forms:

absolute units: $d\Sigma/d\Omega(Q)$ differential cross-section per unit volume per unit solid angle (typical units: 1/cm/sr)

absolute units: $d\sigma/d\Omega(Q)$ differential cross-section per unit atom per unit solid angle (typical units: cm^2)

arbitrary units: $I(Q)$ usually a ratio of two detectors but units are meaningless (typical units: a.u.)

This presents a few problems for analysis software to sort out when reading the data. Fortunately, it is possible to analyze the *units* to determine which type of intensity is being reported and make choices at the time the file is read. But this is an area for consideration and possible improvement.

One problem arises with software that automatically converts data into some canonical units used by that software. The software should not convert units between these different types of intensity indiscriminately.

A second problem is that when arbitrary units are used, then the set of possible analytical results is restricted. With such units, no meaningful volume fraction or number density can be determined directly from $I(Q)$.

In some cases, it is possible to apply a factor to convert the arbitrary units to an absolute scale. This should be considered as a possibility of the analysis process.

@uncertainties: NX_CHAR

Generally, this is the estimate of the uncertainty of each I. Typically the estimated standard deviation. For Poisson statistics, use $1/\sqrt{I}$.

(optional for numerical arrays) Name of the data object (in this SASdata group) that provides the uncertainty to be used for data analysis.

Idev is the canonical name from the 1D standard. The multi-D standard allows for this name to be described in this attribute. Such as:

```
@uncertainties="Idev"
```

@scaling_factor: NX_CHAR

(optional) Names the field (a.k.a. dataset) that contains a factor to multiply `I`. By default, this value is unity. Should an uncertainty be associated with the scaling factor field, the field containing that uncertainty would be designated via the `uncertainties` attribute. Such as:

```
I : NX_NUMBER
    @uncertainties="Idev" : NX_CHAR
    @scaling_factor="I_scaling" : NX_CHAR
Idev : NX_NUMBER
I_scaling : NX_NUMBER
    @uncertainties="I_scaling_dev" : NX_CHAR
I_scaling_dev : NX_NUMBER
```

The exact names for `I_scaling` and `I_scaling_dev` are not defined by NXcanSAS. The user has the flexibility to use names different than those shown in this example.

Idev: (optional) NX_NUMBER {units=NX_PER_LENGTH}

Estimated **uncertainty** (usually standard deviation) in I. Must have the same units as I.

When present, the name of this field is also recorded in the *uncertainties* attribute of *I*, as in:

```
I/@uncertainties="Idev"
```

Qdev: (optional) NX_NUMBER {units=NX_PER_LENGTH}

Estimated **resolution** (usually standard deviation) in Q. Must have the same units as Q.

When present, the name of this field is also recorded in the *resolution* attribute of *Q*, as in:

```
Q/@resolution="Qdev"

Q/@resolution="dQw", "dQl"
```

dQw: (optional) NX_NUMBER {units=NX_PER_LENGTH}

Q **resolution** along the axis of scanning (the high-resolution *slit width* direction). Useful for defining resolution data from slit-smearing instruments such as Bonse-Hart geometry. Must have the same units as Q.

When present, the name of this field is also recorded in the *uncertainties* attribute of *Q*, as in:

```
Q/@uncertainties="dQw", "dQl"
```

dQl: (optional) NX_NUMBER {units=NX_PER_LENGTH}

Q **resolution** perpendicular to the axis of scanning (the low-resolution *slit length* direction). Useful for defining resolution data from slit-smearing instruments such as Bonse-Hart geometry. Must have the same units as Q.

When present, the name of this field is also recorded in the *uncertainties* attribute of *Q*, as in:

```
Q/@uncertainties="dQw", "dQl"
```

Qmean: (optional) NX_NUMBER {units=NX_PER_LENGTH}

Mean value of Q for this data point. Useful when describing data that has been binned from higher-resolution data. It is unexpected for `Q` and `Qmean` to have different units.

ShadowFactor: (optional) NX_CHAR {units=NX_DIMENSIONLESS}

A numerical factor applied to pixels affected by the beam stop penumbra. Used in data files from NIST/NCNR instruments.

See: J.G. Barker and J.S. Pedersen (1995) *J. Appl. Cryst.* **28**, 105-114.

(instrument): (optional) NXinstrument

Description of the small-angle scattering instrument.

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SASinstrument

Obligatory value: `SASinstrument`

(collimator): (optional) NXcollimator

Description of a collimating element in the instrument.

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SAScollimation

Obligatory value: `SAScollimation`

length: (optional) NX_NUMBER {units=NX_LENGTH}

Amount/length of collimation inserted (as on a SANS instrument)

distance: (optional) NX_NUMBER {units=NX_LENGTH}

Distance from this collimation element to the sample

aperture: (optional) NXaperture

Name of “aperture” is only a suggestion. Base class could be either **NXpinhole** or **NXslit**. But **NXaperture** is generic and limits the variation in data files.

shape: NX_CHAR

describe the type of aperture (pinhole, 4-blade slit, Soller slit, ...)

x_gap: (optional) NX_NUMBER {units=NX_LENGTH}

opening along the x axis

y_gap: (optional) NX_NUMBER {units=NX_LENGTH}

opening along the y axis

(detector): (optional) NXdetector

Description of a detector in the instrument.

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SASdetector

Obligatory value: `SASdetector`

name: NX_CHAR

Identifies the name of this detector

SDD: (optional) NX_NUMBER {units=NX_LENGTH}

Distance between sample and detector.

Note: In NXdetector, the `distance` field records the distance to the previous component ... most often the sample. This use is the same as `SDD` for most SAS instruments but not all. For example, Bonse-Hart cameras have one or more crystals between the sample and detector.

We define here the field `SDD` to document without ambiguity the distance between sample and detector.

slit_length: (optional) NX_NUMBER {units=NX_PER_LENGTH}

Slit length of the instrument for this detector, expressed in the same units as Q.

x_position: (optional) NX_CHAR

Location of the detector in x

y_position: (optional) NX_CHAR

Location of the detector in y

roll: (optional) NX_CHAR

Rotation of the detector about the z axis (roll)

pitch: (optional) NX_CHAR

Rotation of the detector about the x axis (roll)

yaw: (optional) NX_CHAR

Rotation of the detector about the y axis (yaw)

beam_center_x: (optional) NX_FLOAT {units=NX_LENGTH}

Position of the beam center on the detector.

This is the x position where the direct beam would hit the detector plane. This is a length, not a pixel position, and can be outside of the actual detector.

beam_center_y: (optional) NX_FLOAT {units=NX_LENGTH}

Position of the beam center on the detector.

This is the y position where the direct beam would hit the detector plane. This is a length, not a pixel position, and can be outside of the actual detector.

x_pixel_size: (optional) NX_FLOAT {units=NX_LENGTH}

Size of each detector pixel. If it is scalar all pixels are the same size

y_pixel_size: (optional) NX_FLOAT {units=NX_LENGTH}

Size of each detector pixel. If it is scalar all pixels are the same size

(source): (optional) NXsource

Description of the radiation source.

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SASsource

Obligatory value: `SASsource`

radiation: NX_CHAR

Name of the radiation used. Note that this is **not** the name of the facility!

Any of these values:

- `Spallation Neutron Source`
- `Pulsed Reactor Neutron Source`
- `Reactor Neutron Source`
- `Synchrotron X-ray Source`
- `Pulsed Muon Source`
- `Rotating Anode X-ray`
- `Fixed Tube X-ray`
- `UV Laser`
- `Free-Electron Laser`
- `Optical Laser`
- `Ion Source`
- `UV Plasma Source`
- `neutron`
- `x-ray`
- `muon`
- `electron`
- `ultraviolet`
- `visible light`
- `positron`
- `proton`

beam_shape: (optional) NX_CHAR

Text description of the shape of the beam (incident on the sample).

incident_wavelength: (optional) NX_NUMBER {units=NX_WAVELENGTH}

wavelength (λ) of radiation incident on the sample

wavelength_min: (optional) NX_NUMBER {units=NX_WAVELENGTH}

Some facilities specify wavelength using a range. This is the lowest wavelength in such a range.

wavelength_max: (optional) NX_NUMBER {units=NX_WAVELENGTH}

Some facilities specify wavelength using a range. This is the highest wavelength in such a range.

incident_wavelength_spread: (optional) NX_NUMBER {units=NX_WAVELENGTH}

Some facilities specify wavelength using a range. This is the width (FWHM) of such a range.

beam_size_x: (optional) NX_NUMBER {units=NX_LENGTH}

Size of the incident beam along the x axis.

beam_size_y: (optional) NX_NUMBER {units=NX_LENGTH}

Size of the incident beam along the y axis.

(sample): NXsample

Description of the sample.

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SASsample

Obligatory value: `SASsample`

name: NX_CHAR

ID: Text string that identifies this sample.

thickness: (optional) NX_FLOAT {units=NX_LENGTH}

Thickness of this sample

transmission: (optional) NX_NUMBER {units=NX_DIMENSIONLESS}

Transmission (I/I_0) of this sample. Note that there is no *units* attribute as this number is dimensionless.

temperature: (optional) NX_NUMBER {units=NX_TEMPERATURE}

Temperature of this sample.

details: (optional) NX_CHAR

Any additional sample details.

x_position: (optional) NX_CHAR

Location of the sample in x

y_position: (optional) NX_CHAR

Location of the sample in y

roll: (optional) NX_CHAR

Rotation of the sample about the z axis (roll)

pitch: (optional) NX_CHAR

Rotation of the sample about the x axis (roll)

yaw: (optional) NX_CHAR

Rotation of the sample about the y axis (yaw)

(process): (optional) NXprocess

Description of a processing or analysis step.

Add additional fields as needed to describe value(s) of any variable, parameter, or term related to the *SASprocess* step. Be sure to include *units* attributes for all numerical fields.

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SASprocess

Obligatory value: `SASprocess`

name: (optional) NX_CHAR

Optional name for this data processing or analysis step

date: (optional) NX_DATE_TIME

Optional date for this data processing or analysis step. [2]

[2] *(1, 2)*

ISO-8601 standard time representation.

NeXus dates and times are reported in ISO-8601 (e.g., `yyyy-mm-ddThh:mm:ss`) or modified ISO-8601 (e.g., `yyyy-mm-dd hh:mm:ss`).

See: http://www.w3.org/TR/NOTE-datetime or http://en.wikipedia.org/wiki/ISO_8601 for more details.

description: (optional) NX_CHAR

Optional description for this data processing or analysis step

term: (optional) NX_CHAR

Specifies the value of a single variable, parameter, or term (while defined here as a string, it could be a number) related to the *SASprocess* step.

Note: The name *term* is not required, it could take any name, as long as the name is unique within this group.

(note): (optional) NXnote

Any additional notes or subprocessing steps will be documented here.

An **NXnote** group can be added to any NeXus group at or below the **NXentry** group. It is shown here as a suggestion of a good place to *consider* its use.

(collection): (optional) NXcollection

Describes anything about *SASprocess* that is not already described.

Any content not defined in the canSAS standard can be placed at this point.

Note: The name of this group is flexible, it could take any name, as long as it is unique within the **NXprocess** group.

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SASprocessnote

Obligatory value: `SASprocessnote`

(collection): (optional) NXcollection

Free form description of anything not covered by other elements.

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SASnote

Obligatory value: `SASnote`

(data): (optional) NXdata

The *SAStransmission_spectrum* element

This describes certain data obtained from a variable-wavelength source such as pulsed-neutron source.

The name of each *SAStransmission_spectrum* group must be unique within a SASentry group. Suggest using names such as `sastransmission_spectrum01`.

@canSAS_class: NX_CHAR

Official canSAS group: NXcanSAS (contributed definition); SAStransmission_spectrum

Obligatory value: `SAStransmission_spectrum`

@signal: NX_CHAR

Name of the default data field.

Obligatory value:

- T: For **SAStransmission_spectrum**, this is always “T”.

@T_axes: NX_CHAR

Obligatory value:

- T: the wavelengths field (as a dimension scale) corresponding to this transmission

@name: NX_CHAR

Identify what type of spectrum is being described. It is expected that this value will take either of these two values:

value	meaning
sample	measurement with the sample and container
can	measurement with just the container

@timestamp: NX_DATE_TIME

ISO-8601 time [2]

lambda: NX_NUMBER {units=NX_WAVELENGTH}

Wavelength of the radiation.

This array is of the same shape as `T` and `Tdev`.

T: NX_NUMBER {units=NX_DIMENSIONLESS}

Transmission value (I/I_0)

This array is of the same shape as `lambda` and `Tdev`.

@uncertainties: NX_CHAR

Estimate of the uncertainty of each transmission T.

Typically:

@uncertainties="Tdev"

Tdev: NX_NUMBER {units=NX_PER_LENGTH}

Estimated uncertainty (usually standard deviation) in T. Must have the same units as T.

When present, the name of this field is also recorded in the *uncertainties* attribute of *T*, as in:

```
T/@uncertainties="Tdev"
```

This array is of the same shape as `lambda` and `T`.

NXDL Source:
https://github.com/nexusformat/definitions/blob/master/applications/NXcanSAS.nxdl.xml