

NeXus: a common data format for neutron, x-ray, and muon science

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http://nexusformat.org

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NeXus is a common data format for neutron, x-ray, and muon science. It is developed as an international standard by scientists and programmers representing major scientific facilities in Europe, Asia, Australia, and North America in order to facilitate greater cooperation in the analysis and visualization of neutron, x-ray, and muon data.

NeXus home: http://nexusformat.org

This manual is also available in a PDF version.

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Part I

Contents

CHAPTER

ONE

PREFACE

With this edition of the manual, NeXus introduces a complete version of the documentation of the NeXus standard. The content from the wiki has been converted, augmented (in some parts significantly), clarified, and indexed. The NeXus Definition Language (NXDL) is introduced now to define base classes and application definitions. NXDL replaces the previous method (meta-DTD) to define NeXus classes. NeXus base classes and instrument definitions are now assigned to one of three classifications:

- 1. base classes (that represent the components used to build a NeXus data file),
- 2. *application definitions* (used to define a minimum set of data for a specific purpose such as scientific data processing or an instrument definition), and
- 3. *contributed definitions* (definitions and specifications that are in an incubation status before ratification by the NIAC).

Additional examples have been added to respond to inquiry from the users of the NeXus standard about implementation and usage. Hopefully, the improved documentation with more examples and the new NXDL will reduce the learning barriers incurred by those new to NeXus.

1.1 Representation of data examples

Most of the examples of data files have been written in a format intended to show the structure of the file rather than the data content. In some cases, where it is useful, some of the data is shown. Consider this prototype example:

```
entry: NXentry
            instrument: NXinstrument
2
                    detector: NXdetector
                             data:[]
4
                                      @axes = "bins"
5
                                      @long name = "strip detector 1-D array"
6
                                      @signal = 1
8
                             bins:[0, 1, 2, ... 1023]
                                      @long_name = "bin index numbers"
            sample:NXsample
10
                    name = "zeolite"
11
            data: NXdata
12
```

```
data --> /entry/instrument/detector/data bins --> /entry/instrument/detector/bins
```

Some words on the notation:

- Hierarchy is represented by indentation. Objects on the same indentation level are in the same group
- The combination name: NXclass denotes a NeXus group with name name and class NXclass.
- A simple name (no following class) denotes a data field. An equal sign is used to show the value, where this is important to the example.
- Sometimes, a data type is specified and possibly a set of dimensions. For example, energy: NX_NUMBER[NE] says energy is a 1-D array of numbers (either integer or floating point) of length NE.
- Attributes are noted as @name=value pairs separated by comma. The @ symbol only indicates this is an attribute. The @ symbol is not part of the attribute name.
- Links are shown with a text arrow --> indicating the source of the link (using HDF5 notation listing the sequence of names).
- [Line 1] shows that there is one group at the root level of the file named entry. This group is of type NXentry which means it conforms to the specification of the NXentry NeXus base class. Using the HDF5 nomenclature, we would refer to this as the /entry group.
- [Lines 2, 10, and 12] The /entry group contains three subgroups: instrument, sample, and data. These groups are of type NXinstrument, NXsample, and NXdata, respectively.
- [Line 4] The data of this example is stored in the /entry/instrument/detector group in the dataset called data (HDF5 path is /entry/instrument/detector/data). The indication of data: [] says that data is an array of unspecified dimension(s).
- [Lines 5-7] There are three attributes of /entry/instrument/detector/data: axes, long name, and signal.
- [Line 8] (reading bins: [0, 1, 2, ... 1023]) shows that bins is a 1-D array of length presumably 1024. A small, representative selection of values are shown.
- [Line 9] an attribute that shows a descriptive name of /entry/instrument/detector/bins. This attribute might be used by a NeXus client while plotting the data.
- [Line 11] (reading name = "zeolite") shows how a string value is represented.
- [Lines 13-14] The /entry/data group has two datasets that are actually linked as shown. (As you will see later, the NXdata group is required and enables NeXus clients to easily determine what to offer for display on a default plot.)

1.2 Class path specification

In some places in this documentation, a path may be shown using the class types rather than names. For example: /NXentry/NXinstrument/NXcrystal/wavelength identifies a dataset called

wavelength that is inside a group of type NXcrystal inside a group of type NXinstrument inside a group of type NSentry. This nomenclature is used when the exact name of each group is either unimportant or not specified. Often, this will be used in a NXDL specification to indicate the connections of a link.



NEXUS: USER MANUAL

Contents:

2.1 NeXus Introduction

In recent years, a community of scientists and computer programmers working in neutron and synchrotron facilities around the world came to the conclusion that a common data format would fulfill a valuable function in the scattering community. As instrumentation becomes more complex and data visualization become more challenging, individual scientists, or even institutions, have found it difficult to keep up with new developments. A common data format makes it easier, both to exchange experimental results and to exchange ideas about how to analyze them. It promotes greater cooperation in software development and stimulates the design of more sophisticated visualization tools. For additional background information see history (not converted yet) (page 157).

quote

The programmers who produce intermediate files for storing analyzed data should agree on simple interchange rules.

This section is designed to give a brief introduction to NeXus, the data format and tools that have been developed in response to these needs. It explains what a modern data format such as NeXus is and how to write simple programs to read and write NeXus files.

2.1.1 What is NeXus?

The NeXus data format has four components:

- 1. A Set of Design Principles (page 10) to help people understand what is in the data files.
- 2. A Set of Data Storage Objects (page 14) (base classes and application definitions) to allow the development of more portable analysis software.
- 3. A Set of Subroutines (page 15) (utilities) to make it easy to read and write NeXus data files.

4. *NeXus Scientific Community* (page 15) provides the scientific data, advice, and continued involvement with the NeXus standard. NeXus provides a forum for the scientific community to exchange ideas in data storage.

The NeXus Application-Programmer Interface (NAPI), which provides the set of subroutines for reading and writing NeXus data files, is described briefly in *NAPI: The NeXus Application Programming Interface* (page 19). (Further details are provided in the NAPI chapter of Volume II of this documentation.)

The principles guiding the design and implementation of the NeXus standard are described in *NeXus Design* (page 22).

Base classes and applications, which comprise the data storage objects used in NeXus data files, are detailed in the *Class Definitions* chapter of Volume II of this documentation.

Additionally, a brief list describing the set of NeXus Utilities available to browse, validate, translate, and visualise NeXus data files is provided in *utilities* (not converted yet) (page 157).

A Set of Design Principles

NeXus data files contain four types of entity: data groups, data fields, attributes, and links. See *Data Groups* (page 23) for more details.

- 1. *Data Groups* (page 23) *Data groups* are like folders that can contain a number of fields and/or other groups.
- 2. *Data Fields* (page 23) *Data fields* can be scalar values or multidimensional arrays of a variety of sizes (1-byte, 2-byte, 4-byte, 8-byte) and types (characters, integers, floats). In HDF, fields are represented as HDF *Scientific Data Sets* (also known as SDS).
- 3. *Data Attributes* (page 23) Extra information required to describe a particular group or field, such as the data units, can be stored as a data attribute.
- 4. *Data Links* (page 25) Links are used to reference the plottable data from *NXdata* (page 54) when the data is provided in other groups such as *NXmonitor* (page 72) or *NXdetector* (page 56).

In fact, a NeXus file can be viewed as a computer file system. Just as files are stored in folders (or subdirectories) to make them easy to locate, so NeXus fields are stored in groups. The group hierarchy is designed to make it easy to navigate a NeXus file.

Example of a NeXus File

The following diagram shows an example of a NeXus data file example; NeXus data file represented as a tree structure. hierarchy; example NeXus data file

Note that each field is identified by a name, such as counts, but each group is identified both by a name and, after a colon as a delimiter, the class type, e.g., monitor: NXmonitor). The class types, which all begin with NX, define the sort of fields that the group should contain, in this case, counts from a beamline monitor. The hierarchical design, with data items nested in groups, makes it easy to identify information if you are browsing through a file.

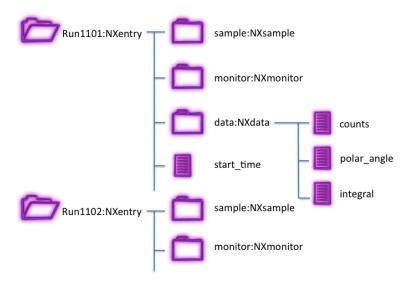


Figure 2.1: Example of a NeXus data file

Important Classes

Here are some of the important classes found in nearly all NeXus files. A complete list can be found in the NeXus Design section (*NeXus Design* (page 22)).

Note: *NXentry* (page 59) and *NXdata* (page 54) are the only two classes **required** in a valid NeXus data file.

- NXentry (page 59) (Required:) The top level of any NeXus file contains one or more groups with the class NXentry. These contain all the data that is required to describe an experimental run or scan. Each NXentry typically contains a number of groups describing sample information (class NXsample), instrument details (class NXinstrument), and monitor counts (class NXmonitor).
- **NXdata** (page 54) (Required:) Each NXentry group contains one or more groups with class NXdata. These groups contain the experimental results in a self-contained way, i.e., it should be possible to generate a sensible plot of the data from the information contained in each NXdata group. That means it should contain the axis labels and titles as well as the data.
- **NXsample** (page 79) A NXentry group will often contain a group with class NXsample. This group contains information pertaining to the sample, such as its chemical composition, mass, and environment variables (temperature, pressure, magnetic field, etc.).
- **NXinstrument** (page 68) There might also be a group with class NXinstrument. This is designed to encapsulate all the instrumental information that might be relevant to a measurement, such as flight paths, collimations, chopper frequencies, etc.

Since an instrument can comprise several beamline components each defined by several parameters, they are each specified by a separate group. This hides the complexity from generic file browsers, but makes the information available in an intuitively obvious way if it is required.

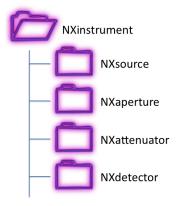


Figure 2.2: NXinstrument excerpt

Simple Data File Example

NeXus data files do not need to be complicated. In fact, the following diagram shows an extremely simple NeXus file (in fact, the simple example shows the minimum information necessary for a NeXus data file) that could be used to transfer data between programs. (Later in this section, we show how to write and read this simple example.)

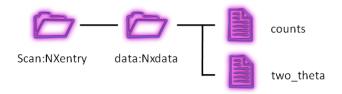


Figure 2.3: Simple Data File Example

This illustrates the fact that the structure of NeXus files is extremely flexible. It can accommodate very complex instrumental information, if required, but it can also be used to store very simple data sets. In the next example, a NeXus data file is shown as XML:

verysimple.xml: A very simple NeXus Data file (in XML)

```
NAPItype="NX INT64[15]"
12
                       long_name="photodiode counts"
13
                       signal="NX_INT32:1"
14
                       axes="two_theta">
15
                                 1193
                                             4474
16
                                53220
                                           274310
17
                               515430
                                          827880
                              1227100
                                         1434640
19
                              1330280
                                        1037070
20
                                          316460
                               598720
21
                                             1000
                                56677
22
                                 1000
23
                     </counts>
24
                     <two theta
25
                       NAPItype="NX_FLOAT64[15]"
26
                       units="degrees"
27
                       long name="two theta (degrees)">
28
                             18.90940
                                                18.90960
                                                                   18.90980
                                                                                       18.91000
29
                              18.91020
                                                18.91040
                                                                   18.91060
                                                                                       18.91080
30
                                                                   18.91140
                             18.91100
                                                18.91120
                                                                                       18.91160
31
                              18.91180
                                                18.91200
                                                                   18.91220
32
                     </two_theta>
33
              </NXdata>
34
            </NXentry>
35
36
```

NeXus files are easy to create. This example NeXus file was created using a short Python program and NeXpy:

verysimple.py: Using NeXpy to write a very simple NeXus Data file (in HDF5)

```
1
   # This example uses NeXpy to build the verysimple.nx5 data file.
2
3
   from nexpy.api import nexus
4
5
   angle = [18.9094, 18.9096, 18.9098, 18.91, 18.9102,
           18.9104, 18.9106, 18.9108, 18.911, 18.9112,
7
        18.9114, 18.9116, 18.9118, 18.912, 18.9122]
8
   diode = [1193, 4474, 53220, 274310, 515430, 827880,
9
            1227100, 1434640, 1330280, 1037070, 598720,
10
        316460, 56677, 1000, 1000]
11
12
   two theta = nexus.SDS(angle, name="two theta",
13
                  units="degrees",
14
              long_name="two_theta (degrees)")
15
   counts = nexus.SDS(diode, name="counts", long_name="photodiode counts")
16
   data = nexus.NXdata(counts,[two_theta])
17
   data.nxsave("verysimple.nx5")
18
19
  # The very simple.xml file was built with this command:
20
  # nxconvert -x verysimple.nx5 verysimple.xml
21
```

```
2 # and then hand-edited (line breaks) for display.
```

A Set of Data Storage Objects

If the design principles are followed, it will be easy for anyone browsing a NeXus file to understand what it contains, without any prior information. However, if you are writing specialized visualization or analysis software, you will need to know precisely what specific information is contained in advance. For that reason, NeXus provides a way of defining the format for particular instrument types, such as time-of-flight small angle neutron scattering. This requires some agreement by the relevant communities, but enables the development of much more portable software.

The set of data storage objects is divided into three parts: base classes, application definitions, and contributed definitions. The base classes represent a set of components that define the dictionary of all possible terms to be used with that component. The application definitions specify the minimum required information to satisfy a particular scientific or data analysis software interest. The contributed definitions have been submitted by the scientific community for incubation before they are adopted by the NIAC or for availability to the community.

These instrument definitions are formalized as XML files, using NXDL, (as described in the NXDL chapter in Volume II of this documentation) to specify the names of data fields, and other NeXus data objects. The following is an example of such a file for the simple NeXus file shown above.

verysimple.nxdl.xml: A very simple NeXus Definition Language (NXDL) file

```
<?xml version="1.0" ?>
   <definition
2
    xmlns="http://definition.nexusformat.org/nxdl/3.1"
3
    xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
4
     xsi:schemaLocation="http://definition.nexusformat.org/nxdl/3.1 .../nxdl.xsd"
5
    category="base"
6
    name="verysimple"
7
     version="1.0"
8
     svnid="$Id: objects.rst 886 2011-09-13 05:32:35Z Pete Jemian $"
9
     type="group" extends="NXobject">
10
11
12
     <doc>
           A very simple NeXus NXDL file
13
     </doc>
14
     <group type="NXentry">
15
           <group type="NXdata">
16
             <field name="counts" type="NX_INT" units="NX_UNITLESS">
17
18
                    <doc>counts recorded by detector</doc>
             </field>
19
              <field name="two_theta" type="NX_FLOAT" units="NX_ANGLE">
20
                    <doc>rotation angle of detector arm</doc>
21
             </field>
22
23
           </group>
     </group>
24
   </definition>
25
```

This chapter has several examples of writing and reading NeXus data files. If you want to define the format of a particular type of NeXus file for your own use, e.g. as the standard output from a program, you are encouraged to *publish* the format using this XML format. An example of how to do this is shown in the section titled Creating a NXDL Specification (*nxdl_tutorial-creatingnxdlspec* (*not converted yet*) (page 157)).

A Set of Subroutines

NeXus data files are high-level so the user only needs to know how the data are referenced in the file but does not need to be concerned where the data are stored in the file. Thus, the data are most easily accessed using a subroutine library tuned to the specifics of the data format.

In the past, a data format was defined by a document describing the precise location of every item in the data file, either as row and column numbers in an ASCII file, or as record and byte numbers in a binary file. It is the job of the subroutine library to retrieve the data. This subroutine library is commonly called an application-programmer interface or API.

For example, in NeXus, a program to read in the wavelength of an experiment would contain lines similar to the following:

Simple example of reading data using the NeXus API

```
NXopendata (fileID, "wavelength");
NXgetdata (fileID, lambda);
NXclosedata (fileID);
```

In this example, the program requests the value of the data that has the label wavelength, storing the result in the variable lambda. fileID is a file identifier that is provided by NeXus when the file is opened.

We shall provide a more complete example when we have discussed the contents of the NeXus files.

NeXus Scientific Community

NeXus began as a group of scientists with the goal of defining a common data storage format to exchange experimental results and to exchange ideas about how to analyze them.

The NeXus Scientific Community provides the scientific data, advice, and continued involvement with the NeXus standard. NeXus provides a forum for the scientific community to exchange ideas in data storage through the NeXus wiki. ¹

The NeXus International Advisory Committee (see *NIAC description* (page 157)) supervises the development and maintenance of the NeXus common data format for neutron, x-ray, and muon science. The NIAC supervises a technical committee to oversee the NeXus Application Programmer Interface (NAPI) and the NeXus class definitions.

¹ http://www.nexusformat.org

2.1.2 Motivations for the NeXus standard in the Scientific Community

By the early 1990s, several groups of scientists in the fields of neutron and X-ray science had recognized a common and troublesome pattern in the data acquired at various scientific instruments and user facilities. Each of these instruments and facilities had a locally defined format for recording experimental data. With lots of different formats, much of the scientists' time was being wasted in the task of writing import readers for processing and analysis programs. As is common, the exact information to be documented from each instrument in a data file evolves, such as the implementation of new high-throughput detectors. Many of these formats lacked the generality to extend to the new data to be stored, thus another new format was devised. In such environments, the documentation of each generation of data format is often lacking.

Three parallel developments have led to NeXus:

- 1. **June 1994:** Mark Koennecke (Paul Scherer Institute, Switzerland) made a proposal using netCDF for the European neutron scattering community while working at the ISIS pulsed neutron facility.
- August 1994: Jon Tischler and Mitch Nelson (Oak Ridge National Laboratory, USA) proposed an HDF-based format as a standard for data storage at the Advanced Photon Source (Argonne National Laboratory, USA).
- 3. **October 1996:** Przemek Klosowski (National Institute of Standards and Technology, USA) produced a first draft of the NeXus proposal drawing on ideas from both sources.

These scientists proposed methods to store data using a self-describing, extensible format that was already in broad use in other scientific disciplines. Their proposals formed the basis for the current design of the NeXus standard which was developed at two workshops, SoftNeSS '95 (NIST Sept. 1995) and SoftNeSS '96 (Argonne Oct. 1996), attended by representatives of a range of neutron and x-ray facilities.

Basic motivations for the NeXus standard

The NeXus API was released in late 1997. Basic motivations for this standard were:

Simple plotting

An important motivation for the design of NeXus was to simplify the creation of a default plot view. While the best representation of a set of observations will vary, depending on various conditions, a good suggestion is often known *a priori*. This suggestion is described in the NXdata element so that any program that is used to browse NeXus data files can provide a *best representation* without request for user input.

A Unified Format for Reduction and Analysis

Another important motivation for NeXus, indeed the *raison d'etre*, was the community need to analyze data from different user facilities. A single data format that is in use at a variety of facilities would provide a major benefit to the scientific community. This unified format should be capable of describing any type of data from the scientific experiments, at any step of the process from data acquisition to data reduction and analysis. This unified format also needs to allow data to be written to storage as efficiently as possible to enable use with high-speed data acquisition.

Self-description, combined with a reliance on a **multi-platform** (and thereby **portable**) data storage format, are valued components of a data storage format where the longevity of the data is expected to be longer than the lifetime of the facility at which it is acquired. As the name implies, self-description within data files is the practice where the structure of the information contained within the file is evident from the file itself. A multi-platform data storage format must faithfully represent the data identically on a variety of computer systems, regardless of the bit order or byte order or word size native to the computer.

The scientific community continues to grow the various types of data to be expressed in data files. This practice is expected to continue as part of the investigative process. To gain broad acceptance in the scientific user community, any data storage format proposed as a standard would need to be **extendable** and continue to provide a means to express the latest notions of scientific data.

The maintenance cost of common data structures meeting the motivations above (self-describing, portable, and extendable) is not insurmountable but is often well-beyond the research funding of individual members of the muon, neutron, and X-ray science communities. Since it is these members that drive the selection of a data storage format, it is necessary for the user cost to be as minimal as possible. In this case, experience has shown that the format must be in the **public-domain** for it to be commonly accepted as a standard. A benefit of the public-domain aspect is that the source code for the API is open and accessible, a point which has received notable comment in the scientific literature.

More recently, NeXus has recognized that part of the scientific community with a desire to write and record scientific data, has small data volumes and a large aversion to the requirement of a complicated API necessary to access data in binary files such as HDF. For such information, the NeXus API has been extended by the addition of the eXtensible Markup Language (XML) ² as an alternative to HDF. XML is a text-based format that supports compression and structured data and has broad usage in business and e-commerce. While possibly complicated, XML files are human readable, and tools for translation and extraction are plentiful. The API has routines to read and write XML data and to convert between HDF and XML.

NeXus as a Common Data Exchange Format By the late 1980s, it had become common practice for a scientific instrument or facility to define its own data format, often at the convenience of the local computer system. Data from these facilities were not easily interchanged due to various differences in computer systems and the compression schemes of binary data. It was necessary to contact the facility to obtain a description so that one could write an import routine in software. Experience with facilities closing (and subsequent lack of access to information describing the facility data format) revealed a significant limitation with this common practice. Further, there existed a N * N number of conversion routines necessary to convert data between various formats. In the next figure, circles represent different data file formats while arrows represent conversion routines. Note that the red circle only maps to one other format.

One early idea has been for NeXus to become the common data exchange format, and thereby reduce the number of data conversion routines from N * N down to 2N, as shown in the next figure.

A Defined Dictionary of Terms

A necessary feature of a standard for the interchange of scientific data is a *defined dictionary* (or *lexicography*) of terms. This dictionary declares the expected spelling and meaning of terms when they are present so that it is not necessary to search for all the variant forms of *energy* when it is used to describe data (e.g., E, e, keV, eV, nrg, ...).

 $^{^2\} XML: http://www.w3.org/XML/.\ There\ are\ many\ other\ descriptions\ of\ XML,\ for\ example:\ http://en.wikipedia.org/wiki/XML$

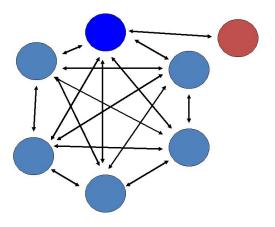


Figure 2.4: *N* separate file formats

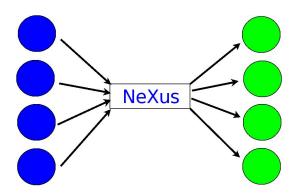


Figure 2.5: N separate file formats joined by a common NeXus converter

NeXus recognized that each scientific specialty has developed a unique dictionary and needs to categorize data using those terms. The NeXus Application Definitions provide the means to document the lexicography for use in data files of that scientific specialty.

2.1.3 NAPI: The NeXus Application Programming Interface

The NeXus API consists of routines to read and write NeXus data files and was written to shield (and hide) the complexity of the HDF API from scientific programmers and users of the NeXus Data Standard.

Further documentation of the NeXus Application Programming Interface (NAPI) for bindings to specific programming language can be obtained from the NeXus development site. ³

For a more detailed description of the internal workings of NAPI that is maintained (mostly) concurrent with code revisions, see the NAPI chapter in Volume II of this documentation and also NeXusIntern.pdf in the NeXus code repository. ⁴ Likely this is only interesting for experienced programmers who wish to hack the NAPI.

How do I write a NeXus file?

The NeXus Application Program Interface (API) provides a set of subroutines that make it easy to read and write NeXus files. These subroutines are available in C, Fortran 77, Fortran 90, Java, Python, C++, and IDL. Access from other languages, such as Python, is anticipated in the near future. It is also possible to read NeXus HDF files in a number of data analysis tools, such as LAMP, ISAW, IgorPro, and Open GENIE. NeXus XML files can be read by any program or library that supports XML.

The API uses a very simple *state* model to navigate through a NeXus file. When you open a file, the API provides a file *handle*, which then stores the current location, i.e. which group and/or field is currently open. Read and write operations then act on the currently open entity. Following the *Simple Data File Example* (page 12), we walk through some parts of a typical NeXus program written in C.

Writing a simple NeXus file

```
#include "napi.h"
2
    int main()
3
4
           NXhandle fileID;
5
           NXopen ('NXfile.nxs', NXACC_CREATE, &fileID);
6
             NXmakegroup (fileID, "Scan", "NXentry");
7
             NXopengroup (fileID, "Scan", "NXentry");
8
                    NXmakegroup (fileID, "data", "NXdata");
9
                    NXopengroup (fileID, "data", "NXdata");
10
                    /\star somehow, we already have arrays tth and counts, each length n\star/
11
                      NXmakedata (fileID, "two_theta", NX_FLOAT32, 1, &n);
12
                      NXopendata (fileID, "two_theta");
13
                            NXputdata (fileID, tth);
14
```

³ http://download.nexusformat.org

⁴ http://svn.nexusformat.org/code/trunk/doc/api/NeXusIntern.pdf

```
NXputattr (fileID, "units", "degrees", 7, NX_CHAR);
15
                      NXclosedata (fileID); /* two_theta */, NX_INT32, 1, &n);
16
                      NXopendata (fileID, "counts");
17
                            NXputdata (fileID, counts);
18
                      NXclosedata (fileID); /* counts */
19
                    NXclosegroup (fileID); /* data */
20
             NXclosegroup (fileID); /* Scan */
21
           NXclose (&fileID);
22
           return;
23
  }
24
```

- [line 6] Open the file NXfile.nxs with *create* access (implying write access). NAPI returns a file identifier of type NXhandle.
- [line 7] Next, we create an NXentry group to contain the scan using NXmakegroup() and then open it for access using NXopengroup().
- [line 9] The plottable data is contained within an NXdata group, which must also be created and opened.
- [line 12] To create a field, call NXmakedata(), specifying the data name, type (NX_FLOAT32), rank (in this case, 1), and length of the array (n). Then, it can be opened for writing.
- [line 14] Write the data using NXputdata().
- [line 15] With the field still open, we can also add some data attributes, such as the data units, which are specified as a character string (type NX_CHAR) that is 7 bytes long.
- [line 16] Then we close the field before opening another. In fact, the API will do this automatically if you attempt to open another field, but it is better style to close it yourself.
- [line 17] The remaining fields in this group are added in a similar fashion. Note that the indentation whenever a new field or group are opened is just intended to make the structure of the NeXus file more transparent.
- [line 20] Finally, close the groups (NXdata and NXentry) before closing the file itself.

How do I read a NeXus file?

Reading a NeXus file is almost identical to writing one. Obviously, it is not necessary to call NXmakedata() since the item already exists, but it is necessary to call one of the query routines to find out the rank and length of the data before allocating an array to store it.

Here is part of a program to read the two-theta array from the file created by Writing a simple NeXus file (page 19) above.

Reading a simple NeXus file

```
NXopen ('NXfile.nxs', NXACC_READ, &fileID);
NXopengroup (fileID, "Scan", "NXentry");
NXopengroup (fileID, "data", "NXdata");
NXopendata (fileID, "two_theta");
NXqetinfo (fileID, &rank, dims, &datatype);
```

```
NXmalloc ((void **) &tth, rank, dims, datatype);
NXgetdata (fileID, tth);
NXclosedata (fileID);
NXclosegroup (fileID);
NXclosegroup (fileID);
NXclose (fileID);
```

How do I browse a NeXus file?

NeXus files can also be viewed by a command-line browser, NXbrowse, which is included with the NeXus API (NAPI: The NeXus Application Programming Interface (page 19)). The following is an example session of using nxbrowse to view a data file from the LRMECS spectrometer at IPNS. The following commands are used in *Using NXbrowse* (page 21) in this session (see the nxbrowse web page):

Using NXbrowse

```
%> nxbrowse lrcs3701.nxs
2
   NXBrowse 3.0.0. Copyright (C) 2000 R. Osborn, M. Koennecke, P. Klosowski
3
           NeXus version = 1.3.3
4
           file name = lrcs3701.nxs
           file time = 2001-02-11 00:02:35-0600
6
           user = EAG/RO
  NX> dir
   NX Group : Histogram1 (NXentry)
    NX Group : Histogram2 (NXentry)
10
  NX> open Histogram1
11
  NX/Histogram1> dir
12
    NX Data : title[44] (NX_CHAR)
13
    NX Data : analysis[7] (NX_CHAR)
14
    NX Data : start_time[24] (NX_CHAR)
15
    NX Data : end_time[24] (NX_CHAR)
    NX Data : run_number (NX_INT32)
17
    NX Group : sample (NXsample)
    NX Group : LRMECS (NXinstrument)
19
    NX Group : monitor1 (NXmonitor)
    NX Group: monitor2 (NXmonitor)
21
    NX Group : data (NXdata)
22
  NX/Histogram1> read title
23
    title[44] (NX_CHAR) = MgB2 PDOS 43.37g 8K 120meV E0@240Hz T0@120Hz
24
  NX/Histogram1> open data
25
  NX/Histogram1/data> dir
26
    NX Data : title[44] (NX CHAR)
27
    NX Data : data[148,750] (NX INT32)
28
    NX Data : time_of_flight[751] (NX_FLOAT32)
29
    NX Data : polar_angle[148] (NX_FLOAT32)
30
  NX/Histogram1/data> read time_of_flight
31
     time_of_flight[751] (NX_FLOAT32) = [ 1900.000000 1902.000000 1904.000000 ...]
32
           units = microseconds
33
           long_name = Time-of-Flight [microseconds]
34
```

```
NX/Histogram1/data> read data
35
     data[148,750] (NX_INT32) = [ 1 1 0 ...]
36
           units = counts
37
           signal = 1
38
           long_name = Neutron Counts
39
           axes = polar_angle:time_of_flight
40
  NX/Histogram1/data> close
  NX/Histogram1> close
42
  NX> quit
```

[line 1] Start NXbrowse from the UNIX command line and open file lrcs3701.nxs from IPNS/LRMECS.

[line 8] List the contents of the current group.

[line 11] Open the NeXus group Histogram1.

[line 23] Print the contents of the NeXus data labelled title.

[line 41] Close the current group.

[line 43] Quits NXbrowse.

The source code of NXbrowse ⁵ provides an example of how to write a NeXus reader. The test programs included in the NeXus API (*NAPI: The NeXus Application Programming Interface* (page 19)) may also be useful to study.

2.2 NeXus Design

This chapter actually defines the rules to use for writing valid NeXus files. An explanation of NeXus objects is followed by the definition of NeXus coordinate systems, the rules for structuring files and the rules for storing single items of data.

Note: In this manual, we use the terms *field*, *data field*, and *data item* synonymously to be consistent with their meaning between NeXus data file instances and NXDL specification files.

The structure of NeXus files is extremely flexible, allowing the storage both of simple data sets, such as a single data array and its axes, and also of highly complex data, such as the simulation results or an entire multi-component instrument. This flexibility is a necessity as NeXus strives to capture data from a wild variety of applications in x-ray, muSR and neutron scattering. The flexibility is achieved through a hierarchical hierarchy structure, with related *fields* data objects; fields collected together into *groups*, making NeXus files easy to navigate, even without any documentation. NeXus files are self-describing, and should be easy to understand, at least by those familiar with the experimental technique.

2.2.1 NeXus Objects and Terms

Before discussing the design of NeXus in greater detail it is necessary to define the objects and terms used by NeXus. These are:

⁵ https://svn.nexusformat.org/code/trunk/applications/NXbrowse/NXbrowse.c

Data Groups (page 23) Group data fields and other groups together. Groups represent levels in the NeXus hierarchy

Data Fields (page 23) Multidimensional arrays and scalars representing the actual data to be stored

Data Attributes (page 23) Additional metadata which can be assigned to groups or data fields

Data Links (page 25) Elements which point to data stored in another place in the file hierarchy

NeXus Classes (page 26) Dictionaries of names possible in the various types of NeXus groups

NeXus Application Definitions (page 27) Describe the content of a NeXus file for a particular usage case

NeXus Coordinate Systems (page 28) Coordinate systems are used to describe the positions and orientations of objects.

Rules for Structuring Information in NeXus Files (page 31)

This section describes where to place data within a NeXus data file.

Rules for Storing Data Items in NeXus Files (page 32) This section describes how to store data in a NeXus data file.

Physical File format (page 38) This section describes how NeXus structures are mapped to features of the underlying physical file format.

In the following sections these elements of NeXus files will be defined in more detail.

Data Groups

NeXus files consist of data groups, which contain fields and/or other groups to form a hierarchical structure. This hierarchy is designed to make it easy to navigate a NeXus file by storing related fields together. Data groups are identified both by a name, which must be unique within a particular group, and a class. There can be multiple groups with the same class but they must have different names (based on the HDF rules). For the class names used with NeXus data groups the prefix NX is reserved. Thus all NeXus class names start with NX.

Data Fields

Data fields contain the essential information stored in a NeXus file. They can be scalar values or multidimensional arrays of a variety of sizes (1-byte, 2-byte, 4-byte, 8-byte) and types (integers, floats, characters). The fields may store both experimental results (counts, detector angles, etc), and other information associated with the experiment (start and end times, user names, etc). Data fields are identified by their names, which must be unique within the group in which they are stored.

Data Attributes

Attributes are extra (meta-)information that are associated with particular fields. They are used to annotate the data, for example with physical units or calibration offsets, and may be scalar numbers or character strings. NeXus also uses attributes to identify plottable data and their axes, etc. A description of possible attributes can be found in the table titled *Example NeXus Data Attributes* (page 24). Finally, NeXus files

themselves have global attributes which are listed in the *NeXus File Global Attributes* (page 25) table that identify the NeXus version, file creation time, etc. Attributes are identified by their names, which must be unique in each field.

Example NeXus Data Attributes

For the full specification of attributes, see NeXus: Reference Documentation (page 45).

Name	Type	Description	
units	NX_CHAR	Data units, given as character strings, must conform to the NeXus units standard. See the "NeXus units" section for details.	
signal	NX_INT	Defines which data set contains the signal to be plotted use signal="1" for main signal	
axes	NX_CHAR	Defines the names of the dimension scales for this data set as a colon-delimited list. For example, suppose data is an array with elements data[j][i](C) or data(i, j) (Fortran), with dimension scales time_of_flight[i] and polar_angle[j], then data would have an attribute axes="polar_angle:time_of_flight" in addition to an attribute signal="1".	
axis	NX_INT	The original way of designating data for plotting, now superceded by the axes attribute. This defines the rank of the signal data for which this data set is a dimension scale in order of the fastest varying index (see a longer discussion in <i>Linking by name using the axes attribute</i> (page 36)), i.e. if the array being stored is data, with elements data[j][i] in C and data(i,j) in Fortran, axis would have the following values: ith dimension (axis="1"), jth dimension (axis="2"), etc.	
primary	NX_INT32	Defines the order of preference for dimension scales which apply to the same rank of signal data. Use <i>primary="1"</i> to indicate preferred dimension scale	
long_name	NX_CHAR	Defines title of signal data or axis label of dimension scale	
calibration_status	NX_CHAR	either Nominal or Measured Defines status of data value.	
offset	NX_INT	Rank values off offsets to use for each dimension if the data is not in C storage order	
stride	NX_INT	Rank values of steps to use when incrementing the dimension	
transformation_type	NX_CHAR	translation or rotation	
vector	NX_FLOAT	3 values describing the axis of rotation or the direction of translation	
interpretation	NX_CHAR	Describes how to display the data. Allowed values include: scaler (0-D data), spectrum (1-D data), image (2-D data), or vertex (3-D data).	

NeXus File Global Attributes

Name	Туре	Description
file_name	NX_CHAR	Original name of NeXus file.
file_time	ISO 8601	Date and time of file creation
file_update_time	ISO 8601	Date and time of last file change at close
NeXus_version	NX_CHAR	Version of NeXus API used in writing the file
creator	NX_CHAR	Facility or program where the file originated

Data Links

Links are pointers to existing data somewhere else. The concept is very much like symbolic links in a unix filesystem. The NeXus definition sometimes requires access to the same data in different groups within the same file. For example: detector data is stored in the NXinstrument/NXdetector group but may be needed in NXdata for automatic plotting. Rather then replicating the data, NeXus uses links in such situations. See the figure *Linking in a NeXus file* (page 25) for a more descriptive representation of the concept of linking.

Linking in a NeXus file

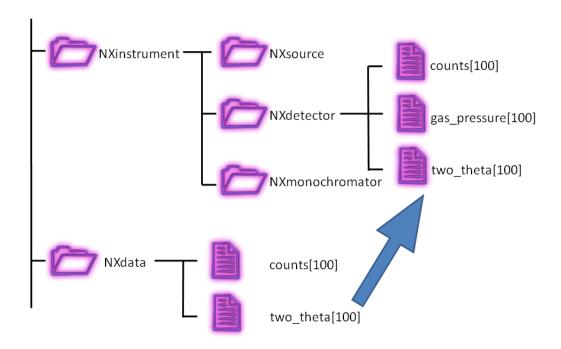


Figure 2.6: Linking in a NeXus file. See example code below: example.data-linking (not converted yet) (page 157)

2.2. NeXus Design

NeXus Classes

Data groups often describe objects in the experiment (monitors, detectors, monochromators, etc.), so that the contents (both data fields and/or other data groups) comprise the properties of that object. NeXus has defined a set of standard objects, or base classes, out of which a NeXus file can be constructed. This is each data group is identified by a name and a class. The group class, defines the type of object and the properties that it can contain, whereas the group name defines a unique instance of that class. These classes are defined in XML using the NeXus Definition Language (NXDL) format. All NeXus class types adopted by the NIAC *must* begin with *NX*. Classes not adopted by the NIAC *must not* start with *NX*.

Not all classes define physical objects. Some refer to logical groupings of experimental information, such as plottable data, sample environment logs, beam profiles, etc. There can be multiple instances of each class. On the other hand, a typical NeXus file will only contain a small subset of the possible classes.

NeXus base classes are not proper classes in the same sense as used in object oriented programming languages. In fact the use of the term classes is actually misleading but has established itself during the development of NeXus. NeXus base classes are rather dictionaries of field names and their meanings which are permitted in a particular NeXus group implementing the NeXus class. This sounds complicated but becomes easy if you consider that most NeXus groups describe instrument components. Then for example, a *NXmonochromator* (page 73) base class describes all the possible field names which NeXus allows to be used to describe a monochromator.

Most NeXus base classes represent instrument components. Some are used as containers to structure information in a file (*NXentry* (page 59), *NXcollection* (page 51), *NXinstrument* (page 68), *NXprocess* (page 78), *NXparameters* (page 75)). But there are some base classes which have special uses that need to be mentioned here:

- *NXdata* (page 54) *NXdata* is used to identify the default plottable data. The notion of a default plot of data is a basic motivation of NeXus.
- *NXlog* (page 69) *NXlog* is used to store time stamped data like the log of a temperature controller. Basically you give a start time, and arrays with a difference in seconds to the start time and the values read.
- **NXnote** (page 73) *NXnote* provides a place to store general notes, images, video or whatever. A mime type is stored together with a binary blob of data. Please use this only for auxiliary information, for example an image of your sample, or a photo of your boss.
- *NXgeometry* (page 65) *NXgeometry* and its subgroups *NXtranslation* (page 85), *NXorientation* (page 75), and *NXshape* (page 82) are used to store absolute positions in the laboratory coordinate system or to define shapes.

These groups can appear anywhere in the NeXus hierarchy, where needed. Preferably close to the component they annotate or in a *NXcollection* (page 51). All of the base classes are documented in the reference manual.

NXdata Facilitates Automatic Plotting

The most notable special base class (also known as *group*) in NeXus is *NXdata* (page 54). *NXdata* is the answer to a basic motivation of NeXus to facilitate automatic plotting of data. NeXus basic motivation; default plot *NXdata* is designed to contain the main dataset and its associated dimension scales (axes) dimension scale of a NeXus data file. The usage scenario is that an automatic data plotting program just opens

a *NXentry* (page 59) and then continues to search for any *NXdata* groups. These *NXdata* groups represent the plottable data. Here is the way an automatic plotting program ought to work:

- 1. Search for NXentry groups
- 2. Open an NXentry
- 3. Search for NXdata groups
- 4. Open an NXdata group
- 5. Identify the plottable data.
 - 1. Search for a dataset with attribute signal=1. This is your main dataset. (There should be only one dataset that matches.)
 - 2. Try to read the axes attribute of the main dataset, if it exists.
 - 1. The value of axes is a colon- or comma-separated list of the datasets describing the dimension scales (such as axes="polar_angle:time_of_flight").
 - 2. Parse axes and open the datasets to describe your dimension scales
 - 3. If axes does not exist:
 - 1. Search for datasets with attributes axis=1, axis=2, etc. These are the datasets describing your axis. There may be several datasets for any axis, i.e. there may be multiple datasets with the attribute axis=1. Among them the dataset with the attribute primary=1 is the preferred one. All others are alternative dimension scales.
 - 2. Open the datasets to describe your dimension scales.
- 6. Having found the default plottable data and its dimension scales: make the plot

NeXus Application Definitions

The objects described so far provide us with the means to store data from a wide variety of instruments, simulations or processed data as resulting from data analysis. But NeXus strives to express strict standards for certain applications of NeXus too. The tool which NeXus uses for the expression of such strict standards is the NeXus Application Definition. A NeXus Application Definition describes which groups and data items have to be present in a file in order to properly describe an application of NeXus. For example for describing a powder diffraction experiment. Typically an application definition will contain only a small subset of the many groups and fields defined in NeXus. NeXus application definitions are also expressed in the NeXus Definition Language (NXDL). A tool exists which allows to validate a NeXus file against a given application definition.

Note: NeXus application definition is a contract

Another way to look at a NeXus application definition is as a contract between a file writer and a file consumer (reader). A contract which reads:

If you write your files following a particular NeXus application definition, I can process these files with my software.

Yet another way to look at a NeXus application definition is to understand it as an interface definition between data files and the software which uses this file. Much like an interface in the Java or other modern object oriented programming languages.

In contrast to NeXus base classes, NeXus supports inheritance in application definitions.

Please note that a NeXus Application Definition will only define the bare minimum of data necessary to perform common analysis with data. Practical files will nearly always contain more data. One of the beauties of NeXus is that it is always possible to add more data to a file without breaking its compliance with its application definition.

NeXus Coordinate Systems

Coordinate systems in NeXus underwent quite some development. Initially, just positions of relevant motors were stored without further standardization. This soon proved to be too little and the *NeXus polar coordinate* system was developed. This system still is very close to angles meaningful to an instrument scientist but allows to define general positions of components easily. Then users from the simulation community approached the NeXus team and asked for a means to store absolute coordinates. This was implemented through the use of the *NXgeometry* class on top of the *McStas* ⁶ system. We soon learned that all the things we do can be expressed through the McStas coordinate system. So the McStas coordinate system became the reference coordinate system for NeXus. *NXgeometry* was expanded to allow the description of shapes when the demand came up. Later members of the CIF ⁷ team convinced the NeXus team of the beauty of transformation matrices and NeXus was enhanced to store the necessary information to fully map CIF concepts. Not much had to be changed though as we choose to document the existing angles in CIF terms. The CIF system allows to store arbitrary operations and nevertheless calculate absolute coordinates in the laboratory coordinate system. It also allows to convert from local, for example detector coordinate systems, to absolute coordinates in the laboratory system.

McStas and NXgeometry System

NeXus uses the *McStas coordinate system* ¹ as its laboratory coordinate system. The instrument is given a global, absolute coordinate system where:

- the z axis points in the direction of the incident beam,
- the x axis is perpendicular to the beam in the horizontal plane pointing left as seen from the source
- the y axis points upwards.

See below for a drawing of the McStas coordinate system. The origin of this coordinate system is the sample position or, if this is ambiguous, the center of the sample holder with all angles and translations set to zero. The McStas coordinate system is illustrated in figure *The McStas Coordinate System* (page 29).

⁶ McStas, http://www.mcstas.org, also http://mcstas.risoe.dk

⁷ CIF (Crystallographic Information Framework), http://www.iucr.org/resources/cif

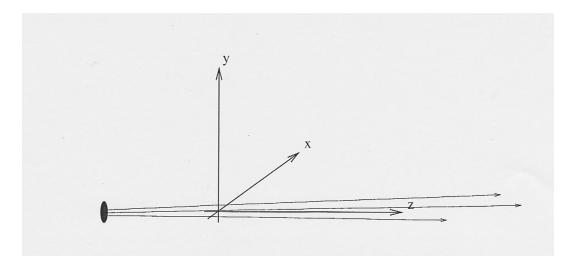


Figure 2.7: The McStas Coordinate System

Note: The NeXus definition of +z is opposite to that in the International Tables for Crystallography, volume G, 8 and consequently, +x is also reversed.

The NeXus NXgeometry class directly uses the McStas coordinate system. NXgeometry classes can appear in any component in order to specify its position. The suggested name to use is geometry. In NXgeometry the NXtranslation/values field defines the absolute position of the component in the McStas coordinate system. The NXorientation/value field describes the orientation of the component as a vector of in the McStas coordinate system.

Simple (Spherical Polar) Coordinate System

In this system, the instrument is considered as a set of components through which the incident beam passes. The variable **distance** is assigned to each component and represents the effective beam flight path length between this component and the sample. A sign convention is used where negative numbers represent components pre-sample and positive numbers components post-sample. At each component there is local spherical coordinate system with the angles *polar_angle* and *azimuthal_angle*. The size of the sphere is the distance to the previous component.

In order to understand this spherical polar coordinate system it is helpful to look initially at the common condition that azimuthal_angle is zero. This corresponds to working directly in the horizontal scattering plane of the instrument. In this case polar_angle maps directly to the setting commonly known as two theta. Now, there are instruments where components live outside of the scattering plane. Most notably detectors. In order to describe such components we first apply the tilt out of the horizontal scattering plane as the azimuthal_angle. Then, in this tilted plane, we rotate to the component. The beauty of this is that polar_angle is always two theta. Which, in the case of a component out of the horizontal scattering plane, is not identical to the value read from the motor responsible for rotating the component. This situation is shown in figure NeXus Simple (Spherical Polar) Coordinate System (page 30).

⁸ **International Tables for Crystallography** *Volume G: Definition and exchange of crystallographic data.* Sydney Hall and Brian McMahon, Editors. Published for the IUCr by Springer, 2005 ISBN 1-4020-3138-6, 594 + xii pages

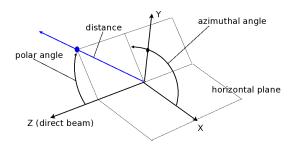


Figure 2.8: NeXus Simple (Spherical Polar) Coordinate System

Coordinate Transformations

Another way to look at coordinates is through the use of transformation matrices. In this world view, the absolute position of a component or a detector pixel with respect to the laboratory corrdinate system is calculated by applying a series of translations and rotations. These operations are commonly expressed as transformation matrices and their combination as matrix multiplication. A very important aspect is that the order of application of the individual operations *does* matter. Another important aspect is that any operation transforms the whole coordinate system and gives rise to a new local coordinate system. The mathematics behind this is well known and used in such applications such as industrial robot control, space flight and computer games. The beauty in this comes from the fact that the operations to apply map easily to instrument settings and constants. It is also easy to analyze the contribution of each individual operation: this can be studied under the condition that all other operations are at a zero setting.

In order to use coordinate transformations, several morsels of information need to be known:

Type The type of operation: rotation or translation

Direction The direction of the translation or the direction of the rotation axis

Value The angle of rotation or the length of the translation

Order The order of operations to apply to move a component into its place.

Actions of standard NeXus field	
	C

Field Name	transformation_type	vector
polar_angle	rotation	010
azimuthal_angle	rotation	0 0 1
meridional_angle	rotation	100
distance	translation	0 0 1
height	translation	010
x_translation	translation	100
chi	rotation	0 0 1
phi	rotation	010

The type and direction of the NeXus standard operations is documented in table *Actions of standard NeXus fields* (page 30). NeXus can now also allow non standard operations to be stored in data files. In such cases additional data attributes are required which describe the operation. These are *transformation_type* which can be either translation or rotation. The other is *vector* which is 3 float values describing the direction of translation or rotation. The value is of course always the value of the data field in the data file.

How NeXus describes the order of operations to apply has not yet been decided upon. The authors favorite scheme is to use a special field at each instrument component, named *transform* which describes the operations to apply to get the component into its position as a list of colon separated paths to the operations to apply relative to the current *NXentry*. For paths in the same group, only the name need to be given. Detectors may need two such fields: the transfrom field to get the detector as a whole into its position and a *transform_pixel* field which describes how the absolute position of a detector pixel can be calculated.

For the NeXus spherical coordinate system, the order is implicit and is given by:

```
azimuthal_angle:polar_angle:distance
```

This is also a nice example of the application of transformation matrices:

- 1. You first apply azimuthal_angle as a rotation around z. This rotates the whole coordinate out of the plane.
- 2. Then you apply polar_angle as a rotation around *y* in the tilted coordinate system.
- 3. This also moves the direction of the *z* vector. Along which you translate the component to place by distance.

Rules for Structuring Information in NeXus Files All NeXus files contain one or many groups of type NXentry at root level. Many files contain only one NXentry group, then the name is entry. The NXentry level of hierarchy is there to support the storage of multiple related experiments in one file. Or to allow the NeXus file to serve as a container for storing a whole scientific workflow from data acquisition to publication ready data. Also, NXentry class groups can contain raw data or processed data. For files with more than one NXentry group, since HDF requires that no two items at the same level in an HDF file may have the same name, the NeXus fashion is to assign names with an incrementing index appended, such as entry1, entry2, entry3, etc.

In order to illustrate what is written in the text, example hierarchies like the one in figure link xlink:href="#table.RawData">RawData

Content of a Raw Data NXentry Group An example raw data hierarchy is shown in the next figure (only showing the relevant parts of the data hierarchy). In the example shown, the data field in the *NXdata* (page 54) group is linked to the 2-D detector data (a 512x512 array of 32-bit integers) which has the attribute signal=1. Note that [,] represents a 2D array.

```
entry:NXentry
2
      instrument: NXinstrument
          source: NXsource
3
4
         detector: NXdetector
5
             data:NX_INT32[512,512]
6
                @signal = 1
7
8
      sample: NXsample
      control: NXmonitor
9
      data: NXdata
10
          data --> /entry/instrument/detector/data
11
```

An *NXentry* (page 59) describing raw data contains at least a *NXsample* (page 79), one *NXmonitor* (page 72), one *NXdata* (page 54) and a *NXinstrument* (page 68) group. It is good practice to use the names sample

for the *NXsample* (page 79) group, control for the *NXmonitor* (page 72) group holding the experiment controlling monitor and instrument for the *NXinstrument* (page 68) group. The *NXinstrument* (page 68) group contains further groups describing the individual components of the instrument as appropriate.

The NXdata group contains links to all those data items in the NXentry hierarchy which are required to put up a default plot of the data. As an example consider a SAXS instrument with a 2D detector. The NXdata will then hold a link to the detector image. If there is only one NXdata group, it is good practice to name it data. Otherwise, the name of the detector bank represented is a good selection.

Rules for Storing Data Items in NeXus Files This section describes the rules which apply for storing single data fields in data files.

Naming Conventions Group and field names used within NeXus follow a naming convention which adheres to these rules: naming The names of NeXus *group* and *field* objects must contain only a restricted set of characters. This set may be described by this regular expression syntax.

```
[A-Za-z_{-}][\w_{-}]*
```

This name pattern starts with a letter (upper or lower case) or "_" (underscore), then letters, numbers, and "_" and is limited to no more than 63 characters (imposed by the HDF5 rules for names). rules; HDF5

Sometimes it is necessary to combine words in order to build a descriptive name for a data field or a group. In such cases lowercase words are connected by underscores.

```
number of lenses
```

For all data fields, only names from the NeXus base class dictionaries are to be used. If a data field name or even a complete component is missing, please suggest the addition to the NIAC. The addition will usually be accepted provided it is adequately documented and not a duplication of an existing field.

Note: The NeXus base classes provide a comprehensive dictionary of terms than can be used for each class. NeXus basic motivation; defined dictionary

NeXus Storage NeXus stores multi dimensional arrays of physical values in C language storage order, dimension; storage order last dimension is the fastest varying. This is the rule.

Good reasons are required to deviate from this rule.

One good reason to deviate from this rule is the situation where data must be streamed to disk as fast as possible and a conversion to NeXus storage order is not possible. In such cases, exceptions can be made. It is possible to store data in other storage orders in NeXus as well as to specify that the data needs to be converted first before being useful.

Non C Storage Order In order to indicate that the storage order dimension; storage order is different from C storage order two additional data set attributes, offset and stride, have to be stored which together define the storage layout of the data. Offset and stride contain rank numbers according to the rank of the multidimensional data set. Offset describes the step to make when the dimension is multiplied by 1. Stride defines the step to make when incrementing the dimension. This is best explained by some examples.

Offset and Stride for 1-D data

```
* raw data = 0 1 2 3 4 5 6 7 8 9
   size[1] = { 10 } // assume uniform overall array dimensions
* default stride:
   stride[1] = \{ 1 \}
   offset[1] = { 0 }
   for i:
      result[i]:
         0 1 2 3 4 5 6 7 8 9
* reverse stride:
  stride[1] = \{ -1 \}
   offset[1] = { 9 }
   for i:
      result[i]:
         9 8 7 6 5 4 3 2 1 0
Offset and Stride for 2-D data
```

```
* raw data = 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
   size[2] = { 4, 5 } // assume uniform overall array dimensions
* row major (C) stride:
   stride[2] = \{ 5, 1 \}
   offset[2] = \{0, 0\}
   for i:
      for j:
         result[i][j]:
            0 1 2 3 4
            5 6 7 8 9
            10 11 12 13 14
            15 16 17 18 19
* column major (Fortran) stride:
   stride[2] = \{ 1, 4 \}
   offset[2] = \{0, 0\}
   for i:
      for j:
         result[i][j]:
            0 4 8 12 16
            1 5 9 13 17
            2 6 10 14 18
            3 7 11 15 19
* "crazy reverse" row major (C) stride:
  stride[2] = \{ -5, -1 \}
   offset[2] = \{4, 5\}
   for i:
      for j:
         result[i][j]:
            19 18 17 16 15
            14 13 12 11 10
```

9 8 7 6 5 4 3 2 1 0

Offset and Stride for 3-D data

```
* raw data = 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19
      20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39
      40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59
   size[3] = { 3, 4, 5 } // assume uniform overall array dimensions
* row major (C) stride:
   stride[3] = \{ 20, 5, 1 \}
   offset[3] = \{0, 0, 0\}
   for i:
      for j:
         for k:
            result[i][j][k]:
               0 1 2 3 4
               5 6 7 8 9
               10 11 12 13 14
               15 16 17 18 19
               20 21 22 23 24
               25 26 27 28 29
               30 31 32 33 34
               35 36 37 38 39
               40 41 42 43 44
               45 46 47 48 49
               50 51 52 53 54
               55 56 57 58 59
* column major (Fortran) stride:
   stride[3] = \{ 1, 3, 12 \}
   offset[3] = \{0, 0, 0\}
   for i:
      for j:
         for k:
            result[i][j][k]:
               0 12 24 36 48
               3 15 27 39 51
               6 18 30 42 54
               9 21 33 45 57
               1 13 25 37 49
               4 16 28 40 52
               7 19 31 43 55
               10 22 34 46 58
               2 14 26 38 50
               5 17 29 41 53
               8 20 32 44 56
               11 23 35 47 59
```

NeXus Data Types Matching regular expressions for NeXus data types

description	matching regular expression
integer	NX_INT(8 16 32 64)
floating-point	NX_FLOAT(32 64)
array	(\[0-9\])?
valid item name	^[A-Za-z_][A-Za-z0-9_]*\$
valid class name	^NX[A-Za-z0-9_] *\$

NeXus supports numeric data as either integer or floating-point numbers. A number follows that indicates the number of bits in the word. The table above shows the regular expressions that matches the data type specifier.

integers NX_INT8, NX_INT16, NX_INT32, or NX_INT64

floating-point numbers NX_FLOAT32 or NX_FLOAT64

date / time stamps NX_DATE_TIME or ISO8601

Dates and times date and time are specified using ISO-8601 standard definitions. Refer to *NeXus dates and times* (page 35).

strings All strings are to be encoded in UTF-8. Since most strings in a NeXus file are restricted to a small set of characters and the first 128 characters are standard across encodings, the encoding of most of the strings in a NeXus file will be a moot point. UTF-8 encoding will be important when recording peoples' names in *NXuser* (page 86) and text notes in *NXnote* (page 73).

Because the few places where encoding is important also have unpredictable content, as well as the way in which current operating systems handle character encoding, it is practically impossible to test the encoding used. Hence, *nxvalidate* utility; nxvalidate provides no messages relating to character encoding.

binary data Binary data is to be written as UINT8.

images Binary image data is to be written using UINT8, the same as binary data, but with an accompanying image mime-type. If the data is text, the line terminator is [CR][LF].

NeXus dates and times NeXus dates and times date and time should be stored using the ISO 8601 ⁹ format, such as:

1996-07-31T21:15:22+0600

Note: The *T* appears literally in the string, to indicate the beginning of the time element, as specified in ISO 8601. It is common to use a space in place of the *T*. While human-readable, compatibility with the ISO 8601 standard is not assured with this substitution.

The standard also allows for time intervals in fractional seconds with 1 or more digits of precision. This avoids confusion, e.g. between U.S. and European conventions, and is appropriate for machine sorting.

NeXus Units Given the plethora of possible applications of NeXus, it is difficult to define units units to use. Therefore, the general rule is that you are free to store data in any unit you find fit. However, any data

⁹ ISO 8601, http://www.w3.org/TR/NOTE-datetime

field must have a units attribute which describes the units, Wherever possible, SI units are preferred. NeXus units are written as a string attribute (*NX_CHAR*) and describe the engineering units. The string should be appropriate for the value. Values for the NeXus units must be specified in a format compatible with Unidata UDunits. ¹⁰ The UDunits specification also includes instructions for derived units. At present, the contents of NeXus *units* attributes are not validated in data files. Application definitions may specify units to be used for fields using an *enumeration*. enumeration

Linking Multi Dimensional Data with Axis Data NeXus allows to store multi dimensional arrays of data. In most cases it is not sufficient to just have the indices into the array as a label for the dimensions of the data. Usually the information which physical value corresponds to an index into a dimension dimension of the multi dimensional data set. To this purpose a means is needed to locate appropriate data arrays which describe what each dimension of a multi dimensional data set actually corresponds too. There is a standard HDF facility to do this: it is called dimension scales. Unfortunately, at a time, there was only one global namespace for dimension scales. Thus NeXus had to come up with its own scheme for locating axis data which is described here. A side effect of the NeXus scheme is that it is possible to have multiple mappings of a given dimension to physical data. For example a TOF data set can have the TOF dimension as raw TOF or as energy.

There are two methods of linking link each data dimension to its respective dimension scale. dimension; dimension scales The preferred method uses the *axes* attribute to specify the names of each dimension scale. The original method uses the *axis* attribute to identify with an integer the axis whose value is the number of the dimension. After describing each of these methods, the two methods will be compared. A prerequisite for both methods is that the data fields describing the axis are stored together with the multi dimensional data set whose axes need to be defined in the same NeXus group. If this leads to data duplication, use links.

Linking by name using the *axes* **attribute** The preferred method is to define an attribute of the data itself called *axes*. axes The *axes* attribute contains the names of each dimension scale dimension; dimension scales as a colon (or comma) separated list in the order they appear in C. For example:

Preferred way of denoting axes

```
data:NXdata
  time_of_flight = 1500.0 1502.0 1504.0 ...
  polar_angle = 15.0 15.6 16.2 ...
  some_other_angle = 0.0 0.0 2.0 ...
  data = 5 7 14 ...
   @axes = polar_angle:time_of_flight
   @signal = 1
```

Linking by dimension number using the *axis* **attribute** The original method is to define an attribute of each dimension scale called *axis*. axis It is an integer whose value is the number of the dimension, in order of fastest varying dimension. dimension; fastest varying That is, if the array being stored is data with elements data[j][i] in C and data(i,j) in Fortran, where i is the time-of-flight index and j is the polar angle index, the NXdata (page 54) group NXdata would contain:

¹⁰ Unidata UDunits, http://www.unidata.ucar.edu/software/udunits/udunits-2-units.html

```
data:NXdata
  time_of_flight = 1500.0 1502.0 1504.0 ...
    @axis = 1
    @primary = 1
  polar_angle = 15.0 15.6 16.2 ...
    @axis = 2
    @primary = 1
  some_other_angle = 0.0 0.0 2.0 ...
    @axis = 1
  data = 5 7 14 ...
    @signal = 1
```

The *axis* attribute must be defined for each dimension scale. The *primary* attribute is unique to this method of linking.

There are limited circumstances in which more than one dimension scale dimension; dimension scales for the same data dimension can be included in the same *NXdata* (page 54) group. NXdata The most common is when the dimension scales are the three components of an (*hkl*) scan. In order to handle this case, we have defined another attribute of type integer called *primary* whose value determines the order in which the scale is expected to be chosen for plotting, NeXus basic motivation; default plot i.e.

Note: The *primary* attribute can only be used with the first method of defining dimension scales dimension; dimension scales discussed above. In addition to the *signal* data, this group could contain a data set of the same rank rank and dimensions called *errors* containing the standard deviations of the data.

```
1st choice: primary="1"
2nd choice: primary="2"
etc.
```

If there is more than one scale with the same value of the *axis* attribute, one of them must have set *primary*="1". Defining the *primary* attribute for the other scales is optional.

Discussion of the two linking methods In general the method using the *axes* attribute on the multi dimensional data set dimension; data set should be preferred. This leaves the actual axis describing data sets unannotated and allows them to be used as an axis for other multi dimensional data. This is especially a concern as an axis describing a data set may be linked into another group where it may describe a completely different dimension of another data set.

Only when alternative axes definitions are needed, the *axis* method should be used to specify an axis of a data set. This is shown in the example above for the *some_other_angle* field where *axis="1"* denotes another possible primary axis for plotting. The default axis for plotting carries the *primary="1"* attribute.

Both methods of linking data axes will be supported in NeXus utilities that identify dimension scales, dimension; dimension scales such as *NXUfindaxis()*.

Storing Detectors There are very different types of detectors out there. Storing their data can be a challenge. As a general guide line: if the detector has some well defined form, this should be reflected in the data file. A linear detector becomes a linear array, a rectangular detector becomes an array of size *xsize* times

ysize. Some detectors are so irregular that this does not work. Then the detector data is stored as a linear array, with the index being detector number till *ndet*. Such detectors must be accompanied by further arrays of length *ndet* which give *azimuthal_angle*, *polar_angle* and distance for each detector.

If data from a time of flight (TOF) instrument must be described, then the TOF dimension becomes the last dimension, for example an area detector of *xsize vs. ysize* is stored with TOF as an array with dimensions *xsize*, *ysize*, *ntof*.

Monitors are Special Monitors, monitor detectors that measure the properties of the experimental probe rather than the sample, have a special place in NeXus files. Monitors are crucial to normalize data. To emphasize their role, monitors are not stored in the *NXinstrument* (page 68) hierarchy but as *NXmonitor* (page 72) group(s) as direct children of the *NXentry* (page 59) level, as there might be multiple monitors. Of special importance is the monitor in a group called *control*. This is the main monitor against which the data has to be normalized. This group also contains the counting control information, i.e. counting mode, times, etc.

Monitor data may be multidimensional. Good examples are scan monitors where a monitor value per scan point is expected or time-of-flight monitors.

Physical File format This section describes how NeXus structures are mapped to features of the underlying physical file format. This can also be considered a guide for people who wish to create NeXus files without using the NeXus-API.

Choice of HDF as Underlying File Format At its beginnings, the founders of NeXus identified the Hierarchical Data Format (HDF) ¹¹, as a multi-platform data storage format with capacity for conveying large data payloads and a substantial user community. HDF (now HDF5) was provided with software to read and write data (this is the application-programmer interface, or API) using a large number of computing systems in common use for neutron and X-ray science. HDF is a binary data file format that supports compression and structured data.

Mapping NeXus into HDF NeXus data structures map directly to HDF structures.

NeXus *groups* HDF4 *vgroups* or HDF5 *groups*

NeXus data sets (or fields) HDF4 SDS (scientific data sets) or HDF5 datasets

Attributes HDF group or dataset attributes.

The only special case is the NeXus class name. HDF4 supports a group class which is set with the Vsetclass() call and read with VGetclass(). HDF-5 has no group class. Thus the NeXus class is stored as a group attribute with the name NX_class.

NeXus links directly map to the HDF linking mechanisms.

¹¹ HDF: http://www.hdfgroup.org, initially from the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign (UIUC) and later spun off into its own group called The HDF Group (THG).

Mapping NeXus into XML This takes a bit more work than HDF. At the root of NeXus XML file is a XML element with the name NXroot. Further XML attributes to NXroot define the NeXus file level attributes.

NeXus groups are encoded into XML as elements with the name of the NeXus class and an XML attribute name which defines the NeXus name of the group. Further group attributes become XML attributes. An example of a NeXus group element in XML:

```
1 <NXentry name="entry">
2 </NXentry>
```

NeXus data sets are encoded as XML elements with the name of the data. An attribute NAPItype defines the type and dimensions of the data. The actual data is stored as PCDATA 12 in the element. An example of two NeXus data elements in XML:

Data are printed in appropriate formats and in C storage order. The codes understood for NAPItype are all the NeXus data type names. The dimensions are given in square brackets as a comma separated list. No dimensions need to be given if the data is just a single value. Data attributes are represented as XML attributes. If the attribute is not a text string, then the attribute is given in the form: *type:value*, for example: signal="NX_INT32:1".

NeXus links are stored in XML as XML elements with the name NAPIlink and a XML attribute target which stores the path to the linked entity in the file. If the item is linked under a different name, then this name is specified as a XML attribute name to the element NAPIlink.

The authors of the NeXus API worked with the author of the miniXML XML ¹³ library to create a reasonably efficient way of handling numeric data with XML. Using the NeXus API handling something like 400 detectors versus 2000 time channels in XML is not a problem. But you may hit limits with XML as the file format when data becomes to large or you try to process NeXus XML files with general XML tools. General XML tools are normally ill-prepared to process large amounts of numbers.

Special Attributes NeXus makes use of some special attributes for its internal purposes. These attributes are stored as normal group or data set attributes in the respective file format. These are:

target The *target* attribute is automatically created when items get linked. The target attribute contains a text string with the path to the source of the item linked.

napimount The napimount attribute is used to implement external linking in NeXus. The string is a URL to the file and group in the external file to link too. The system is meant to be extended. But as of now, the only format supported is: nxfile://path-to-file#path-infile. This is a NeXus file in the file system at path-to-file and the group path-infile in that NeXus file.

¹² PCDATA is the XML term for *parsed character data* (see: http://www.w3schools.com/xml/xml_cdata.asp)

¹³ MiniXML: http://www.minixml.org/

NAPILINK NeXus supports linking items in another group under another name. This is only supported natively in HDF-5. For HDF-4 and XML a crutch is needed. This crutch is a special class name or attribute NAPILink combined with the target attribute. For groups, NAPILink is the group class, for data items a special attribute with the name NAPILink.

2.3 Frequently Asked Questions

This is a list of commonly asked questions concerning the NeXus data format.

2.3.1 How many facilities use NeXus?

This is not easy to say, not all facilities using NeXus actively participate in the committee. Some facilities have reported their adoption status on the :ref:Facilities Wiki page. Please have a look at this list. Keep in mind that it is not complete.

2.3.2 NeXus files are binary? This is crazy! How am I supposed to see my data?

NeXus files are not binary *per se*. If you use the XML backend the data are stored in a relatively human readable form (see *this example*). This backend however is only recommended for very small data sets. With the multidimensional data that is routinely recorded on many modern instruments it is very difficult anyway to retrieve useful information on a VT100 terminal. If you want to try, for example nxbrowse is a utility provided by the NeXus community that can be very helpful to those who want to inspect their files and avoid graphical applications. For larger data volumes the binary backends used with the appropriate tools are by far superior in terms of efficiency and speed and most users happily accept that after having worked with supersized "human readable" files for a while.

2.3.3 What on-disk file format should I choose for my data?

HDF5 is the default file container to use for NeXus data. It is the recommended format for all applications. HDF4 is still supported as a on disk format for NeXus but for new installations preference should be given to HDF5. The XML backend is available for special use cases. Choose this option with care considering the space and speed implications.

2.3.4 Why are the NeXus classes so complicated? I'll never store all that information

The NeXus classes are essentially *glossaries of terms*. If you need to store a piece of information, consult the class definitions to see if it has been defined. If so, use it. It is not compulsory to include every item that has been defined in the base class if it is not relevant to your experiment. On the other hand, a NeXus application definition lists a smaller set of compulsory items that should allow other researchers or software to analyze your data. You should really follow the application definition that corresponds to your experiment to take full advantage of NeXus.

2.3.5 I don't like NeXus. It seems much faster and simpler to develop my own file format. Why should I even consider NeXus?

If you consider using an efficient on disk storage format, HDF5 is a better choice than most others. It is fast and efficient and well supported in all main stream programming languages and a fair share of popular analysis packages. The format is so widely used and backed by a big organisation that it will continue to be supported for the foreseeable future. So if you are going to use HDF5 anyway, why not use the NeXus definition to lay out the data in a standardised way? The NeXus community spent years trying to get the standard right and while you will not agree with every single choice they made in the past, you should be able to store the data you have in a quite reasonable way. If you do not comply with NeXus chances are most people will perceive your format as different but not necessarily better than NeXus by any large measure. So it may not be worth the effort. Seriously. If you encounter any problems because the classes are not sufficient to describe your configuration, please contact the NIAC Executive Secretary explaining the problem, and post a suggestion at the relevant class wiki page. Or raise the problem in one of the *mailing lists*. The NIAC is always willing to consider new proposals.

2.3.6 I want to produce an application definition. How do I go about it?

Read the NXDL Tutorial in *nxdl_tutorial-creatingnxdlspec* (*not converted yet*) (page 157). The procedures for acceptance are defined in the NIAC constitution. Refer to the most recent version of the NIAC constitution on the NIAC wiki ¹⁴.

2.3.7 What is the purpose of NXdata?

NXdata contains links to the data stored elsewhere in the NXentry. It identifies the default plottable data. This is one of the basic motivations (see *Simple plotting* (page 16)) for the NeXus standard. The choice of the name NXdata is historic and does not really reflect its function.

2.3.8 How do I identify the plottable data?

Any program whose aim is to identify plottable data should use the following procedure:

- 1. Open the first top level NeXus group with class NXentry.
- 2. Open the first NeXus group with class NXdata.
- 3. Loop through NeXus fields in this group searching for the item with attribute signal="1" indicating this field has the plottable data.
- 4. Check to see if this field has an attribute called axes. If so, the attribute value contains a colon (or comma) delimited list (in the C-order of the data array) with the names of the dimension scales associated with the plottable data. And then you can skip the next two steps.

¹⁴ NIAC wiki: http://www.nexusformat.org/NIAC

- 5. If the axes attribute is not defined, search for the one-dimensional NeXus fields with attribute primary="1".
- 6. These are the dimension scales to label the axes of each dimension of the data.
- 7. Link each dimension scale to the respective data dimension by the axis attribute (axis="1", axis="2", ... up to the rank of the data).
- 8. If necessary, close the NXdata group, open the next one and repeat steps 3 to 6.
- 9. If necessary, close the NXentry group, open the next one and repeat steps 2 to 7.

Consult the *NeXus API* section, which describes the routines available to program these operations. In the course of time, generic NeXus browsers will provide this functionality automatically.

2.3.9 How can I specify reasonable axes for my data?

See the section: *NXdata Facilitates Automatic Plotting* (page 26).

2.3.10 Why aren't NXsample and NXmonitor groups stored in the NXinstrument group?

A NeXus file can contain a number of NXentry groups, which may represent different scans in an experiment, or sample and calibration runs, etc. In many cases, though by no means all, the instrument has the same configuration so that it would be possible to save space by storing the NXinstrument group once and using multiple links in the remaining NXentry groups. It is assumed that the sample and monitor information would be more likely to change from run to run, and so should be stored at the top level.

2.3.11 Specifications are boring. Where can I find some good example data files?

There are a few checked into the *definitions repository*. At the moment the selection is quite limited and not very representative.

2.3.12 Can I use a NXDL specification to parse a NeXus data file?

This should be possible as there is nothing in the NeXus specifications to prevent this but it is not implemented in NAPI. You would need to implement it for yourself. You would be wise to consult the algorithms in the Java version of NXvalidate (see NXvalidate-java) for more details.

2.3.13 Why do I need to specify the NAPItype?

My programming language does not need that information and I don't care about C and colleagues. Can I leave it out?

NAPItype is necessary. When implementing the NeXus-XML API we strived to make this as general as HDF and reasonably efficient for medium sized datasets. This is why we store arrays as a large bunch of numbers in C-storage order. And we need the NAPItype to figure out the dimensions of the dataset.

2.3.14 Do I have to use the NAPI subroutines? Can't I read (or write) the NeXus data files with my own routines?

You are not required to use the NAPI to write valid NeXus data files. It is possible to avoid the NAPI to write and read valid NeXus data files. But, the programmer who chooses this path must have more understanding of how the NeXus HDF or XML data file is written. Validation of data files written without the NAPI is strongly encouraged.

2.3.15 I'm using links to place data in two places. Which one should be the data and which one is the link?

NeXus uses HDF5 hard links. Both places have pointers to the actual data. That is the way hard links work in HDF5. There is no need for a preference to either location. NeXus defines a target attribute to label one directory entry as the source of the data (in this, the link *target*). This has value in only a few situations such as when converting the data from one format to another. By identifying the original in place, duplicate copies of the data are not converted. In HDF, a hard link points to a data object. A soft link points to a directory entry. Since NeXus uses hard links, there is no need to distinguish between two (or more) directory entries that point to the same data.



CHAPTER THREE

NEXUS: REFERENCE DOCUMENTATION

Contents:

3.1 NXDL Class Descriptions

Contents:

3.1.1 NeXus Base Classes

Contents:

NXaperture

category: base_classes

NXDL source: NXaperture

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXaperture.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXaperture.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: *NXgeometry* (page 65), *NXnote* (page 73)

symbol list: none

documentation: Template of a beamline aperture.

Basic Structure of NXaperture

```
NXaperture (base class, version 1.0)
description:NX_CHAR
material:NX_CHAR
NXgeometry
NXgeometry
NXnote
```

Comprehensive Structure of NXaperture

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXattenuator

category: base_classes

NXDL source: NXattenuator

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXattenuator.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXattenuator.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: Template of a beamline attenuator. If uncertain whether to use NXfilter (band-pass filter) or NXattenuator (reduces beam intensity), then use NXattenuator.

Basic Structure of NXattenuator

```
NXattenuator (base class, version 1.0)
absorption_cross_section:NX_FLOAT
attenuator_transmission:NX_FLOAT
distance:NX_FLOAT
scattering_cross_section:NX_FLOAT
status:NX_CHAR
@time
thickness:NX_FLOAT
type:NX_CHAR
```

Comprehensive Structure of NXattenuator

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXbeam

category: base_classes
NXDL source: NXbeam

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXbeam.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXbeam.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54)

symbol list: none

documentation: Template of the state of the neutron or X-ray beam at any location. It will be referenced by beamline component groups within the NXinstrument group or by the NXsample group. Note that variables such as the incident energy could be scalar values or arrays. This group is especially valuable in storing the results of instrument simulations in which it is useful to specify the beam profile, time distribution etc. at each beamline component. Otherwise, its most likely use is in the NXsample group in which it defines the results of the neutron scattering by the sample, e.g., energy transfer, polarizations.

Basic Structure of NXbeam

```
NXbeam (base class, version 1.0)
distance:NX_FLOAT
energy_transfer:NX_FLOAT[i]
final_beam_divergence:NX_FLOAT[2,j]
final_energy:NX_FLOAT[i]
final_polarization:NX_FLOAT[2,j]
final_wavelength:NX_FLOAT[i]
final_wavelength_spread:NX_FLOAT[i]
flux:NX_FLOAT[i]
incident_beam_divergence:NX_FLOAT[2,j]
incident_energy:NX_FLOAT[i]
incident_polarization:NX_FLOAT[2,j]
incident_wavelength:NX_FLOAT[i]
incident_wavelength:NX_FLOAT[i]
NXdata
```

Comprehensive Structure of NXbeam

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXbeam_stop

category: base_classes

NXDL source: NXbeam_stop

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXbeam_stop.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXbeam_stop.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXgeometry (page 65)

symbol list: none

documentation: A class for a beamstop. Beamstops and their positions are important for SANS and SAXS

experiments.

Basic Structure of NXbeam_stop

```
NXbeam_stop (base class, version 1.0)
  description:NX_CHAR
  distance_to_detector:NX_FLOAT
  size:NX_FLOAT
  status:NX_CHAR
  x:NX_FLOAT
  y:NX_FLOAT
  NXgeometry
```

Comprehensive Structure of NXbeam_stop

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXbending_magnet

category: base_classes

NXDL source: NXbending_magnet

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXbending_magnet.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXbending_magnet.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXgeometry (page 65)

symbol list: none

documentation: description for a bending magnet

Basic Structure of NXbending magnet

```
NXbending_magnet (base class, version 1.0)
accepted_photon_beam_divergence:NX_FLOAT
bending_radius:NX_FLOAT
critical_energy:NX_FLOAT
divergence_x_minus:NX_FLOAT
divergence_x_plus:NX_FLOAT
divergence_y_minus:NX_FLOAT
divergence_y_plus:NX_FLOAT
source_distance_x:NX_FLOAT
source_distance_y:NX_FLOAT
spectrum:NXdata
NXgeometry
```

Comprehensive Structure of NXbending_magnet

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXcapillary

category: base_classes

NXDL source: NXcapillary

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXcapillary.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXcapillary.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: NXdata (page 54)

symbol list: none

documentation: This is a dictionary of field names to use for describing a capillary as used in X-ray beam-

Basic Structure of NXcapillary

```
NXcapillary (base class, version 1.0)
accepting_aperture:NX_FLOAT
focal_size:NX_FLOAT
manufacturer:NX_CHAR
maximum_incident_angle:NX_FLOAT
type:NX_CHAR
working_distance:NX_FLOAT
gain:NXdata
transmission:NXdata
```

Comprehensive Structure of NXcapillary

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXcharacterization

category: base_classes

NXDL source: NXcharacterization

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXcharacterization.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXcharacterization.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none
documentation:

Basic Structure of NXcharacterization

```
NXcharacterization (base class, version 1.0)
@source
@location
@mime_type
definition:NX_CHAR
@version
@URL
```

Comprehensive Structure of NXcharacterization

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXcollection

category: base_classes

NXDL source: NXcollection

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXcollection.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXcollection.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: Use NXcollection to gather together any set of terms. The original suggestion is to use this as a container class for the description of a beamline.

For NeXus validation, NXcollection will always generate a warning since it is always an optional group. Anything (groups, fields, or attributes) placed in an NXcollection group will not be validated.

Basic Structure of NXcollection

NXcollection (contributed definition, version 1.0) beamline: NX_CHAR

Comprehensive Structure of NXcollection

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXcollimator

category: base_classes

NXDL source: NXcollimator

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXcollimator.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXcollimator.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: *NXgeometry* (page 65), *NXlog* (page 69)

symbol list: none

documentation: Template of a beamline collimator.

Basic Structure of NXcollimator

```
NXcollimator (base class, version 1.0)
  absorbing_material:NX_CHAR
 blade_spacing:NX_FLOAT
 blade_thickness:NX_FLOAT
  divergence_x:NX_FLOAT
  divergence_y:NX_FLOAT
  frequency:NX_FLOAT
  soller_angle:NX_FLOAT
  transmitting_material:NX_CHAR
  type:NX_CHAR
  NXgeometry
  frequency_log:NXlog
```

Comprehensive Structure of NXcollimator

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXcrystal

category: base_classes

NXDL source: NXcrystal

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXcrystal.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXcrystal.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXgeometry (page 65), NXlog (page 69), NXshape (page 82)

symbol list: These symbols will be used below to coordinate dimensions with the same lengths.

n comp number of different unit cells to be described

i number of wavelengths

documentation: Template of a crystal monochromator or analyzer. Permits double bent monochromator comprised of multiple segments with anisotropic Gaussian mosaic.

If curvatures are set to zero or are absent, array is considered to be flat.

Scattering vector is perpendicular to surface. Crystal is oriented parallel to beam incident on crystal before rotation, and lies in vertical plane.

Basic Structure of NXcrystal

```
NXcrystal (base class, version 1.0)
  azimuthal_angle:NX_FLOAT[i]
 bragg_angle:NX_FLOAT[i]
  chemical_formula:NX_CHAR
  curvature_horizontal:NX_FLOAT
  curvature_vertical:NX_FLOAT
  cut_angle:NX_FLOAT
  cylindrical_orientation_angle:NX_NUMBER
  d_spacing:NX_FLOAT
  density:NX_NUMBER
  is cylindrical:NX BOOLEAN
  mosaic_horizontal:NX_FLOAT
  mosaic_vertical:NX_FLOAT
  order_no:NX_INT
  orientation matrix:NX FLOAT[3,3]
  polar_angle:NX_FLOAT[i]
  reflection: NX INT[3]
  scattering_vector:NX_FLOAT
  segment_columns:NX_FLOAT
  segment_gap:NX_FLOAT
  segment_height:NX_FLOAT
  segment_rows:NX_FLOAT
  segment_thickness:NX_FLOAT
  segment_width:NX_FLOAT
  space_group:NX_CHAR
  temperature: NX_FLOAT
  temperature coefficient:NX FLOAT
  thickness:NX FLOAT
  type:NX CHAR
  unit_cell:NX_FLOAT[n_comp,6]
  unit_cell_a:NX_FLOAT
  unit cell alpha: NX FLOAT
  unit_cell_b:NX_FLOAT
  unit cell beta:NX FLOAT
  unit_cell_c:NX_FLOAT
  unit_cell_gamma:NX_FLOAT
  unit_cell_volume:NX_FLOAT
  usage:NX_CHAR
  wavelength:NX_FLOAT[i]
  reflectivity: NXdata
  transmission: NXdata
  NXgeometry
  temperature_log:NXlog
  shape: NXshape
```

Comprehensive Structure of NXcrystal

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXdata

category: base_classes
NXDL source: NXdata

(http://svn.nexusformat.org/definitions/trunk/base classes/NXdata.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXdata.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: These symbols will be used below to coordinate datasets with the same shape.

dataRank rank of the data field

n length of the variable field

nx length of the x field

ny length of the y field

nz length of the z field

documentation: (required) NXdata is a template of plottable data and their dimension scales.

NeXus basic motivation default plot

It is mandatory that there is at least one NXdata group in each NXentry group. Note that the variable and data can be defined with different names. The signal and axes attribute of the data item define which items are plottable data and which are dimension scales.

NeXus basic motivation default plot

Each NXdata group will consist of only one data set containing plottable data and their standard deviations.

This data set may be of arbitrary rank up to a maximum of NX_MAXRANK=32.

The plottable data will be identified by the attribute: signal="1"

The plottable data will identify the dimension scale(s) in the axes attribute.

If available, the standard deviations of the data are to be stored in a data set of the same rank and dimensions, with the name errors.

For each data dimension, there should be a one-dimensional array of the same length.

These one-dimensional arrays are the dimension scales of the data, i.e. the values of the independent variables at which the data is measured, such as scattering angle or energy transfer.

There are two methods of linking

link

each data dimension to its respective dimension scale.

The preferred (and recommended) method uses the axes

axes

attribute to specify the names of each dimension scale.

The older method uses the axis attribute on each dimension scale to identify with an integer the axis whose value is the number of the dimension.

NXdata is used to implement one of the basic motivations in NeXus, to provide a default plot for the data of this NXentry. The actual data might be stored in another group and (hard) linked to the NXdata group.

Basic Structure of NXdata

```
NXdata (base class, version 1.0)
  data:NX_NUMBER[n]
    @signal
    @axes
    Quncertainties
    @long_name
  errors:NX_NUMBER[n]
  offset:NX FLOAT
  scaling factor: NX FLOAT
  variable:NX_NUMBER[n]
    @long name
    @distribution
    @first good
    @last_good
    @axis
  variable_errors:NX_NUMBER[n]
  x:NX_FLOAT[nx]
  y:NX_FLOAT[ny]
  z:NX_FLOAT[nz]
```

Comprehensive Structure of NXdata

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXdetector

```
category: base classes
NXDL source: NXdetector
      (http://svn.nexusformat.org/definitions/trunk/base_classes/NXdetector.nxdl.xml)
version: 1.0
SVN Id: $Id: NXdetector.rst 917 2011-10-16 21:04:30Z Pete Jemian $
extends class: NXobject (page 74)
other classes included: NXcharacterization (page 50), NXdata (page 54), NXgeometry (page 65), NXnote
      (page 73)
symbol list: none
documentation: Template of a detector, detector bank, or multidetector. The indices require explanation:
     np
     the number of points in a scan. This dimension is only present in scanning measurements.
     tof
     the number of points in a scan. This dimension is only present in scanning measurements.
     i
     the number of pixels in the slowest varying direction. This is only missing in the point detector.
     j
     the number of pixels in the fastest varying direction. This exists only in "area" detectors.
```

Basic Structure of NXdetector

```
NXdetector (base class, version 1.0)
  azimuthal_angle:NX_FLOAT[np,i,j]
 beam_center_x:NX_FLOAT
 beam_center_y:NX_FLOAT
  calibration_date:NX_DATE_TIME
  count_time:NX_NUMBER[np]
  crate:NX_INT[i, j]
    @local_name
  data:NX_NUMBER[np,i,j,tof]
    @signal
    @axes
    @long_name
    @check sum
  data_error:NX_NUMBER[np,i,j,tof]
    @units
    @link
```

```
dead_time:NX_FLOAT[np,i,j]
description: NX_CHAR
detection_gas_path:NX_FLOAT
detector_number:NX_INT[i,j]
diameter:NX_FLOAT
distance:NX_FLOAT[np,i,j]
frame_start_number:NX_INT
gas_pressure:NX_FLOAT[i,j]
input:NX_INT[i,j]
  @local_name
layout:NX_CHAR
local_name:NX_CHAR
polar_angle:NX_FLOAT[np,i,j]
raw_time_of_flight:NX_INT[tof+1]
  @frequency
sequence_number:NX_CHAR
slot:NX INT[i, j]
  @local_name
solid_angle:NX_FLOAT[i, j]
time_of_flight:NX_FLOAT[tof+1]
  @axis
  @primary
  @long_name
  @link
type:NX_CHAR
x_pixel_offset:NX_FLOAT[i]
  @axis
  @primary
  @long_name
  @link
x_pixel_size:NX_FLOAT[i,j]
y_pixel_offset:NX_FLOAT[j]
  @axis
  @primary
  @long_name
y_pixel_size:NX_FLOAT[i, j]
NXcharacterization
efficiency: NXdata
  efficiency:NX_FLOAT[i,j,k]
  real_time:NX_NUMBER[i,j,k]
  wavelength:NX_FLOAT[i,j,k]
NXgeometry
calibration_method:NXnote
data file:NXnote
```

Comprehensive Structure of NXdetector

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXdetector group

category: base_classes

NXDL source: NXdetector_group

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXdetector_group.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXdetector_group.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: This class is used to allow a logical grouping of detector elements (e.g. which tube, bank or group of banks) to be recorded in the file. As well as allowing you to e.g just select the "left" or "east" detectors, it may also be useful for determining which elements belong to the same PSD tube and hence have e.g. the same dead time.

For example, if we had "bank1" composed of "tube1", "tube2" and "tube3" then group_names would be the string "bank1, bank1/tube1, bank1/tube2,bank1/tube3" group_index would be {1,2,3,4} group_parent would be {-1,1,1,1}

The mapping array is interpreted as group 1 is a top level group containing groups 2, 3 and 4

A group_index array in NXdetector give the base group for a detector element.

Basic Structure of NXdetector_group

```
NXdetector_group (base class, version 1.0)
  group_index:NX_INT[i]
  group_names:NX_CHAR
  group_parent:NX_INT[]
  group_type:NX_INT[]
```

Comprehensive Structure of NXdetector group

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXdisk chopper

category: base_classes

NXDL source: NXdisk_chopper

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXdisk_chopper.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXdisk_chopper.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: *NXgeometry* (page 65)

symbol list: none

documentation: No documentation provided.

Basic Structure of NXdisk chopper

```
NXdisk_chopper (base class, version 1.0)
distance:NX_FLOAT
pair_separation:NX_FLOAT
phase:NX_FLOAT
radius:NX_FLOAT
ratio:NX_INT
rotation_speed:NX_FLOAT
slit_angle:NX_FLOAT
slit_height:NX_FLOAT
slits:NX_INT
type:NX_CHAR
wavelength_range:NX_FLOAT[2]
NXgeometry
```

Comprehensive Structure of NXdisk chopper

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXentry

category: base_classes
NXDL source: NXentry

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXentry.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXentry.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXcharacterization (page 50), NXdata (page 54), NXinstrument (page 68), NXmonitor (page 72), NXnote (page 73), NXprocess (page 78), NXsample (page 79), NXsubentry (page 83), NXuser (page 86)

symbol list: none

documentation: (required) Template of the top-level NeXus group which contains all the data and associated information that comprise a single measurement. It is mandatory that there is at least one group of this type in the NeXus file.

Basic Structure of NXentry

```
NXentry (base class, version 1.0)
  @IDF_Version
  collection_description:NX_CHAR
  collection_identifier:NX_CHAR
  collection_time:NX_FLOAT
  definition:NX_CHAR
    @version
    @URL
  definition_local:NX_CHAR
    @version
    @URL
  duration: NX INT
  end_time:NX_DATE_TIME
  entry_identifier:NX_CHAR
  experiment_description:NX_CHAR
  experiment identifier: NX CHAR
  pre_sample_flightpath:NX_FLOAT
  program_name:NX_CHAR
    @version
    @configuration
  revision:NX_CHAR
    @comment
  run_cycle:NX_CHAR
  start_time:NX_DATE_TIME
  title:NX_CHAR
 NXcharacterization
 NXdata
 NXinstrument
 NXmonitor
  experiment documentation: NXnote
  notes:NXnote
  thumbnail:NXnote
    @mime_type
 NXprocess
 NXsample
 NXsubentry
 NXuser
```

Comprehensive Structure of NXentry

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXenvironment

category: base_classes

NXDL source: NXenvironment

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXenvironment.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXenvironment.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXgeometry (page 65), NXnote (page 73), NXsensor (page 81)

symbol list: none

documentation: This class describes an external condition applied to the sample

Basic Structure of NXenvironment

NXenvironment (base class, version 1.0)
description:NX_CHAR
name:NX_CHAR
program:NX_CHAR
short_name:NX_CHAR
type:NX_CHAR
position:NXgeometry
NXnote
NXsensor

Comprehensive Structure of NXenvironment

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXevent data

category: base_classes

NXDL source: NXevent_data

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXevent_data.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXevent_data.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: Time-of-flight events

Basic Structure of NXevent_data

```
NXevent_data (base class, version 1.0)
  events_per_pulse:NX_INT[j]
  pixel_number:NX_INT[i]
  pulse_height:NX_FLOAT[i,k]
  pulse_time:NX_INT[j]
    @offset
  time_of_flight:NX_INT[i]
```

Comprehensive Structure of NXevent data

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXfermi_chopper

category: base_classes

NXDL source: NXfermi_chopper

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXfermi_chopper.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXfermi chopper.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: *NXgeometry* (page 65)

symbol list: none

documentation: Description of a Fermi chopper, possibly with curved slits.

Basic Structure of NXfermi chopper

```
NXfermi_chopper (base class, version 1.0)
absorbing_material:NX_CHAR
distance:NX_FLOAT
energy:NX_FLOAT
height:NX_FLOAT
number:NX_INT
r_slit:NX_FLOAT
radius:NX_FLOAT
rotation_speed:NX_FLOAT
```

slit:NX_FLOAT
transmitting_material:NX_CHAR
type:NX_CHAR
wavelength:NX_FLOAT
width:NX_FLOAT
NXgeometry

Comprehensive Structure of NXfermi chopper

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXfilter

category: base_classes
NXDL source: NXfilter

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXfilter.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXfilter.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXgeometry (page 65), NXlog (page 69), NXsensor (page 81)

symbol list: none

documentation: Template for specifying the state of band pass filters. If uncertain whether to use NXfilter (band-pass filter) or NXattenuator (reduces beam intensity), then use NXattenuator.

Basic Structure of NXfilter

```
NXfilter (base class, version 1.0)
  chemical_formula:NX_CHAR
  coating_material:NX_CHAR
  coating_roughness:NX_FLOAT[nsurf]
  density:NX_NUMBER
  description: NX_CHAR
  m_value:NX_FLOAT
  orientation matrix: NX FLOAT[n comp, 3, 3]
  status:NX CHAR
  substrate_material:NX_CHAR
  substrate_roughness:NX_FLOAT
  substrate_thickness:NX_FLOAT
  temperature: NX_FLOAT
  thickness:NX_FLOAT
  unit_cell_a:NX_FLOAT
  unit_cell_alpha:NX_FLOAT
```

```
unit_cell_b:NX_FLOAT
unit_cell_beta:NX_FLOAT
unit_cell_c:NX_FLOAT
unit_cell_gamma:NX_FLOAT
unit_cell_volume:NX_FLOAT[n_comp]
transmission:NXdata
NXgeometry
temperature_log:NXlog
sensor_type:NXsensor
```

Comprehensive Structure of NXfilter

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXflipper

category: base_classes

NXDL source: NXflipper

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXflipper.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXflipper.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: Template of a beamline spin flipper.

Basic Structure of NXflipper

```
NXflipper (base class, version 1.0)
comp_current:NX_FLOAT
comp_turns:NX_FLOAT
flip_current:NX_FLOAT
flip_turns:NX_FLOAT
guide_current:NX_FLOAT
guide_turns:NX_FLOAT
thickness:NX_FLOAT
type:NX_CHAR
```

Comprehensive Structure of NXflipper

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXgeometry

category: base_classes

NXDL source: NXgeometry

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXgeometry.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXgeometry.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXorientation (page 75), NXshape (page 82), NXtranslation (page 85)

symbol list: none

documentation: This is the description for a general position of a component. It is recommended to name an instance of NXgeometry as "geometry" to aid in the use of the definition in simulation codes such as McStas. Also, in HDF, linked items must share the same name. However, it might not be possible or practical in all situations.

Basic Structure of NXgeometry

NXgeometry (base class, version 1.0)
component_index:NX_INT
description:NX_CHAR
NXorientation
NXshape
NXtranslation

Comprehensive Structure of NXgeometry

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXguide

category: base_classes
NXDL source: NXguide

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXguide.nxdl.xml)

```
version: 1.0
SVN Id: $Id: NXguide.rst 917 2011-10-16 21:04:30Z Pete Jemian $
extends class: NXobject (page 74)
other classes included: NXdata (page 54), NXgeometry (page 65)
symbol list:
    nsurf number of reflecting surfaces
    nwl number of wavelengths
```

documentation: NXguide is used by neutron instruments to describe a guide consists of several mirrors building a shape through which neutrons can be guided or directed. The simplest such form is box shaped although elliptical guides are gaining in popularity. The individual parts of a guide usually have common characteristics but there are cases where they are different. For example, a neutron guide might consist of 2 or 4 coated walls or a supermirror bender with multiple, coated vanes.

To describe polarizing supermirrors such as used in neutron reflection, it may be necessary to revise this definition of NXguide to include NXpolarizer and/or NXmirror.

When even greater complexity exists in the definition of what constitutes a guide, it has been suggested that NXguide be redefined as a NXcollection of NXmirrors each having their own NXgeometries describing their location(s).

For the more general case when describing mirrors, consider using NXmirror.

NOTE: The NeXus International Advisory Committee welcomes comments for revision and improvement of this definition of NXguide.

Basic Structure of NXquide

```
NXguide (base class, version 1.0)
 bend angle x:NX FLOAT
 bend_angle_y:NX_FLOAT
  coating material:NX FLOAT[nsurf]
  coating_roughness:NX_FLOAT[nsurf]
  description: NX CHAR
  external_material:NX_CHAR
  incident angle: NX FLOAT
  interior_atmosphere:NX_CHAR
  m_value:NX_FLOAT[nsurf]
  number_sections:NX_INT
  substrate_material:NX_FLOAT[nsurf]
  substrate_roughness:NX_FLOAT[nsurf]
  substrate_thickness:NX_FLOAT[nsurf]
  reflectivity: NXdata
    data:NX_NUMBER[nsurf,nwl]
      @signal
      @axes
    surface:NX_NUMBER[nsurf]
```

```
wavelength:NX_NUMBER[nwl]
NXgeometry
```

Comprehensive Structure of NXguide

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXinsertion device

category: base_classes

NXDL source: NXinsertion_device

(http://svn.nexusformat.org/definitions/trunk/base classes/NXinsertion device.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXinsertion_device.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXgeometry (page 65)

symbol list: none

documentation: Description of an insertion device, as in a synchrotron.

Basic Structure of NXinsertion_device

```
NXinsertion_device (base class, version 1.0)
bandwidth:NX_FLOAT
energy:NX_FLOAT
gap:NX_FLOAT
harmonic:NX_INT
k:NX_FLOAT
length:NX_FLOAT
magnetic_wavelength:NX_FLOAT
phase:NX_FLOAT
poles:NX_INT
power:NX_FLOAT
taper:NX_FLOAT
type:NX_CHAR
spectrum:NXdata
NXgeometry
```

Comprehensive Structure of NXinsertion_device

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXinstrument

category: base_classes

NXDL source: NXinstrument

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXinstrument.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXinstrument.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXaperture (page 45), NXattenuator (page 46), NXbeam_stop (page 48), NXbeam (page 47), NXbending_magnet (page 48), NXcollimator (page 51), NXcrystal (page 52), NXdetector (page 56), NXdisk_chopper (page 58), NXfermi_chopper (page 62), NXfilter (page 63), NXflipper (page 64), NXguide (page 65), NXinsertion_device (page 67), NXmirror (page 70), NXmoderator (page 71), NXpolarizer (page 76), NXsource (page 82), NXvelocity_selector (page 86)

symbol list: none

documentation: Template of instrument descriptions comprising various beamline components. Each component will also be a NeXus group defined by its distance from the sample. Negative distances represent beamline components that are before the sample while positive distances represent components that are after the sample. This device allows the unique identification of beamline components in a way that is valid for both reactor and pulsed instrumentation.

Basic Structure of NXinstrument

NXinstrument (base class, version 1.0) name:NX_CHAR @short name NXaperture NXattenuator NXbeam NXbeam_stop NXbending_magnet NXcollimator NXcrystal NXdetector NXdisk_chopper NXfermi_chopper NXfilter NXflipper NXquide

NXinsertion_device NXmirror NXmoderator NXpolarizer NXsource NXvelocity_selector

Comprehensive Structure of NXinstrument

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXlog

category: base_classes **NXDL source:** NXlog

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXlog.nxdl.xml)

version: 1.0

(CI SIUII. 1.0

SVN Id: \$Id: NXlog.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: Definition of information that is recorded against time, such as information monitored during the run. It contains the logged values and the times at which they were measured as elapsed time since a starting time recorded in ISO8601 format. This method of storing logged data helps to distinguish instances in which a variable is a dimension scale of the data, in which case it is stored in an NXdata group, and instances in which it is logged during the run, when it should be stored in an NXlog group. Note: When using multiple NXlog groups, it is suggested to place them inside a NXcollection group. In such cases, when NXlog is used in another class, NXcollection/NXlog is then constructed.

Basic Structure of NXlog

NXlog (base class, version 1.0)
average_value:NX_FLOAT
average_value_error:NX_FLOAT
description:NX_CHAR
duration:NX_FLOAT
maximum_value:NX_FLOAT
minimum_value:NX_FLOAT
raw_value:NX_NUMBER
time:NX_FLOAT

@start
value:NX_NUMBER

Comprehensive Structure of NXlog

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXmirror

category: base_classes

NXDL source: NXmirror

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXmirror.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXmirror.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXgeometry (page 65), NXshape (page 82)

symbol list: none

documentation: Template of a beamline mirror or supermirror.

Basic Structure of NXmirror

NXmirror (base class, version 1.0) bend angle x:NX FLOAT bend_angle_y:NX_FLOAT coating_material:NX_CHAR coating_roughness:NX_FLOAT description: NX_CHAR even layer density: NX FLOAT even_layer_material:NX_CHAR external_material:NX_CHAR incident_angle:NX_FLOAT interior_atmosphere:NX_CHAR layer_thickness:NX_FLOAT m_value:NX_FLOAT odd_layer_density:NX_FLOAT odd_layer_material:NX_CHAR substrate_density:NX_FLOAT substrate_material:NX_CHAR substrate_roughness:NX_FLOAT substrate thickness:NX FLOAT type:NX_CHAR reflectivity: NXdata

figure_data:NXdata
NXgeometry
shape:NXshape

Comprehensive Structure of NXmirror

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXmoderator

category: base_classes

NXDL source: NXmoderator

(http://svn.nexusformat.org/definitions/trunk/base classes/NXmoderator.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXmoderator.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXgeometry (page 65), NXlog (page 69)

symbol list: none

documentation: This is the description for a general moderator

Basic Structure of NXmoderator

NXmoderator (base class, version 1.0)
coupled:NX_BOOLEAN
coupling_material:NX_CHAR
distance:NX_FLOAT
poison_depth:NX_FLOAT
poison_material:NX_CHAR
temperature:NX_FLOAT
type:NX_CHAR
pulse_shape:NXdata
NXgeometry
temperature_log:NXlog

Comprehensive Structure of NXmoderator

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXmonitor

category: base_classes

NXDL source: NXmonitor

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXmonitor.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXmonitor.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXgeometry (page 65), NXlog (page 69)

symbol list: none

documentation: Template of monitor data. It is similar to the NXdata groups containing monitor data and its associated dimension scale, e.g. time_of_flight or wavelength in pulsed neutron instruments. However, it may also include integrals, or scalar monitor counts, which are often used in both in both pulsed and steady-state instrumentation.

Basic Structure of NXmonitor

```
NXmonitor (base class, version 1.0)
  count_time:NX_FLOAT
  data:NX_NUMBER[n]
    @signal
    @axes
  distance: NX FLOAT
  efficiency: NX_NUMBER[]
  end_time:NX_DATE_TIME
  integral:NX_NUMBER
  mode:NX_CHAR
  preset:NX_NUMBER
  range:NX_FLOAT[2]
  sampled_fraction:NX_FLOAT
  start_time:NX_DATE_TIME
  time_of_flight:NX_FLOAT[]
  type:NX_CHAR
  NXgeometry
  integral_log:NXlog
```

Comprehensive Structure of NXmonitor

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXmonochromator

category: base_classes

NXDL source: NXmonochromator

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXmonochromator.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXmonochromator.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXcrystal (page 52), NXdata (page 54), NXgeometry (page 65), NXveloc-

ity_selector (page 86)

symbol list: none

documentation: This is a base class for everything which selects a wavelength or energy, be it a monochro-

mator crystal, a velocity selector, a undulator or whatever.

The expected units are:

wavelength: angstrom

energy: eV

Basic Structure of NXmonochromator

```
NXmonochromator (base class, version 1.0)
energy:NX_FLOAT
energy_error:NX_FLOAT
wavelength:NX_FLOAT
wavelength_error:NX_FLOAT
NXcrystal
distribution:NXdata
geometry:NXgeometry
NXvelocity_selector
```

Comprehensive Structure of NXmonochromator

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXnote

category: base_classes
NXDL source: NXnote

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXnote.nxdl.xml)

NeXus: a common data format for neutron, x-ray, and muon science, Release 2011-10

version: 1.0

SVN Id: \$Id: NXnote.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: This class can be used to store additional information in a NeXus file e.g. pictures, movies,

audio, additional text logs

Basic Structure of NXnote

NXnote (base class, version 1.0)
author:NX_CHAR
data:NX_BINARY
date:NX_DATE_TIME
description:NX_CHAR
file_name:NX_CHAR
type:NX_CHAR

Comprehensive Structure of NXnote

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXobject

category: base_classes
NXDL source: NXobject

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXobject.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXobject.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: none

other classes included: none

symbol list: none

documentation: This is the base object of NeXus

Basic Structure of NXobject

NXobject (base class, version 1.0)

Comprehensive Structure of NXobject

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXorientation

category: base_classes

NXDL source: NXorientation

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXorientation.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXorientation.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: *NXgeometry* (page 65)

symbol list: none

documentation: This is the description for a general orientation of a component - it is used by the NXge-

ometry class

Basic Structure of NXorientation

```
NXorientation (base class, version 1.0)
value:NX_FLOAT[numobj, 6]
NXgeometry
```

Comprehensive Structure of NXorientation

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXparameters

category: base_classes

NXDL source: NXparameters

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXparameters.nxdl.xml)

NeXus: a common data format for neutron, x-ray, and muon science, Release 2011-10

version: 1.0

SVN Id: \$Id: NXparameters.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: Container for parameters, usually used in processing or analysis.

Basic Structure of NXparameters

```
NXparameters (base class, version 1.0) term: NX_CHAR @units
```

Comprehensive Structure of NXparameters

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXpolarizer

category: base_classes

NXDL source: NXpolarizer

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXpolarizer.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXpolarizer.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: none

symbol list: none

documentation: Template of a beamline spin polarizer.

This is a draft and is subject to revision.

Basic Structure of NXpolarizer

```
NXpolarizer (base class, version 1.0)
  composition:NX_CHAR
  efficiency:NX_FLOAT
  reflection:NX_INT[3]
  type:NX_CHAR
```

Comprehensive Structure of NXpolarizer

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXpositioner

category: base_classes

NXDL source: NXpositioner

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXpositioner.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXpositioner.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: This group describes a generic positioner such as a motor or piezo-electric transducer. It is used to document the current information of a piece of beam line equipment. Note: When using multiple NXpositioner groups, it is suggested to place them inside a NXcollection group. In such cases, when NXpositioner is used in another class, NXcollection/NXpositioner is then constructed.

Basic Structure of NXpositioner

```
NXpositioner (base class, version 1.0)
acceleration_time:NX_NUMBER
controller_record:NX_CHAR
description:NX_CHAR
name:NX_CHAR
raw_value:NX_NUMBER[n]
soft_limit_max:NX_NUMBER
soft_limit_min:NX_NUMBER
target_value:NX_NUMBER[n]
tolerance:NX_NUMBER[n]
value:NX_NUMBER[n]
velocity:NX_NUMBER
```

Comprehensive Structure of NXpositioner

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXprocess

category: base_classes

NXDL source: NXprocess

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXprocess.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXprocess.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXnote (page 73)

symbol list: none

documentation: Document an event of data processing, reconstruction, or analysis for this data.

Basic Structure of NXprocess

```
NXprocess (base class, version 1.0)
  date:NX_DATE_TIME
  program:NX_CHAR
  version:NX_CHAR
  NXnote
```

Comprehensive Structure of NXprocess

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXroot

category: base_classes
NXDL source: NXroot

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXroot.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXroot.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXentry (page 59)

symbol list: none

documentation: Definition of the root NeXus group.

Basic Structure of NXroot

```
NXroot (base class, version 1.0)

@NX_class

@file_time

@file_name

@file_update_time

@NeXus_version

@HDF_version

@HDF5_Version

@XML_version

@creator

NXentry
```

Comprehensive Structure of NXroot

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsample

category: base_classes

NXDL source: NXsample

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXsample.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXsample.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: NXbeam (page 47), NXdata (page 54), NXenvironment (page 61), NXgeometry

(page 65), *NXlog* (page 69)

symbol list: symbolic array lengths to be coordinated between various fields

n_comp number of compositions

n_Temp number of temperatures

n_eField number of values in applied electric field

n_mField number of values in applied magnetic field

n_pField number of values in applied pressure field

n_sField number of values in applied stress field

documentation: Template of the state of the sample. This could include scanned variables that are associated with one of the data dimensions, e.g. the magnetic field, or logged data, e.g. monitored temperature vs elapsed time.

Basic Structure of NXsample

```
NXsample (base class, version 1.0)
  changer_position:NX_INT
  chemical_formula:NX_CHAR
  component:NX_CHAR
  concentration:NX_FLOAT[n_comp]
  density:NX_FLOAT[n_comp]
  description: NX CHAR
  distance: NX_FLOAT
  electric_field:NX_FLOAT[n_eField]
    @direction
  external_DAC:NX_FLOAT
  magnetic_field:NX_FLOAT[n_mField]
    @direction
  mass:NX_FLOAT[n_comp]
  name:NX_CHAR
  orientation_matrix:NX_FLOAT[n_comp,3,3]
  path_length:NX_FLOAT
  path_length_window:NX_FLOAT
  preparation_date:NX_DATE_TIME
  pressure:NX_FLOAT[n_pField]
  relative_molecular_mass:NX_FLOAT[n_comp]
  rotation_angle:NX_FLOAT
  sample_component:NX_CHAR
  sample orientation:NX FLOAT[3]
  scattering_length_density:NX_FLOAT[n_comp]
  short title:NX CHAR
  situation:NX_CHAR
  stress_field:NX_FLOAT[n_sField]
    @direction
  temperature:NX_FLOAT[n_Temp]
  thickness:NX_FLOAT
  type:NX_CHAR
  unit_cell:NX_FLOAT[n_comp,6]
  unit_cell_class:NX_CHAR
  unit_cell_group:NX_CHAR
  unit_cell_volume:NX_FLOAT[n_comp]
  volume_fraction:NX_FLOAT[n_comp]
  x_translation:NX_FLOAT
 NXbeam
  transmission: NXdata
  temperature env:NXenvironment
  magnetic_field_env:NXenvironment
  geometry:NXgeometry
  temperature_log:NXlog
  magnetic_field_log:NXlog
  external_ADC:NXlog
```

Comprehensive Structure of NXsample

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsensor

category: base_classes

NXDL source: NXsensor

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXsensor.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXsensor.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXgeometry (page 65), NXlog (page 69), NXorientation (page 75)

symbol list: none

documentation: This class describes a sensor used to monitor an external condition - the condition itself is

described in NXenvironment

Basic Structure of NXsensor

```
NXsensor (base class, version 1.0)
 attached_to:NX_CHAR
  external_field_brief:NX_CHAR
 high_trip_value:NX_FLOAT
  low_trip_value:NX_FLOAT
 measurement:NX_CHAR
 model:NX_CHAR
  name:NX_CHAR
  run_control:NX_BOOLEAN
  short name: NX CHAR
  type:NX_CHAR
  value:NX FLOAT[n]
  value_deriv1:NX_FLOAT[]
  value_deriv2:NX_FLOAT[]
  geometry:NXgeometry
  value_log:NXlog
  value_deriv1_log:NXlog
  value_deriv2_log:NXlog
  external_field_full:NXorientation
```

Comprehensive Structure of NXsensor

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXshape

category: base_classes
NXDL source: NXshape

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXshape.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXshape.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: This is the description of the general shape and size of a component, which may be made

up of "numobj" separate elements - it is used by the NXgeometry class

Basic Structure of NXshape

NXshape (base class, version 1.0)
 direction:NX_CHAR
 shape:NX_CHAR
 size:NX_FLOAT[numobj,nshapepar]

Comprehensive Structure of NXshape

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsource

category: base_classes
NXDL source: NXsource

(http://svn.nexusformat.org/definitions/trunk/base classes/NXsource.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXsource.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXgeometry (page 65), NXnote (page 73)

symbol list: none

documentation: Template of the neutron or x-ray source, insertion devices and/or moderators.

Basic Structure of NXsource

```
NXsource (base class, version 1.0)
 bunch distance: NX FLOAT
 bunch_length:NX_FLOAT
  current:NX_FLOAT
  distance: NX_FLOAT
  emittance_x:NX_FLOAT
  emittance_y:NX_FLOAT
  energy:NX_FLOAT
  flux:NX_FLOAT
  frequency:NX_FLOAT
  last_fill:NX_NUMBER
    @time
 mode:NX_CHAR
  name:NX CHAR
    @short_name
  number_of_bunches:NX_INT
  period:NX_FLOAT
  power: NX_FLOAT
  probe:NX_CHAR
  pulse_width:NX_FLOAT
  sigma_x:NX_FLOAT
  sigma_y:NX_FLOAT
  target_material:NX_CHAR
  top_up:NX_BOOLEAN
  type:NX_CHAR
  voltage:NX_FLOAT
 bunch_pattern:NXdata
    title:NX_CHAR
  pulse_shape:NXdata
  distribution: NXdata
  geometry:NXgeometry
  notes:NXnote
```

Comprehensive Structure of NXsource

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsubentry

category: base_classes

NXDL source: NXsubentry

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXsubentry.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXsubentry.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXcharacterization (page 50), NXdata (page 54), NXinstrument (page 68), NXmonitor (page 72), NXnote (page 73), NXprocess (page 78), NXsample (page 79), NXuser (page 86)

symbol list: none

documentation: NXsubentry is a base class virtually identical to NXentry and is used as the (overlay) location for application definitions. Use a separate NXsubentry for each application definition.

To use NXsubentry with a hypothetical application definition called NXmyappdef:

Create a group with attribute NX_class="NXsubentry".

Within that group, create a field called definition="NXmyappdef".

There are two optional attributes of definition: version and URL

The intended use is to define application definitions for a multi-technique NXentry. Previously, an application definition replaced NXentry with its own definition. With the increasing popularity of instruments combining multiple techniques for data collection (such as SAXS/WAXS instruments), it was recognized the application definitions must be entered in the NeXus data file tree as children of NXentry.

Basic Structure of NXsubentry

```
NXsubentry (base class, version 1.0)
  @IDF_Version
  collection_description:NX_CHAR
  collection identifier: NX CHAR
  collection time: NX FLOAT
  definition: NX CHAR
    @version
    QURL
  definition_local:NX_CHAR
    @version
    @URL
  duration:NX_INT
  end_time:NX_DATE_TIME
  entry_identifier:NX_CHAR
  experiment_description:NX_CHAR
  experiment_identifier:NX_CHAR
  pre_sample_flightpath:NX_FLOAT
 program_name:NX_CHAR
    @version
    @configuration
  revision: NX CHAR
```

@comment
run_cycle:NX_CHAR
start_time:NX_DATE_TIME
title:NX_CHAR
NXcharacterization
NXdata
NXinstrument
NXmonitor
experiment_documentation:NXnote
notes:NXnote
thumbnail:NXnote
@mime_type
NXprocess
NXsample
NXuser

Comprehensive Structure of NXsubentry

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXtranslation

category: base_classes

NXDL source: NXtranslation

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXtranslation.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXtranslation.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXgeometry (page 65)

symbol list: none

documentation: This is the description for the general spatial location of a component - it is used by the

NXgeometry class

Basic Structure of NXtranslation

```
NXtranslation (base class, version 1.0)
  distances:NX_FLOAT[numobj,3]
  geometry:NXgeometry
```

Comprehensive Structure of NXtranslation

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXuser

category: base_classes
NXDL source: NXuser

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXuser.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXuser.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: Template of user's contact information. The format allows more than one user with the same affiliation and contact information, but a second NXuser group should be used if they have different affiliations, etc.

Basic Structure of NXuser

NXuser (base class, version 1.0)
address:NX_CHAR
affiliation:NX_CHAR
email:NX_CHAR
facility_user_id:NX_CHAR
fax_number:NX_CHAR
name:NX_CHAR
role:NX_CHAR
telephone_number:NX_CHAR

Comprehensive Structure of NXuser

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXvelocity_selector

category: base_classes

NXDL source: NXvelocity_selector

(http://svn.nexusformat.org/definitions/trunk/base classes/NXvelocity selector.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXvelocity_selector.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: *NXgeometry* (page 65)

symbol list: none

documentation: This is the description for a (typically neutron) velocity selector

Basic Structure of NXvelocity_selector

```
NXvelocity_selector (base class, version 1.0)
height:NX_FLOAT
length:NX_FLOAT
num:NX_INT
radius:NX_FLOAT
rotation_speed:NX_FLOAT
spwidth:NX_FLOAT
table:NX_FLOAT
table:NX_FLOAT
twist:NX_FLOAT
type:NX_CHAR
wavelength:NX_FLOAT
wavelength_spread:NX_FLOAT
width:NX_FLOAT
geometry:NXgeometry
```

Comprehensive Structure of NXvelocity selector

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxraylens

category: base_classes

NXDL source: NXxraylens

(http://svn.nexusformat.org/definitions/trunk/base_classes/NXxraylens.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXxraylens.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXnote (page 73)

symbol list: none

documentation: This is a dictionary of field names to use dor describing a X-ray lens as used at synchrotron

beam lines. Based on information provided by Gerd Wellenreuther.

Basic Structure of NXxraylens

```
NXxraylens (base class, version 1.0)
aperture:NX_FLOAT
curvature:NX_FLOAT
cylindrical:NX_BOOLEAN
focus_type:NX_CHAR
gas:NX_CHAR
gas_pressure:NX_FLOAT
lens_geometry:NX_CHAR
lens_length:NX_FLOAT
lens_material:NX_CHAR
lens_thickness:NX_FLOAT
number_of_lenses:NX_INT
symmetric:NX_BOOLEAN
cylinder_orientation:NXnote
```

Comprehensive Structure of NXxraylens

Name and Attributes	Type	Units	Description (and Occurrences)
class			

3.1.2 NeXus Application Definitions Classes

Contents:

NXarchive

category: applications

NXDL source: NXarchive

(http://svn.nexusformat.org/definitions/trunk/applications/NXarchive.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXarchive.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: NXentry (page 59), NXinstrument (page 68), NXsample (page 79), NXsource

(page 82), *NXuser* (page 86)

symbol list: none

documentation: This is a definition for data to be archived by ICAT (see: http://www.icatproject.org/),

the database (with supporting software) that provides an interface to all ISIS experimental data and will provide a mechanism to link all aspects of ISIS research from proposal through to publication.

Basic Structure of NXarchive

```
NXarchive (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    @index
    collection_description:NX_CHAR
    collection_identifier:NX_CHAR
    collection_time:NX_FLOAT
    definition: NX_CHAR
    duration: NX_FLOAT
    end time: NX DATE TIME
    entry_identifier:NX_CHAR
    experiment_description:NX_CHAR
    experiment_identifer:NX_CHAR
    program: NX_CHAR
      @version
    release_date:NX_CHAR
    revision: NX CHAR
    run_cycle:NX_CHAR
    start_time:NX_DATE_TIME
    title:NX_CHAR
    instrument: NXinstrument
      description: NX_CHAR
      name:NX_CHAR
      NXsource
        name:NX_CHAR
        probe: NX_CHAR
        type:NX_CHAR
    sample: NXsample
      chemical_formula:NX_CHAR
      description: NX_CHAR
      electric_field:NX_FLOAT
      magnetic field:NX FLOAT
      name:NX_CHAR
      preparation date: NX CHAR
      pressure: NX_FLOAT
      sample_id:NX_CHAR
      situation: NX_CHAR
      stress_field:NX_FLOAT
      temperature: NX_FLOAT
      type:NX_CHAR
    user:NXuser
      facility_user_id:NX_CHAR
      name: NX_CHAR
      role:NX CHAR
```

Comprehensive Structure of NXarchive

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXdirecttof

category: applications

NXDL source: NXdirecttof

(http://svn.nexusformat.org/definitions/trunk/applications/NXdirecttof.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXdirecttof.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXtofraw (page 107)

other classes included: NXentry (page 59), NXfermi_chopper (page 62), NXinstrument (page 68)

symbol list: none

documentation: This is a application definition for raw data from a direct geometry TOF spectrometer

Basic Structure of NXdirecttof

```
NXdirecttof (application definition, version 1.0b)
  (overlays NXentry)
  entry:NXentry
   definition:NX_CHAR
   start_time:NX_DATE_TIME
   title:NX_CHAR
   NXinstrument
    fermi_chopper:NXfermi_chopper
       energy:NX_FLOAT
      rotation_speed:NX_FLOAT
```

Comprehensive Structure of NXdirecttof

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXfluo

category: applications **NXDL source:** NXfluo

(http://svn.nexusformat.org/definitions/trunk/applications/NXfluo.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXfluo.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument (page 68), NXmonitor (page 72), NXmonochromator (page 73), NXsample (page 79), NXsource

(page 82)

symbol list: none

documentation: This is an application definition for raw data from an X-ray fluorescence experiment

Basic Structure of NXfluo

```
NXfluo (application definition, version 1.0)
  (overlays NXentry)
  entry: NXentry
    definition: NX CHAR
    start_time:NX_DATE_TIME
    title:NX CHAR
    NXdata
     data --> /entry/instrument/fluorecence/data
     energy --> /entry/instrument/fluorecence/energy
    NXinstrument
      fluorescence:NXdetector
        data:NX_INT[nenergy]
        energy:NX_FLOAT[nenergy]
     monochromator: NXmonochromator
        wavelength: NX_FLOAT
     NXsource
       name:NX_CHAR
       probe:NX_CHAR
        type:NX_CHAR
    NXmonitor
     data:NX INT
     mode: NX_CHAR
      preset:NX FLOAT
    NXsample
      name:NX CHAR
```

Comprehensive Structure of NXfluo

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXindirecttof

category: applications

NXDL source: NXindirecttof

(http://svn.nexusformat.org/definitions/trunk/applications/NXindirecttof.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXindirecttof.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXtofraw (page 107)

other classes included: NXentry (page 59), NXinstrument (page 68), NXmonochromator (page 73)

symbol list: none

documentation: This is a application definition for raw data from a direct geometry TOF spectrometer

Basic Structure of NXindirecttof

```
NXindirecttof (application definition, version 1.0b)
  (overlays NXentry)
  entry:NXentry
   definition:NX_CHAR
   start_time:NX_DATE_TIME
   title:NX_CHAR
   NXinstrument
    analyser:NXmonochromator
      distance:NX_FLOAT[ndet]
      energy:NX_FLOAT[nDet]
      polar_angle:NX_FLOAT[ndet]
```

Comprehensive Structure of NXindirecttof

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXiqproc

category: applications

NXDL source: NXiqproc

(http://svn.nexusformat.org/definitions/trunk/applications/NXiqproc.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXiqproc.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXentry (page 59), NXinstrument (page 68), NXparameters

(page 75), NXprocess (page 78), NXsample (page 79), NXsource (page 82)

symbol list: none

documentation: Actually this is a template from which to start an application definition.

Basic Structure of NXiqproc

```
NXiqproc (application definition, version 1.0b)
  (overlays NXentry)
 NXentry
    @entry
    definition: NX_CHAR
    title:NX_CHAR
    NXdata
      data:NX_INT[NE,NQX,NQY]
      qx:NX_CHAR
      qy:NX_CHAR
      variable:NX CHAR
        @varied_variable
    instrument: NXinstrument
      name:NX_CHAR
      NXsource
        name:NX_CHAR
        probe: NX_CHAR
        type:NX_CHAR
    reduction: NXprocess
      program: NX_CHAR
      version:NX_CHAR
      input:NXparameters
        filenames:NX_CHAR
      output: NXparameters
    NXsample
      name:NX_CHAR
```

Comprehensive Structure of NXiqproc

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXlauetof

category: applicationsNXDL source: NXlauetof

(http://svn.nexusformat.org/definitions/trunk/applications/NXlauetof.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXlauetof.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument (page 68), NXmonitor (page 72), NXsample (page 79)

symbol list: none

documentation: This is the application definition for a TOF laue diffractometer

Basic Structure of NXIauetof

```
NXlauetof (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX_CHAR
    name:NXdata
      data --> /NXentry/NXinstrument/NXdetector/data
     time_of_flight --> /NXentry/NXinstrument/NXdetector/time_of_flight
    instrument: NXinstrument
      detector: NXdetector
        azimuthal_angle:NX_FLOAT
        data:NX_INT[number of x pixels, number of y pixels, nTOF]
          @signal
        distance:NX_FLOAT
        polar_angle:NX_FLOAT
        time_of_flight:NX_FLOAT[nTOF]
        x_pixel_size:NX_FLOAT
        y_pixel_size:NX_FLOAT
    control: NXmonitor
      data:NX_INT[nTOF]
     mode:NX_CHAR
     preset:NX_FLOAT
     time_of_flight:NX_FLOAT[nTOF]
    sample: NXsample
      name:NX_CHAR
      orientation_matrix:NX_FLOAT[3,3]
      unit_cell:NX_FLOAT[6]
```

Comprehensive Structure of NXIauetof

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXmonopd

category: applications

NXDL source: NXmonopd

(http://svn.nexusformat.org/definitions/trunk/applications/NXmonopd.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXmonopd.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXcrystal (page 52), NXdata (page 54), NXdetector (page 56), NXentry (page 59),

NXinstrument (page 68), NXmonitor (page 72), NXsample (page 79), NXsource (page 82)

symbol list: none

documentation: Monochromatic Neutron and X-Ray Powder Diffraction. Instrument definition for a powder diffractometer at a monochromatic neutron or X-ray beam. This is both suited for a powder diffractometer with a single detector or a powder diffractometer with a position sensitive detector.

Basic Structure of NXmonopd

```
NXmonopd (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX CHAR
    start time: NX DATE TIME
    title:NX_CHAR
    NXdata
     data --> /NXentry/NXinstrument/NXdetector/data
      polar_angle --> /NXentry/NXinstrument/NXdetector/polar_angle
    NXinstrument
     NXcrystal
        wavelength:NX_FLOAT[i]
     NXdetector
        data:NX_INT[ndet]
       polar_angle:NX_FLOAT[ndet]
     NXsource
        name:NX_CHAR
        probe: NX_CHAR
        type:NX_CHAR
    NXmonitor
      integral:NX FLOAT
     mode: NX CHAR
      preset:NX_FLOAT
    NXsample
     name:NX_CHAR
      rotation_angle:NX_FLOAT
```

Comprehensive Structure of NXmonopd

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXrefscan

category: applications

documentation: This is an application definition for a monochromatic scanning reflectometer. It does not have the information to calculate the resolution since it does not have any apertures.

Basic Structure of NXrefscan

```
NXrefscan (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX_CHAR
    end_time:NX_DATE_TIME
    start_time:NX_DATE_TIME
    title:NX CHAR
    data:NXdata
      data --> /NXentry/NXinstrument/NXdetector/data
      polar_angle --> /NXentry/NXinstrument/NXdetector/polar_angle
      rotation_angle --> /NXentry/NXsample/rotation_angle
    instrument: NXinstrument
      NXdetector
        data:NX_INT[NP]
        polar_angle:NX_FLOAT[NP]
      monochromator: NXmonochromator
        wavelength:NX_FLOAT
      NXsource
        name:NX_CHAR
        probe: NX_CHAR
        type:NX_CHAR
    control: NXmonitor
      data:NX_FLOAT[NP]
      mode:NX CHAR
      preset:NX_FLOAT
    sample: NXsample
      name:NX CHAR
      rotation_angle:NX_FLOAT[NP]
```

Comprehensive Structure of NXrefscan

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXreftof

category: applications **NXDL source:** NXreftof

(http://svn.nexusformat.org/definitions/trunk/applications/NXreftof.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXreftof.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXdisk_chopper (page 58), NXentry

(page 59), NXinstrument (page 68), NXmonitor (page 72), NXsample (page 79)

symbol list: none

documentation: This is an application definition for raw data from a TOF reflectometer.

Basic Structure of NXreftof

```
NXreftof (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX_CHAR
    end_time:NX_DATE_TIME
    start_time:NX_DATE_TIME
    title:NX_CHAR
    data:NXdata
      data --> /NXentry/NXinstrument/NXdetector/data
      time binning --> /NXentry/NXinstrument/NXdetector/time binning
    instrument: NXinstrument
      name:NX CHAR
      detector:NXdetector
        data:NX_INT[xsize, ysize, nTOF]
        distance: NX FLOAT
        polar_angle:NX_FLOAT
        time_of_flight:NX_FLOAT[nTOF]
        x_pixel_size:NX_FLOAT
        y_pixel_size:NX_FLOAT
      chopper:NXdisk_chopper
        distance: NX_FLOAT
    control:NXmonitor
      data:NX_INT
      integral:NX_INT
```

```
mode:NX_CHAR
preset:NX_FLOAT
time_of_flight:NX_FLOAT
sample:NXsample
name:NX_CHAR
rotation_angle:NX_FLOAT
```

Comprehensive Structure of NXreftof

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsas

category: applications **NXDL source:** NXsas

(http://svn.nexusformat.org/definitions/trunk/applications/NXsas.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXsas.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXcollimator (page 51), NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXgeometry (page 65), NXinstrument (page 68), NXmonitor (page 72), NXmonochromator (page 73), NXsample (page 79), NXshape (page 82), NXsource (page 82)

symbol list: none

documentation: This is an application definition for 2-D small angle scattering data collected with a monochromatic beam and an area detector. It is meant to be suitable both for neutron SANS and X-ray SAXS data. It covers all SAS techniques: SAS, WSAS, grazing incidence, GISAS

Basic Structure of NXsas

```
NXsas (application definition, version 1.0b)
  (overlays NXentry)
  NXentry
    @entry
    definition:NX_CHAR
    end_time:NX_DATE_TIME
    start_time:NX_DATE_TIME
    title:NX_CHAR
    data:NXdata
        data --> /NXentry/NXinstrument/NXdetector/data
    instrument:NXinstrument
        name:NX CHAR
```

```
collimator: NX collimator
   geometry:NXgeometry
      shape: NXshape
        shape:NX_CHAR
        size:NX_FLOAT
 detector: NXdetector
   aequatorial_angle:NX_FLOAT
   azimuthal_angle:NX_FLOAT
   beam_center_x:NX_FLOAT
   beam_center_y:NX_FLOAT
   data:NX NUMBER[nXPixel, nYPixel]
   distance: NX FLOAT
   polar_angle:NX_FLOAT
   rotation_angle:NX_FLOAT
   x_pixel_size:NX_FLOAT
   y_pixel_size:NX_FLOAT
 monochromator: NXmonochromator
   wavelength: NX_FLOAT
   wavelength_spread:NX_FLOAT
 source: NXsource
   name:NX_CHAR
   probe: NX_CHAR
   type:NX_CHAR
control: NXmonitor
 integral:NX_FLOAT
 mode: NX_CHAR
 preset:NX_FLOAT
sample: NXsample
 aequatorial_angle:NX_FLOAT
 name:NX_CHAR
```

Comprehensive Structure of NXsas

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsastof

category: applicationsNXDL source: NXsastof

(http://svn.nexusformat.org/definitions/trunk/applications/NXsastof.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXsastof.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXcollimator (page 51), NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXgeometry (page 65), NXinstrument (page 68), NXmonitor (page 72), NXsample

```
(page 79), NXshape (page 82), NXsource (page 82)
```

symbol list: none

documentation: This is an application definition for small angle scattering using a 2D detector in TOF mode. It strives to cover all the SAS techniques in the file again

Basic Structure of NXsastof

```
NXsastof (application definition, version 1.0b)
  (overlays NXentry)
 NXentry
    @entry
    definition: NX_CHAR
    start_time:NX_DATE_TIME
    title:NX_CHAR
    data:NXdata
      data --> /NXentry/NXinstrument/NXdetector/data
      time_of_flight --> /NXentry/NXinstrument/NXdetector/time_of_flight
    instrument: NXinstrument
      name:NX CHAR
      collimator: NX collimator
        geometry:NXgeometry
          shape: NXshape
            shape:NX_CHAR
            size:NX FLOAT
      detector: NXdetector
        aequatorial_angle:NX_FLOAT
        azimuthal_angle:NX_FLOAT
        beam_center_x:NX_FLOAT
        beam_center_y:NX_FLOAT
        data:NX_NUMBER[nXPixel,nYPixel,nTOF]
        distance:NX_FLOAT
        polar_angle:NX_FLOAT
        rotation_angle:NX_FLOAT
        time_of_flight:NX_FLOAT[nTOF]
        x_pixel_size:NX_FLOAT
        y pixel size:NX FLOAT
      source: NXsource
        name:NX CHAR
        probe: NX_CHAR
        type:NX CHAR
    control: NXmonitor
      data:NX_INT[nTOF]
      mode: NX CHAR
      preset:NX_FLOAT
      time_of_flight:NX_FLOAT[nTOF]
    sample: NXsample
      aequatorial_angle:NX_FLOAT
      name:NX_CHAR
```

Comprehensive Structure of NXsastof

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXscan

category: applications

NXDL source: NXscan

(http://svn.nexusformat.org/definitions/trunk/applications/NXscan.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXscan.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument

(page 68), NXmonitor (page 72), NXsample (page 79)

symbol list: none

documentation: Application definition for a generic scan instrument. This definition is more an example then a stringent definition as the content of a given NeXus scan file needs to differ for different types of scans. This example definition shows a scan like done on a rotation camera: the sample is rotated and a detector image, the rotation angle and a monitor value is stored at each step in the scan. In the following I use the symbol NP as a placeholder for the number of scan points. These are the rules for storing scan data in NeXus files which are implemented in this example:

Each value varied throughout a scan is stored as an array of length NP at its respective location within the NeXus hierarchy.

For area detectors, NP is the first dimension, example for a detector of 256x256: data[NP,256,256]

The NXdata group contains links to all variables varied in the scan and the data. This to give an equivalent to the more familiar classical tabular representation of scans.

These rules exist for a reason: HDF allows the first dimension of a data set to be unlimited. This means the data can be appended too. Thus a NeXus file built according to the rules given above can be used in the following way:

At the start of a scan, write all the static information.

At each scan point, append new data from varied variables and the detector to the file.

Basic Structure of NXscan

```
NXscan (application definition, version 1.0b)
(overlays NXentry)
NXentry
definition:NX_CHAR
```

```
end_time:NX_DATE_TIME
start_time:NX_DATE_TIME
title:NX_CHAR
NXdata
  data --> /NXentry/NXinstrument/NXdetector/data
  rotation_angle --> /NXentry/NXsample/rotation_angle
NXinstrument
  NXdetector
    data:NX_INT[NP,xdim,ydim]
NXmonitor
  data:NX_INT[NP]
NXsample
  rotation_angle:NX_FLOAT[NP]
```

Comprehensive Structure of NXscan

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXspe

category: applications **NXDL source:** NXspe

(http://svn.nexusformat.org/definitions/trunk/applications/NXspe.nxdl.xml)

version: 1.0 SVN Id: none

extends class: NXobject (page 74)

other classes included: NXcollection (page 51), NXdata (page 54), NXentry (page 59), NXfermi_chopper

(page 62), NXinstrument (page 68), NXsample (page 79)

symbol list: none

documentation: NXSPE Inelastic Format. Application definition for NXSPE file format.

Basic Structure of NXspe

```
NXspe (application definition, version 1.0)
  (overlays NXentry)
  NXentry
    definition:NX_CHAR
      @version
    program_name:NX_CHAR
      NXSPE_info:NXcollection
      fixed_energy:NX_FLOAT
      ki_over_kf_scaling:NX_BOOLEAN
```

psi:NX_FLOAT data:NXdata azimuthal:NX_FLOAT azimuthal_width:NX_FLOAT data:NX_NUMBER distance: NX_FLOAT energy: NX_FLOAT error:NX_NUMBER polar:NX_FLOAT polar_width:NX_FLOAT NXinstrument name:NX CHAR NXfermi_chopper energy: NX_NUMBER NXsample rotation_angle:NX_NUMBER seblock:NX CHAR temperature: NX_NUMBER

Comprehensive Structure of NXspe

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsqom

category: applications

NXDL source: NXsqom

(http://svn.nexusformat.org/definitions/trunk/applications/NXsqom.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXsqom.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXentry (page 59), NXinstrument (page 68), NXparameters

(page 75), NXprocess (page 78), NXsample (page 79), NXsource (page 82)

symbol list: none

documentation: This is the application definition for S(Q,OM) processed data. As this kind of data is in general not on a rectangular grid after data reduction, it is stored as Q,E positions plus their intensity, table like. It is the task of a possible visualisation program to regrid this data in a sensible way.

Basic Structure of NXsqom

```
NXsqom (application definition, version 1.0b)
  (overlays NXentry)
 NXentry
    @entry
    definition: NX_CHAR
   title:NX CHAR
    NXdata
      data:NX_INT[NP]
      en:NX FLOAT[NP]
      qx:NX_CHAR
      qy:NX_CHAR
      qz:NX_CHAR
    instrument: NXinstrument
      name:NX_CHAR
      NXsource
       name:NX_CHAR
        probe: NX_CHAR
        type:NX_CHAR
    reduction: NXprocess
      program: NX_CHAR
      version:NX_CHAR
      input:NXparameters
        filenames:NX CHAR
      output: NXparameters
    NXsample
      name:NX CHAR
```

Comprehensive Structure of NXsqom

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXtas

category: applications **NXDL source:** NXtas

(http://svn.nexusformat.org/definitions/trunk/applications/NXtas.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXtas.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: NXcrystal (page 52), NXdata (page 54), NXdetector (page 56), NXentry (page 59),

NXinstrument (page 68), NXmonitor (page 72), NXsample (page 79), NXsource (page 82)

symbol list: none

documentation: This is an application definition for a triple axis spectrometer. It is for the trademark scan of the TAS, the Q-E scan. For your alignment scans use the rules in NXscan.

Basic Structure of NXtas

```
NXtas (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX_CHAR
    start_time:NX_DATE_TIME
    title:NX_CHAR
    NXdata
      data --> /NXentry/NXinstrument/NXdetector/data
      ef --> /NXentry/NXinstrument/analyzer:NXcrystal/ef
      ei --> /NXentry/NXinstrument/monochromator:NXcrystal/ei
      en --> /NXentry/NXsample/en
      qh --> /NXentry/NXsample/qh
      gk --> /NXentry/NXsample/gk
      ql --> /NXentry/NXsample/ql
    NXinstrument
     monochromator: NXcrystal
        ei:NX_FLOAT[np]
        rotation_angle:NX_FLOAT[np]
      analyser: NXcrystal
        ef:NX_FLOAT[np]
        polar_angle:NX_FLOAT[np]
        rotation_angle:NX_FLOAT[np]
     NXdetector
        data:NX_INT[np]
        polar_angle:NX_FLOAT[np]
      NXsource
        name:NX_CHAR
       probe:NX CHAR
    NXmonitor
      data:NX_FLOAT[np]
     mode: NX CHAR
      preset:NX_FLOAT
    NXsample
      en:NX_FLOAT[np]
      name:NX_CHAR
      orientation_matrix:NX_FLOAT[9]
      polar_angle:NX_FLOAT[np]
      qh:NX_FLOAT[np]
      qk:NX_FLOAT[np]
      ql:NX_FLOAT[np]
      rotation_angle:NX_FLOAT[np]
      sgl:NX_FLOAT[np]
      squ:NX FLOAT[np]
      unit_cell:NX_FLOAT[6]
```

Comprehensive Structure of NXtas

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXtofnpd

category: applicationsNXDL source: NXtofnpd

(http://svn.nexusformat.org/definitions/trunk/applications/NXtofnpd.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXtofnpd.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument

(page 68), NXmonitor (page 72), NXsample (page 79), NXuser (page 86)

symbol list: none

documentation: This is a application definition for raw data from a TOF neutron powder diffractometer

Basic Structure of NXtofnpd

```
NXtofnpd (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX_CHAR
    pre_sample_flightpath:NX_FLOAT
    start_time:NX_DATE_TIME
    title:NX_CHAR
    data:NXdata
      data --> /NXentry/NXinstrument/NXdetector/data
      detector number --> /NXentry/NXinstrument/NXdetector/detector number
      time_of_flight --> /NXentry/NXinstrument/NXdetector/time_of_flight
    NXinstrument
      detector: NXdetector
        azimuthal_angle:NX_FLOAT[ndet]
        data:NX INT[ndet,ntimechan]
        detector_number:NX_INT[ndet]
        distance:NX_FLOAT[ndet]
        polar_angle:NX_FLOAT[ndet]
        time_of_flight:NX_FLOAT[ntimechan]
    NXmonitor
      data:NX_INT[ntimechan]
      distance: NX_FLOAT
      mode: NX_CHAR
      preset:NX_FLOAT
```

```
time_of_flight:NX_FLOAT[ntimechan]
NXsample
  name:NX_CHAR
user:NXuser
  name:NX_CHAR
```

Comprehensive Structure of NXtofnpd

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXtofraw

category: applications

NXDL source: NXtofraw

(http://svn.nexusformat.org/definitions/trunk/applications/NXtofraw.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXtofraw.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument

(page 68), NXmonitor (page 72), NXsample (page 79), NXuser (page 86)

symbol list: none

documentation: This is an application definition for raw data from a generic TOF instrument

Basic Structure of NXtofraw

```
NXtofraw (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX_CHAR
    duration: NX_FLOAT
    pre_sample_flightpath:NX_FLOAT
    run_number:NX_INT
    start_time:NX_DATE_TIME
    title:NX_CHAR
    data:NXdata
      data --> /NXentry/NXinstrument/NXdetector/data
      detector_number --> /NXentry/NXinstrument/NXdetector/detector_number
      time_of_flight --> /NXentry/NXinstrument/NXdetector/time_of_flight
    instrument: NXinstrument
      detector: NXdetector
        azimuthal angle:NX FLOAT[ndet]
        data:NX_INT[ndet,ntimechan]
```

```
detector_number:NX_INT[ndet]
    distance:NX_FLOAT[ndet]
    polar_angle:NX_FLOAT[ndet]
    time_of_flight:NX_FLOAT[ntimechan]
NXmonitor
  data:NX_INT[ntimechan]
  distance: NX_FLOAT
  integral_counts:NX_INT
 mode:NX_CHAR
 preset:NX_FLOAT
 time_of_flight:NX_FLOAT[ntimechan]
NXsample
 name:NX_CHAR
 nature:NX_CHAR
user:NXuser
 name:NX_CHAR
```

Comprehensive Structure of NXtofraw

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXtofsingle

category: applications

NXDL source: NXtofsingle

(http://svn.nexusformat.org/definitions/trunk/applications/NXtofsingle.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXtofsingle.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument

(page 68), NXmonitor (page 72), NXsample (page 79), NXuser (page 86)

symbol list: none

documentation: This is a application definition for raw data from a generic TOF instrument

Basic Structure of NXtofsingle

```
NXtofsingle (application definition, version 1.0b)
  (overlays NXentry)
  entry:NXentry
   definition:NX_CHAR
   duration:NX_FLOAT
    pre_sample_flightpath:NX_FLOAT
```

```
start_time:NX_DATE_TIME
title:NX_CHAR
data:NXdata
  data --> /NXentry/NXinstrument/NXdetector/data
  detector_number --> /NXentry/NXinstrument/NXdetector/detector_number
  time_of_flight --> /NXentry/NXinstrument/NXdetector/time_of_flight
NXinstrument
  detector: NXdetector
    azimuthal_angle:NX_FLOAT[ndet]
    data:NX_INT[xsize, ysize, ntimechan]
    distance: NX FLOAT[1]
    polar angle:NX FLOAT[ndet]
    time_of_flight:NX_FLOAT[ntimechan]
NXmonitor
  data:NX_INT[ntimechan]
  distance: NX_FLOAT
 mode: NX CHAR
 preset:NX FLOAT
  time_of_flight:NX_FLOAT[ntimechan]
NXsample
  name:NX_CHAR
  nature: NX_CHAR
user:NXuser
  name:NX_CHAR
```

Comprehensive Structure of NXtofsingle

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXtomo

category: applications

NXDL source: NXtomo

(http://svn.nexusformat.org/definitions/trunk/applications/NXtomo.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXtomo.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument

(page 68), NXmonitor (page 72), NXsample (page 79), NXsource (page 82)

symbol list: none

documentation: This is the application definition for x-ray or neutron tomography raw data. In tomography first some dark field images are measured, some bright field images and, of course the sample. In order to properly sort the order of the images taken, a sequence number is stored with each image.

Basic Structure of NXtomo

```
NXtomo (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX CHAR
    end_time:NX_DATE_TIME
    start_time:NX_DATE_TIME
    title:NX CHAR
    data:NXdata
      data --> /NXentry/NXinstrument/data:NXdetector/data
      rotation_angle --> /NXentry/NXsample/rotation_angle
    instrument: NXinstrument
      bright_field:NXdetector
        data:NX_INT[nBrightFrames, xsize, ysize]
        sequence_number:NX_CHAR
      dark_field:NXdetector
        data:NX_INT[nDarkFrames, xsize, ysize]
        sequence_number:NX_CHAR
      sample:NXdetector
        data:NX_INT[nSampleFrames,xsize,ysize]
        distance:NX_FLOAT
        sequence_number:NX_CHAR
        x_pixel_size:NX_FLOAT
        y_pixel_size:NX_FLOAT
      NXsource
        name:NX_CHAR
        probe:NX CHAR
        type:NX_CHAR
    control: NXmonitor
      integral:NX_FLOAT[nDarkFrames + nBrightFrames + nSampleFrame]
    sample: NXsample
      name:NX_CHAR
      rotation_angle:NX_FLOAT[nSampleFrames]
      x_translation:NX_FLOAT[nSampleFrames]
      y_translation:NX_FLOAT[nSampleFrames]
      z_translation:NX_FLOAT[nSampleFrames]
```

Comprehensive Structure of NXtomo

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXtomophase

category: applications

NXDL source: NXtomophase

(http://svn.nexusformat.org/definitions/trunk/applications/NXtomophase.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXtomophase.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument

(page 68), NXmonitor (page 72), NXsample (page 79), NXsource (page 82)

symbol list: none

documentation: This is the application definition for x-ray or neutron tomography raw data with phase contrast variation at each point. In tomography first some dark field images are measured, some bright field images and, of course the sample. In order to properly sort the order of the images taken, a sequence number is stored with each image.

Basic Structure of NXtomophase

```
NXtomophase (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX CHAR
    end time: NX DATE TIME
    start_time:NX_DATE_TIME
    title:NX_CHAR
    data:NXdata
      data --> /NXentry/NXinstrument/sample: NXdetector/data
      rotation_angle --> /NXentry/NXsample/rotation_angle
    instrument: NXinstrument
      bright_field:NXdetector
        data:NX_INT[nBrightFrames, xsize, ysize]
        sequence_number:NX_CHAR
      dark field: NXdetector
        data:NX_INT[nDarkFrames, xsize, ysize]
        sequence_number:NX_CHAR
      sample:NXdetector
        data:NX_INT[nSampleFrames, nPhase, xsize, ysize]
        distance: NX FLOAT
        sequence number: NX CHAR
        x_pixel_size:NX_FLOAT
        y_pixel_size:NX_FLOAT
      NXsource
        name:NX_CHAR
        probe: NX CHAR
        type:NX_CHAR
    control: NXmonitor
      integral:NX_FLOAT[nDarkFrames + nBrightFrames + nSampleFrame]
    sample: NXsample
      name: NX_CHAR
      rotation_angle:NX_FLOAT[nSampleFrames]
      x_translation:NX_FLOAT[nSampleFrames]
      y_translation:NX_FLOAT[nSampleFrames]
      z_translation:NX_FLOAT[nSampleFrames]
```

Comprehensive Structure of NXtomophase

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXtomoproc

category: applications

NXDL source: NXtomoproc

(http://svn.nexusformat.org/definitions/trunk/applications/NXtomoproc.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXtomoproc.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXentry (page 59), NXinstrument (page 68), NXparameters

(page 75), NXprocess (page 78), NXsample (page 79), NXsource (page 82)

symbol list: none

documentation: This is an application definition for the final result of a tomography experiment: a 3D

construction of some volume of physical properties.

Basic Structure of NXtomoproc

```
NXtomoproc (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX_CHAR
    title:NX_CHAR
    data:NXdata
      data:NX_INT[nx,nx,nz]
        @transform
        @offset
        @scaling
      x:NX_FLOAT[nx]
      y:NX_FLOAT[ny]
      z:NX FLOAT[nz]
    NXinstrument
      NXsource
        name:NX_CHAR
        probe: NX_CHAR
        type:NX_CHAR
    reconstruction: NXprocess
      date:NX_DATE_TIME
      program: NX_CHAR
      version:NX_CHAR
      parameters: NXparameters
```

```
raw_file:NX_CHAR
NXsample
name:NX_CHAR
```

Comprehensive Structure of NXtomoproc

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxas

category: applications **NXDL source:** NXxas

(http://svn.nexusformat.org/definitions/trunk/applications/NXxas.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXxas.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument (page 68), NXmonitor (page 72), NXmonochromator (page 73), NXsample (page 79), NXsource (page 82)

symbol list: none

documentation: This is an application definition for raw data from an X-ray absorption spectroscopy experiment. This is essentially a scan on energy versus incoming/ absorbed beam

Basic Structure of NXxas

```
NXxas (application definition, version 1.0)
  (overlays NXentry)
  NXentry
    @entry
    definition:NX_CHAR
    start_time:NX_DATE_TIME
    title:NX_CHAR
    NXdata
     absorbed_beam --> /entry/instrument/absorbed_beam
     energy --> /entry/instrument/monochromator/energy
    NXinstrument
    incoming_beam:NXdetector
        data:NX_INT[np]
    absorbed_beam:NXdetector
        data:NX_INT[np]
    monochromator:NXmonochromator
```

```
energy:NX_CHAR
NXsource
name:NX_CHAR
probe:NX_CHAR
type:NX_CHAR
NXmonitor
data:NX_INT[np]
mode:NX_CHAR
preset:NX_FLOAT
NXsample
name:NX_CHAR
```

Comprehensive Structure of NXxas

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxasproc

category: applications

NXDL source: NXxasproc

(http://svn.nexusformat.org/definitions/trunk/applications/NXxasproc.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXxasproc.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXentry (page 59), NXparameters (page 75), NXprocess (page 78), NXsample (page 79)

symbol list: none

documentation: This is an application definition for processed data from XAS. This is energy versus I(i)/I(a)

Basic Structure of NXxasproc

```
NXxasproc (application definition, version 1.0)
(overlays NXentry)
NXentry
@entry
definition:NX_CHAR
title:NX_CHAR
NXdata
data:NX_FLOAT[np]
energy:NX_CHAR
XAS_data_reduction:NXprocess
```

```
date:NX_DATE_TIME
program:NX_CHAR
version:NX_CHAR
parameters:NXparameters
   raw_file:NX_CHAR
NXsample
name:NX_CHAR
```

Comprehensive Structure of NXxasproc

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxbase

category: applications

NXDL source: NXxbase

(http://svn.nexusformat.org/definitions/trunk/applications/NXxbase.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXxbase.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument (page 68), NXmonitor (page 72), NXmonochromator (page 73), NXsample (page 79), NXsource (page 82)

symbol list: none

documentation: This definition covers the common parts of all monochromatic single crystal raw data application definitions

Basic Structure of NXxbase

```
NXxbase (application definition, version 1.0b)
  (overlays NXentry)
  entry:NXentry
  definition:NX_CHAR
   start_time:NX_DATE_TIME
  title:NX_CHAR
  NXdata
    data --> /NXentry/NXinstrument/NXdetector/data
  instrument:NXinstrument
    detector:NXdetector
    data:NX_INT[np,number of x pixels,number of y pixels]
     @signal
```

```
distance:NX FLOAT
    frame_start_number:NX_INT
   x_pixel_size:NX_FLOAT
   y_pixel_size:NX_FLOAT
 monochromator: NXmonochromator
   wavelength: NX FLOAT
 source: NXsource
   name:NX_CHAR
   probe: NX_CHAR
   type:NX_CHAR
control: NXmonitor
 integral:NX FLOAT
 mode:NX_CHAR
 preset:NX_FLOAT
sample: NXsample
 distance: NX_FLOAT
 name:NX CHAR
 orientation_matrix:NX_FLOAT[3,3]
 temperature:NX_FLOAT[NP]
 unit_cell:NX_FLOAT[6]
 x_translation:NX_FLOAT
 y_translation:NX_FLOAT
```

Comprehensive Structure of NXxbase

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxeuler

category: applications

NXDL source: NXxeuler

(http://svn.nexusformat.org/definitions/trunk/applications/NXxeuler.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXxeuler.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXxbase* (page 115)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument

(page 68), NXsample (page 79)

symbol list: none

documentation: This is the application definition for raw data from a four circle diffractometer with an eulerian cradle. It extends NXxbase, so the full definition is the content of NXxbase plus the data defined here. All four angles are logged in order to support arbitray scans in reciprocal space.

Basic Structure of NXxeuler

```
NXxeuler (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX CHAR
    name:NXdata
     chi --> /NXentry/NXsample/chi
     phi --> /NXentry/NXsample/phi
     polar_angle --> /NXentry/NXinstrument/NXdetector/polar_angle
     rotation_angle --> /NXentry/NXsample/rotation_angle
    instrument:NXinstrument
      detector: NXdetector
        polar_angle:NX_FLOAT[np]
    sample: NXsample
      chi:NX_FLOAT[np]
     phi:NX_FLOAT[np]
      rotation_angle:NX_FLOAT[np]
```

Comprehensive Structure of NXxeuler

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxkappa

category: applications

NXDL source: NXxkappa

(http://svn.nexusformat.org/definitions/trunk/applications/NXxkappa.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXxkappa.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXxbase* (page 115)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument

(page 68), NXsample (page 79)

symbol list: none

documentation: This is the application definition for raw data from a kappa geometry (CAD4) single crystal diffractometer. It extends NXxbase, so the full definition is the content of NXxbase plus the data defined here.

Basic Structure of NXxkappa

```
NXxkappa (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX CHAR
    name:NXdata
     kappa --> /NXentry/NXsample/kappa
     phi --> /NXentry/NXsample/phi
      polar_angle --> /NXentry/NXinstrument/NXdetector/polar_angle
     rotation_angle --> /NXentry/NXsample/rotation_angle
    instrument:NXinstrument
      detector: NXdetector
        polar_angle:NX_FLOAT[np]
    sample: NXsample
      alpha:NX_FLOAT
      kappa:NX_FLOAT[np]
      phi:NX_FLOAT[np]
      rotation_angle:NX_FLOAT[np]
```

Comprehensive Structure of NXxkappa

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxIaue

category: applications

NXDL source: NXxlaue

(http://svn.nexusformat.org/definitions/trunk/applications/NXxlaue.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXxlaue.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXxrot (page 121)

other classes included: NXdata (page 54), NXentry (page 59), NXinstrument (page 68), NXsource

(page 82)

symbol list: none

documentation: This is the application definition for raw data from a single crystal laue camera. It extends

NXxrot.

Basic Structure of NXxlaue

```
NXxlaue (application definition, version 1.0b)
  (overlays NXentry)
  entry:NXentry
   definition:NX_CHAR
   instrument:NXinstrument
     source:NXsource
     distribution:NXdata
        data:NX_CHAR
        wavelength:NX_CHAR
```

Comprehensive Structure of NXxlaue

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxlaueplate

category: applications

NXDL source: NXxlaueplate

(http://svn.nexusformat.org/definitions/trunk/applications/NXxlaueplate.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXxlaueplate.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXxlaue (page 118)

other classes included: NXdetector (page 56), NXentry (page 59), NXinstrument (page 68)

symbol list: none

documentation: This is the application definition for raw data from a single crystal laue camera witha an image plate as a detector. It extends NXxlaue.

Basic Structure of NXxlaueplate

```
NXxlaueplate (application definition, version 1.0b)
(overlays NXentry)
entry:NXentry
definition:NX_CHAR
instrument:NXinstrument
detector:NXdetector
diameter:NX FLOAT
```

Comprehensive Structure of NXxlaueplate

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxnb

category: applications **NXDL source:** NXxnb

(http://svn.nexusformat.org/definitions/trunk/applications/NXxnb.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXxnb.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXxbase* (page 115)

other classes included: NXdata (page 54), NXdetector (page 56), NXentry (page 59), NXinstrument

(page 68), NXsample (page 79)

symbol list: none

documentation: This is the application definition for raw data from a single crystal diffractometer measuring in normal beam mode. It extends NXxbase, so the full definition is the content of NXxbase plus the data defined here. All angles are logged in order to support arbitray scans in reciprocal space.

Basic Structure of NXxnb

```
NXxnb (application definition, version 1.0b)
  (overlays NXentry)
  entry:NXentry
  definition:NX_CHAR
  name:NXdata
    polar_angle --> /NXentry/NXinstrument/NXdetector/polar_angle
    rotation_angle --> /NXentry/NXsample/rotation_angle
    tilt --> /NXentry/NXinstrument/NXdetector/tilt
  instrument:NXinstrument
    detector:NXdetector
        polar_angle:NX_FLOAT[np]
        tilt_angle:NX_FLOAT[np]
    sample:NXsample
    rotation_angle:NX_FLOAT[np]
```

Comprehensive Structure of NXxnb

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXxrot

category: applications **NXDL source:** NXxrot

(http://svn.nexusformat.org/definitions/trunk/applications/NXxrot.nxdl.xml)

version: 1.0b

SVN Id: \$Id: NXxrot.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXxbase* (page 115)

other classes included: NXattenuator (page 46), NXdata (page 54), NXdetector (page 56), NXentry

(page 59), NXinstrument (page 68), NXsample (page 79)

symbol list: none

documentation: This is the application definition for raw data from a rotation camera. It extends NXxbase,

so the full definition is the content of NXxbase plus the data defined here.

Basic Structure of NXxrot

```
NXxrot (application definition, version 1.0b)
  (overlays NXentry)
  entry: NXentry
    definition: NX CHAR
    name:NXdata
      rotation_angle --> /NXentry/NXsample/rotation_angle
    instrument: NXinstrument
      attenuator: NXattenuator
        attenuator_transmission:NX_FLOAT
      detector: NXdetector
        beam_center_x:NX_FLOAT
        beam_center_y:NX_FLOAT
        polar_angle:NX_FLOAT
    sample:NXsample
      rotation angle:NX FLOAT[np]
      rotation_angle_step:NX_FLOAT[np]
```

Comprehensive Structure of NXxrot

Name and Attributes	Type	Units	Description (and Occurrences)
class			

3.1.3 NeXus Contributed Definitions Classes

Contents:

NXbeamline

category: contributed_definitions

NXDL source: NXbeamline

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXbeamline.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXbeamline.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXaperture (page 45), NXbending_magnet (page 48), NXcollection (page 51), NX-electrostatic_kicker (page 122), NXmagnetic_kicker (page 123), NXquadrupole_magnet (page 124), NXseparator (page 125), NXsolenoid_magnet (page 133), NXspin_rotator (page 133)

symbol list: none

documentation: container for elements describing beamline.

Basic Structure of NXbeamline

NXbeamline (contributed definition, version 1.0)
(base class definition, NXentry or NXsubentry not found)
beamline:NX_CHAR
NXaperture
NXbending_magnet
diagnostics:NXcollection
NXelectrostatic_kicker
NXmagnetic_kicker
NXquadrupole_magnet
NXseparator
NXsolenoid_magnet
NXspin_rotator

Comprehensive Structure of NXbeamline

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXelectrostatic kicker

category: contributed_definitions

NXDL source: NXelectrostatic_kicker

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXelectrostatic_kicker.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXelectrostatic_kicker.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXlog (page 69)

symbol list: none

documentation: definition for a electrostatic kicker.

Basic Structure of NXelectrostatic_kicker

```
NXelectrostatic_kicker (contributed definition, version 1.0)
  (base class definition, NXentry or NXsubentry not found)
 beamline_distance:NX_FLOAT
  description: NX_CHAR
  set_current:NX_FLOAT
  set_voltage:NX_FLOAT
  timing:NX_FLOAT
    @description
  read_current:NXlog
   value:NX_CHAR
  read_voltage:NXlog
   value:NX CHAR
```

Comprehensive Structure of NXelectrostatic kicker

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXmagnetic kicker

category: contributed definitions

NXDL source: NXmagnetic_kicker

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXmagnetic_kicker.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXmagnetic_kicker.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXlog (page 69)

symbol list: none

documentation: definition for a magnetic kicker.

Basic Structure of NXmagnetic_kicker

```
NXmagnetic_kicker (contributed definition, version 1.0)
(base class definition, NXentry or NXsubentry not found)
beamline_distance:NX_FLOAT
description:NX_CHAR
set_current:NX_FLOAT
set_voltage:NX_FLOAT
timing:NX_FLOAT
@description
read_current:NXlog
value:NX_CHAR
read_voltage:NXlog
value:NX CHAR
```

Comprehensive Structure of NXmagnetic_kicker

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXquadrupole_magnet

category: contributed_definitions

NXDL source: NXquadrupole_magnet

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXquadrupole_magnet.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXquadrupole_magnet.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: NXlog (page 69)

symbol list: none

documentation: definition for a quadrupole magnet.

Basic Structure of NXquadrupole_magnet

```
NXquadrupole_magnet (contributed definition, version 1.0)
(base class definition, NXentry or NXsubentry not found)
beamline_distance:NX_FLOAT
description:NX_CHAR
set_current:NX_FLOAT
read_current:NXlog
value:NX_CHAR
read_voltage:NXlog
value:NX_CHAR
```

Comprehensive Structure of NXquadrupole_magnet

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsai_controller

category: contributed_definitionsNXDL source: NXsai_controller

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXsai_controller.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXsai_controller.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXtechnical_data (page 134)

symbol list: none

documentation: (definition implied by usage) Subclass of NXinstrument used by Soleil. This class appears in the example data files provided from Soleil. This class should be considered as a base class (and relocated there, once approved by the NIAC).

Basic Structure of NXsai controller

NXsai_controller (contributed definition, version 1.0)
(base class definition, NXentry or NXsubentry not found)
Frequency:NXtechnical_data
IntegrationTime:NXtechnical_data
TriggerNumber:NXtechnical_data

Comprehensive Structure of NXsai controller

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXseparator

category: contributed_definitions

NXDL source: NXseparator

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXseparator.nxdl.xml)

version: 1.0

NeXus: a common data format for neutron, x-ray, and muon science, Release 2011-10

SVN Id: \$Id: NXseparator.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXlog (page 69)

symbol list: none

documentation: definition for an electrostatic separator.

Basic Structure of NXseparator

```
NXseparator (contributed definition, version 1.0)
(base class definition, NXentry or NXsubentry not found)
beamline_distance:NX_FLOAT
description:NX_CHAR
set_Bfield_current:NX_FLOAT
set_Efield_voltage:NX_FLOAT
read_Bfield_current:NXlog
value:NX_CHAR
read_Bfield_voltage:NXlog
value:NX_CHAR
read_Efield_current:NXlog
value:NX_CHAR
read_Efield_voltage:NXlog
value:NX_CHAR
read_Efield_voltage:NXlog
value:NX_CHAR
```

Comprehensive Structure of NXseparator

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsnsevent

category: contributed_definitions

NXDL source: NXsnsevent

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXsnsevent.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXsnsevent.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: NXaperture (page 45), NXattenuator (page 46), NXcollection (page 51), NXcrystal (page 52), NXdata (page 54), NXdetector (page 56), NXdisk_chopper (page 58), NXentry (page 59), NXevent_data (page 61), NXgeometry (page 65), NXinstrument (page 68), NXlog (page 69), NXmoderator (page 71), NXmonitor (page 72), NXnote (page 73), NXorientation (page 75), NXpolarizer

```
(page 76), NXpositioner (page 77), NXsample (page 79), NXshape (page 82), NXsource (page 82), NXtranslation (page 85), NXuser (page 86)
```

symbol list: none

documentation: This is a definition for event data from Spallation Neutron Source (SNS) at ORNL.

Basic Structure of NXsnsevent

```
NXsnsevent (contributed definition, version 1.0)
  (overlays NXentry)
  NXentry
    collection_identifier:NX_CHAR
    collection_title:NX_CHAR
    definition: NX_CHAR
    duration: NX FLOAT
    end_time:NX_DATE_TIME
    entry_identifier:NX_CHAR
    experiment_identifier:NX_CHAR
    notes:NX_CHAR
    proton_charge:NX_FLOAT
    raw_frames:NX_INT
    run_number:NX_CHAR
    start_time:NX_DATE_TIME
    title:NX_CHAR
    total_counts:NX_UINT
    total uncounted counts: NX UINT
    DASlogs: NXcollection
      NXloq
        average_value:NX_FLOAT
        average_value_error:NX_FLOAT
        description: NX_CHAR
        duration: NX FLOAT
        maximum_value:NX_FLOAT
        minimum_value:NX_FLOAT
        time:NX_FLOAT[nvalue]
        value:NX_FLOAT[nvalue]
      NXpositioner
        average_value:NX_FLOAT
        average_value_error:NX_FLOAT
        description: NX_CHAR
        duration: NX_FLOAT
        maximum value:NX FLOAT
        minimum_value:NX_FLOAT
        time: NX FLOAT [numvalue]
        value:NX_FLOAT[numvalue]
    NXdata
      data_x_y --> /NXentry/NXinstrument/NXdetector/data_x_y
      x_pixel_offset --> /NXentry/NXinstrument/NXdetector/x_pixel_offset
      y_pixel_offset --> /NXentry/NXinstrument/NXdetector/y_pixel_offset
    NXevent_data
      event_index --> /NXentry/NXinstrument/NXdetector/event_index
      event_pixel_id --> /NXentry/NXinstrument/NXdetector/event_pixel_id
```

```
event_time_of_flight --> /NXentry/NXinstrument/NXdetector/event_time_of_flight
 pulse_time --> /NXentry/NXinstrument/NXdetector/pulse_time
instrument: NXinstrument
  SNSdetector_calibration_id:NX_CHAR
 SNSgeometry_file_name:NX_CHAR
 SNStranslation service: NX CHAR
 beamline: NX_CHAR
 name:NX_CHAR
 NXaperture
   x_pixel_offset:NX_FLOAT
   origin: NXgeometry
      orientation: NX orientation
        value:NX FLOAT[6]
      shape: NXshape
        description: NX_CHAR
        shape:NX_CHAR
        size:NX FLOAT[3]
      translation: NXtranslation
        distance:NX_FLOAT[3]
 NXattenuator
   distance: NX_FLOAT
 NXcrystal
   type:NX_CHAR
   wavelength: NX_FLOAT
   origin: NXgeometry
      description: NX_CHAR
      orientation: NX orientation
        value:NX_FLOAT[6]
      shape: NXshape
        description: NX_CHAR
        shape:NX_CHAR
        size:NX FLOAT
      translation: NXtranslation
        distance: NX FLOAT[3]
 NXdetector
    azimuthal_angle:NX_FLOAT[numx,numy]
   data_x_y:NX_UINT[numx, numy]
    distance:NX_FLOAT[numx, numy]
    event_index:NX_UINT[numpulses]
    event_pixel_id:NX_UINT[numevents]
   event_time_of_flight:NX_FLOAT[numevents]
   pixel_id:NX_UINT[numx, numy]
   polar_angle:NX_FLOAT[numx,numy]
   pulse_time:NX_FLOAT[numpulses]
   total_counts:NX_UINT
   x_pixel_offset:NX_FLOAT[numx]
   y_pixel_offset:NX_FLOAT[numy]
   origin: NXgeometry
      orientation: NX orientation
        value:NX_FLOAT[6]
      shape: NXshape
        description: NX_CHAR
        shape:NX_CHAR
```

```
size:NX_FLOAT[3]
      translation: NXtranslation
        distance:NX_FLOAT[3]
  NXdisk_chopper
    distance: NX_FLOAT
 moderator: NXmoderator
    coupling_material:NX_CHAR
    distance:NX_FLOAT
    temperature: NX_FLOAT
    type:NX_CHAR
  NXpolarizer
  SNS: NXsource
    frequency: NX_FLOAT
    name:NX_CHAR
    probe:NX_CHAR
    type:NX_CHAR
NXmonitor
  data:NX_UINT[numtimechannels]
  distance: NX_FLOAT
  mode: NX_CHAR
  time_of_flight:NX_FLOAT[numtimechannels + 1]
SNSHistoTool:NXnote
  SNSbanking_file_name:NX_CHAR
  SNSmapping_file_name:NX_CHAR
  author: NX_CHAR
  command1:NX_CHAR
  date:NX_CHAR
  description: NX_CHAR
  version:NX CHAR
sample: NXsample
  changer_position:NX_CHAR
  holder:NX_CHAR
  identifier:NX_CHAR
  name:NX CHAR
  nature:NX_CHAR
  facility_user_id:NX_CHAR
  name:NX_CHAR
  role:NX_CHAR
```

Comprehensive Structure of NXsnsevent

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsnshisto

category: contributed_definitions

NXDL source: NXsnshisto

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXsnshisto.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXsnshisto.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXaperture (page 45), NXattenuator (page 46), NXcollection (page 51), NXcrystal (page 52), NXdata (page 54), NXdetector (page 56), NXdisk_chopper (page 58), NXentry (page 59), NXfermi_chopper (page 62), NXgeometry (page 65), NXinstrument (page 68), NXlog (page 69), NXmoderator (page 71), NXmonitor (page 72), NXnote (page 73), NXorientation (page 75), NXpolarizer (page 76), NXpositioner (page 77), NXsample (page 79), NXshape (page 82), NXsource (page 82), NXtranslation (page 85), NXuser (page 86)

symbol list: none

documentation: This is a definition for histogram data from Spallation Neutron Source (SNS) at ORNL.

Basic Structure of NXsnshisto

```
NXsnshisto (contributed definition, version 1.0)
  (overlays NXentry)
 NXentry
    collection_identifier:NX_CHAR
    collection_title:NX_CHAR
    definition: NX CHAR
    duration: NX_FLOAT
    end_time:NX_DATE TIME
    entry identifier: NX CHAR
    experiment_identifier:NX_CHAR
    notes:NX_CHAR
    proton_charge:NX_FLOAT
    raw frames:NX INT
    run number: NX CHAR
    start_time:NX_DATE_TIME
    title:NX_CHAR
    total_counts:NX_UINT
    total_uncounted_counts:NX_UINT
    DASlogs: NXcollection
      NXloa
        average_value:NX_FLOAT
        average_value_error:NX_FLOAT
        description: NX CHAR
        duration: NX_FLOAT
        maximum value:NX FLOAT
        minimum value: NX FLOAT
        time:NX FLOAT[nvalue]
        value:NX_FLOAT[nvalue]
      NXpositioner
        average value: NX FLOAT
        average_value_error:NX_FLOAT
        description: NX_CHAR
```

```
duration: NX FLOAT
    maximum_value:NX_FLOAT
    minimum_value:NX_FLOAT
    time:NX_FLOAT[numvalue]
    value:NX_FLOAT[numvalue]
NXdat.a
  data --> /NXentry/NXinstrument/NXdetector/data
  data_x_time_of_flight --> /NXentry/NXinstrument/NXdetector/data_x_time_of_flight
  data_x_y --> /NXentry/NXinstrument/NXdetector/data_x_y
  data_y_time_of_flight --> /NXentry/NXinstrument/NXdetector/data_y_time_of_flight
  pixel id --> /NXentry/NXinstrument/NXdetector/pixel id
  time of flight --> /NXentry/NXinstrument/NXdetector/time of flight
  total counts --> /NXentry/NXinstrument/NXdetector/total counts
  x_pixel_offset --> /NXentry/NXinstrument/NXdetector/x_pixel_offset
  y_pixel_offset --> /NXentry/NXinstrument/NXdetector/y_pixel_offset
instrument: NXinstrument
  SNSdetector calibration id:NX CHAR
  SNSgeometry_file_name:NX_CHAR
  SNStranslation_service:NX_CHAR
 beamline: NX_CHAR
  name:NX_CHAR
 NXaperture
    x_pixel_offset:NX_FLOAT
    origin: NXgeometry
      orientation: NX orientation
        value:NX_FLOAT[6]
      shape: NXshape
        description: NX CHAR
        shape:NX CHAR
        size:NX FLOAT[3]
      translation: NXtranslation
        distance: NX FLOAT[3]
 NXattenuator
    distance: NX FLOAT
 NXcrystal
    type:NX_CHAR
    wavelength: NX_FLOAT
    origin: NXgeometry
      description:NX_CHAR
      orientation: NX orientation
        value:NX_FLOAT[6]
      shape: NXshape
        description: NX_CHAR
        shape:NX CHAR
        size:NX_FLOAT
      translation: NXtranslation
        distance: NX FLOAT[3]
 NXdetector
    azimuthal_angle:NX_FLOAT[numx,numy]
    data:NX_UINT[numx, numy, numtof]
    data x time of flight: NX UINT[numx, numtof]
    data_x_y:NX_UINT[numx, numy]
    data_y_time_of_flight:NX_UINT[numy, numtof]
```

```
distance:NX FLOAT[numx, numy]
    pixel_id:NX_UINT[numx, numy]
    polar_angle:NX_FLOAT[numx, numy]
    time_of_flight:NX_FLOAT[numtof + 1]
    total_counts:NX_UINT
    x pixel offset:NX FLOAT[numx]
    y_pixel_offset:NX_FLOAT[numy]
    origin: NXgeometry
      orientation: NX orientation
        value:NX_FLOAT[6]
      shape: NXshape
        description: NX CHAR
        shape:NX_CHAR
        size:NX_FLOAT[3]
      translation: NXtranslation
        distance:NX_FLOAT[3]
  NXdisk chopper
    distance:NX_FLOAT
 NXfermi_chopper
    distance:NX_FLOAT
 moderator: NXmoderator
    coupling_material:NX_CHAR
    distance:NX_FLOAT
    temperature: NX_FLOAT
    type:NX_CHAR
 NXpolarizer
  SNS: NXsource
    frequency: NX FLOAT
    name:NX CHAR
    probe:NX_CHAR
    type:NX_CHAR
NXmonitor
  data:NX_UINT[numtimechannels]
  distance: NX FLOAT
 mode: NX_CHAR
  time_of_flight:NX_FLOAT[numtimechannels + 1]
SNSHistoTool:NXnote
  SNSbanking_file_name:NX_CHAR
  SNSmapping_file_name:NX_CHAR
  author: NX CHAR
  command1:NX_CHAR
  date:NX_CHAR
  description: NX_CHAR
  version:NX CHAR
sample: NXsample
  changer position:NX CHAR
  holder:NX CHAR
  identifier: NX CHAR
  name:NX CHAR
  nature:NX CHAR
NXuser
  facility_user_id:NX_CHAR
  name:NX_CHAR
```

role:NX CHAR

Comprehensive Structure of NXsnshisto

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXsolenoid_magnet

category: contributed_definitions

NXDL source: NXsolenoid_magnet

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXsolenoid_magnet.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXsolenoid_magnet.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: *NXobject* (page 74)

other classes included: NXlog (page 69)

symbol list: none

documentation: definition for a solenoid magnet.

Basic Structure of NXsolenoid magnet

```
NXsolenoid_magnet (contributed definition, version 1.0)
(base class definition, NXentry or NXsubentry not found)
beamline_distance:NX_FLOAT
description:NX_CHAR
set_current:NX_FLOAT
read_current:NXlog
value:NX_CHAR
read_voltage:NXlog
value:NX CHAR
```

Comprehensive Structure of NXsolenoid_magnet

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXspin_rotator

category: contributed_definitions

NXDL source: NXspin_rotator

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXspin_rotator.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXspin_rotator.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: NXlog (page 69)

symbol list: none

documentation: definition for a spin rotator.

Basic Structure of NXspin rotator

```
NXspin_rotator (contributed definition, version 1.0)
(base class definition, NXentry or NXsubentry not found)
beamline_distance:NX_FLOAT
description:NX_CHAR
set_Bfield_current:NX_FLOAT
set_Efield_voltage:NX_FLOAT
read_Bfield_current:NXlog
   value:NX_CHAR
read_Bfield_voltage:NXlog
   value:NX_CHAR
read_Efield_current:NXlog
   value:NX_CHAR
read_Efield_voltage:NXlog
   value:NX_CHAR
read_Efield_voltage:NXlog
   value:NX_CHAR
```

Comprehensive Structure of NXspin rotator

Name and Attributes	Type	Units	Description (and Occurrences)
class			

NXtechnical_data

category: contributed_definitionsNXDL source: NXtechnical_data

(http://svn.nexusformat.org/definitions/trunk/contributed_definitions/NXtechnical_data.nxdl.xml)

version: 1.0

SVN Id: \$Id: NXtechnical_data.rst 917 2011-10-16 21:04:30Z Pete Jemian \$

extends class: NXobject (page 74)

other classes included: none

symbol list: none

documentation: (definition implied by usage) Some measure of metadata not already considered by the other base classes. This class appears in the example data files provided from Soleil. This class should be considered as a base class (and relocated there, once approved by the NIAC). This class is used by Soleil as a child of (at least) these classes: NXsai_controller, NXdetector, NXsource

Basic Structure of NXtechnical_data

```
NXtechnical_data (contributed definition, version 1.0)
(base class definition, NXentry or NXsubentry not found)
data:NX_NUMBER
@units
@timestamp
@description
description:NX_CHAR
@description
```

Comprehensive Structure of NXtechnical_data

Name and Attributes	Type	Units	Description (and Occurrences)
class			



DOCUMENTATION AUTHORS

These people have made substantial contributions to the NeXus manual:

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- Tobias Richter, Diamond Light Source Ltd., <Tobias.Richter@diamond.ac.uk>
- genindex
- search



CHAPTER

FIVE

TODO ITEMS

- fix math source formatting between html and pdf * see examples at http://theoretical-physics.net/dev/src/math/integration.html
- tables, examples, and figures: treat them consistently with titles, captions, and cross-references
- stop the section numbering for very deep subsections (2.1.4.1.2.1.3.1.4.5.1.4.1... is just ridiculous)
- Should we produce two or more separate books?
- Convert NXDL doc strings into ReST
- note there is a figure number extension: https://bitbucket.org/arjones6/sphinx-numfig/wiki/Home



CHAPTER

SIX

NEXUS HOME PAGE

We've had a request for examples to improve the NeXus home page. Here are some examples that use sphinx in one way or another:

- http://doc.openerp.com/v6.0/
- https://docs.djangoproject.com/en/1.3/



Part II

Cheatsheet

This is a cheat sheet and will be removed later.

Section headings automatically get labels assigned. For example, see this: Demo list-table (page 151)

symbol	description
#	with overline, for parts
*	with overline, for chapters
=	for sections
-	for subsections
٨	for subsubsections
"	for paragraphs

NeXus: a common data format for neutron, x-ray, and muon science, Release 2011-10

TYPESETTING MATH AND EQUATIONS

Enjoy inline math such as: $E=mc^2$ using LaTeX markup. You will need the matplotlib package in your Python. There is also separate math.

TODO:

adjust conf.py?

Sphinx has some inconsistency with this expression:

Tip: Perhaps some modification of *conf.py* would help?

The Sphinx HTML renderer handles simple math this way but not all LaTeX markup. The HTML renderer needs two backslashes while the LaTeX renderer only needs one.

This was possible with this definition in *conf.py*:

```
extensions = ['sphinx.ext.pngmath', 'sphinx.ext.ifconfig']
extensions.append( 'matplotlib.sphinxext.mathmpl' )
```



CHAPTER EIGHT

OTHER LINKS

Here are some links to more help about reStructuredText formatting.

reST home page http://docutils.sourceforge.net/rst.html

Docutils http://docutils.sourceforge.net/

Very useful! http://docutils.sourceforge.net/docs/ref/rst/directives.html

Independent Overview http://www.siafoo.net/help/reST

Wikipedia http://en.wikipedia.org/wiki/ReStructuredText

reST Quick Reference http://docutils.sourceforge.net/docs/user/rst/quickref.html

Comparison: text v. reST v. DocBook http://www.ibm.com/developerworks/library/x-matters24/

Curious http://rst2a.com/

NeXus: a common data format for neutron, x-ray, and muon science	e, Relea	se 2011-	10
		0 0::	

CHAPTER NINE

DEMO LIST-TABLE

Does this work?

It was found on this page http://docutils.sourceforge.net/docs/ref/rst/directives.html

Table 9.1: Frozen Delights!

Treat	Quantity	Description
Albatross	2.99	On a stick!
Crunchy Frog	1.49	If we took the bones out, it wouldn't be crunchy, now would it?
Gannet Ripple	1.99	On a stick!

NeXus: a common data format for neutron, x-ray, and muon science, Rele	ase 2011-10

NUMBERED LISTS

What about automatically numbering a list?

- 1. How will the numbering look?
- 2. Will it look great?
- 3. Even more great? What about more than one line of text in the source code?
- 8. Made a jump in the numbering. But that started a new list and produced a compile error. What about more than one line of text in the source code? Cannot use multiple paragraphs in a list, it seems. Maybe there is a way.
- 9. And another ...
- 6. Perhaps we can switch to lettering? Only if we start a new list. But we needed a blank line at the switch.
- 7. Another lettered item.

NeXus: a common of	data format for	neutron, x-ray,	and muon scier	nce, Release 201	11-10

CHAPTER ELEVEN

ABOUT LINKING

What about a link to *Indirect Hyperlinks* (page 178) on another page?

The reSt documentation says that links can be written as:

```
'NeXus: User Manual'_
```

This works for sphinx, as long as the link target is in the same .rst document. **But**, when the link is in a different document, sphinx requires the citation to use:

```
:ref:'NeXus User Manual'
```

and the target must be a section with an explicit hyperlink definition, such as on the top page of these docs:

This is the correct link: NeXus: User Manual (page 9).



MISSING LINKS

These sections show up as missing links.

Can you find the history (page 157) link below? What about the history (page 157) link below? This works: history (not converted yet) (page 157) (or history (not converted yet) (page 157)).

12.1 history (not converted yet)

12.2 utilities (not converted yet)

12.3 nxdl_tutorial-creatingnxdlspec (not converted yet)

nxdata-structure (not converted yet)

12.4 NIAC description

12.5 example.data-linking (not converted yet)

12.5.1 Section to cross-reference

This is the text of the section.

It refers to the section itself, see *Section to cross-reference* (page 157). What about a section on another page, such as *Footnote References* (page 179)?



Part III reStructuredText Markup Specification

Author: David Goodger Contact: dgoodger@bigfoot.com Version: 0.2 Date: 2001-05-29

Help for reST authors

This document, while old, presents information useful to authors of reST documents, such as this manual.

This will be removed in the released version of the NeXus documentation.

reStructuredText is plain text that uses simple and intuitive constructs to indicate the structure of a document. These constructs are equally easy to read in raw and processed forms. This document is itself an example of reStructuredText (raw, if you are reading the text file, or processed, if you are reading an HTML document, for example). reStructuredText is a candidate markup syntax for the Python Docstring Processing System.

Simple, implicit markup is used to indicate special constructs, such as section headings, bullet lists, and emphasis. The markup used is as minimal and unobtrusive as possible. Less often-used constructs and extensions to the basic reStructuredText syntax may have more elaborate or explicit markup.

The first section gives a quick overview of the syntax of the reStructuredText markup by example. More details are given in the Syntax Details (page 165) section.

Literal blocks (page 171) are used for examples throughout this document.

NeXus: a common data format for ne	eutron, x-ray, and	muon science, I	Release 2011-10

QUICK SYNTAX OVERVIEW

A reStructuredText document is made up of body elements, and may be structured into sections. Section Structure (page 166) is indicated through title style (underlines & optional overlines). Sections contain body elements and/or subsections.

Here are examples of body elements:

• Paragraphs (page 167) (and inline markup (page 176)):

```
Paragraphs contain text and may contain inline markup: *emphasis*, **strong emphasis**, 'interpreted text', 'inline literals'', standalone hyperlinks (http://www.python.org), indirect hyperlinks (Python_), internal cross-references (example_), footnote references ([1] ).
```

Paragraphs are separated by blank lines and are flush left.

- Three types of lists:
 - 1. Bullet lists (page 167):

```
- This is a bullet list.
```

- Bullets can be '-', '*', or '+'.
- 2. Enumerated lists (page 168):
 - 1. This is an enumerated list.
 - 2. Enumerators may be arabic numbers, letters, or roman numerals.
- 3. Definition lists (page 169):

```
what
```

Definition lists associate a term with a definition.

how

The term is a one-line phrase, and the definition is one or more paragraphs or body elements, indented relative to the term.

• Literal blocks (page 171):

```
Literal blocks are indented, and indicated with a double-colon ('::')
 at the end of the preceeding paragraph::
    if literal_block:
        text = 'is left as-is'
        spaces_and_linebreaks = 'are preserved'
        markup_processing = None
• Block quotes (page 172):
 Block quotes consist of indented body elements:
    This theory, that is mine, is mine.
    Anne Elk (Miss)
• Tables (page 173):
 +----+
 | Header row, column 1 | Header 2 | Header 3 |
 | body row 1, column 1 | column 2 | column 3 |
 +----+
                      | Cells may span
 | body row 2
 +----+
• Comments (page 173):
 .. Comments begin with two dots and a space. Anything may follow,
   except for the syntax of directives, footnotes, and hyperlink
   targets, described below.
• Directives (page 174):
 .. graphic:: mylogo.png
• Footnotes (page 175):
 .. _[1] A footnote contains indented body elements.
   It is a form of hyperlink target.
• Hyperlink targets (page 175):
 .. _Python: http://www.python.org
 .. _example:
 The '_example' target above points to this paragraph.
```

FOURTEEN

SYNTAX DETAILS

Below is a diagram of the hierarchy of element types in reStructuredText. Elements may contain other elements below them. Element types in parentheses indicate recursive or one-to-many relationships: sections may contain (sub)sections, tables contain further body elements, etc.

For definitive element hierarchy details, see the "Generic Plaintext Document Interface DTD" XML document type definition, gpdi.dtd. Descriptions below list 'DTD elements' (XML 'generic identifiers') corresponding to syntax constructs.

14.1 Whitespace

Blank lines are used to separate paragraphs and other elements. Blank lines may be omitted when the markup makes element separation unambiguous.

Indentation is used to indicate, and is only significant in indicating:

- multiple body elements within a list item (including nested lists),
- the definition part of a definition list item,
- · block quotes, and

• the extent of literal blocks.

Although spaces are recommended for indentation, tabs may also be used. Tabs will be converted to spaces. Tab stops are at every 8th column.

14.2 Escaping Mechanism

The character set available in plain text documents, 7-bit ASCII, is limited. No matter what characters are used for markup, they will already have multiple meanings in written text. Therefore markup characters *will* sometimes appear in text **without being intended as markup**.

Any serious markup system requires an escaping mechanism to override the default meaning of the characters used for the markup. In reStructuredText we use the backslash, commonly used as an escaping character in other domains.

A backslash followed by any character escapes the character. The escaped character represents the character itself, and is prevented from playing a role in any markup interpretation. The backslash is removed from the output. A literal backslash is represented by two backslashes in a row.

There are two contexts in which backslashes have no special meaning: literal blocks and inline literals. In these contexts, a single backslash represents a literal backslash.

14.3 Section Structure

DTD elements: section, title.

Sections are identified through their titles, which are marked up with 'underlines' below the title text (and, in some cases, 'overlines' above the title). An underline/overline is a line of non-alphanumeric characters that begins in column 1 and extends at least as far as the right edge of the title text. When there an overline is used, the length and character used must match the underline. There may be any number of levels of section titles.

Rather than imposing a fixed number and order of section title styles, the order enforced will be the order as encountered. The first style encountered will be an outermost title (like HTML H1), the second style will be a subtitle, the third will be a subsubtitle, and so on.

Below are examples of section title styles:

===========
Section Title
=======================================
Section Title
Section Title
========
Section Title

When a title has both an underline and an overline, the title text may be inset, as in the first two examples above. This is merely aesthetic and not significant. Underline-only title text may not be inset.

A blank line after a title is optional. All text blocks up to the next title of the same or higher level are included in a section (or subsection, etc.).

All section title styles need not be used, nor must any specific section title style be used. However, a document must be consistent in its use of section titles: once a hierarchy of title styles is established, sections must use that hierarchy.

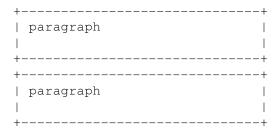
14.4 Body Elements

14.4.1 Paragraphs

DTD element: paragraph.

Paragraphs consist of blocks of left-aligned text with no markup indicating any other body element. Blank lines separate paragraphs from each other and from other body elements. Paragraphs may contain inline markup (page 176).

Syntax diagram:



14.4.2 Bullet Lists

DTD elements: bullet_list, list_item.

A text block which begins with a '-', '*', or '+', followed by whitespace, is a bullet list item (a.k.a. 'unordered' list item). For example:

- This is the first bullet list item. The blank line above the first list item is required; blank lines between list items (such as below this paragraph) are optional. Text blocks must be left-aligned, indented relative to the bullet.
- This is the first paragraph in the second item in the list.

This is the second paragraph in the second item in the list. The blank line above this paragraph is required. The left edge of this paragraph lines up with the paragraph above, both indented relative to the bullet.

- This is a sublist. The bullet lines up with the left edge of the text blocks above. A sublist is a new list so requires a blank line above and below.
- This is the third item of the main list.

This paragraph is not part of the list.

Here are examples of **incorrectly** formatted bullet lists:

- This first line is fine.

 A blank line is required between list items and paragraphs. (Warning)
- The following line appears to be a new sublist, but it is not:
 - This is a paragraph contination, not a sublist (no blank line).
 - Warnings may be issued by the implementation.

Syntax diagram:

14.4.3 Enumerated Lists

DTD elements: enumerated list, list item.

Enumerated lists (a.k.a. 'ordered' lists) are similar to bullet lists, but use enumerators instead of bullets. An enumerator consists of an enumeration sequence member and formatting, followed by whitespace. The following enumeration sequences are recognized:

- arabic numerals: 1, 2, 3, ... (no upper limit).
- uppercase alphabet characters: A, B, C, ..., Z.
- lower-case alphabet characters: a, b, c, ..., z.
- uppercase Roman numerals: I, II, III, IV, ... (no upper limit).

• lowercase Roman numerals: i, ii, iii, iv, ... (no upper limit).

The following formatting types are recognized:

- suffixed with a period: '1.', 'A.', 'a.', 'I.', 'i.'.
- surrounded by parentheses: '(1)', '(A)', '(a)', '(I)', '(i)'.
- suffixed with a right-parenthesis: '1)', 'A)', 'a)', 'I)', 'i)'.

For an enumerated list to be recognized, the following must hold true:

- 1. The list must consist of multiple adjacent list items (2 or more).
- 2. The enumerators must all have the same format and sequence type.
- 3. The enumerators must be in sequence (i.e., '1.', '3.' is not allowed).

It is recommended that the enumerator of the first list item be ordinal-1 ('1', 'A', 'a', 'I', or 'i'). Although other start-values will be recognized, they may not be supported by the output format.

Nested enumerated lists must be created with indentation. For example:

```
    Item 1.
    a) item 1a.
    b) Item 1b.
```

14.4.4 Definition Lists

DTD elements: definition list, definition list item, term, definition.

Each definition list item contains a term and a definition. A term is a simple one-line paragraph. A definition is a block indented relative to the term, and may contain multiple paragraphs and other body elements. Blank lines are required before the term and after the definition, but there may be no blank line between a term and a definition (this distinguishes definition lists from block quotes (page 172)).

```
term 1
Definition 1.

term 2
Definition 2, paragraph 1.
Definition 2, paragraph 2.

Syntax diagram:
```

```
+----+
| term |
+--+--+
| definition |
| (body elements)+ |
```

14.4.5 Field Lists

DTD elements: field_list, field, field_name, field_argument, field_body.

Field lists are mappings from field names to field bodies, modeled on RFC822 headers. A field name is made up of one or more letters, numbers, and punctuation, except colons (':') and whitespace. A single colon and whitespace follows the field name, and this is followed by the field body. The field body may contain multiple body elements.

Applications of reStructuredText may recognize field names and transform fields or field bodies in certain contexts. Field names are case-insensitive. Any untransformed fields remain in the field list as the document's first body element.

The syntax for field lists has not been finalized. Syntax alternatives:

1. Unadorned RFC822 everywhere:

```
Author: Me Version: 1
```

Advantages: clean, precedent. Disadvantage: ambiguous (these paragraphs are a prime example).

Conclusion: rejected.

2. Special case: use unadorned RFC822 for the very first or very last text block of a docstring:

```
Author: Me
Version: 1

The rest of the docstring...
```

Advantages: clean, precedent. Disadvantages: special case, flat (unnested) field lists only.

Conclusion: accepted, see below.

3. Use a directive:

```
.. fields::

Author: Me
Version: 1
```

Advantages: explicit and unambiguous. Disadvantage: cumbersome.

4. Use Javadoc-style:

```
@Author: Me
@Version: 1
@param a: integer
```

Advantages: unambiguous, precedent, flexible. Disadvantages: non-intuitive, ugly.

One special context is defined for field lists. A field list as the very first non-comment block, or the second non-comment block immediately after a title, is interpreted as document bibliographic data. No special syntax is required, just unadorned RFC822. The first block ends with a blank line, therefore field bodies

must be single paragraphs only and there may be no blank lines between fields. The following field names are recognized and transformed to the corresponding DTD elements listed, child elements of the 'document' element. No ordering is imposed on these fields:

• Title: title

· Subtitle: subtitle

Author/Authors: author

• Organization: organization

Contact: contactVersion: version

• Status: status

• Date: date

• Copyright: copyright

This field-name-to-element mapping can be extended, or replaced for other languages. See the implementation documentation for details.

14.4.6 Literal Blocks

DTD element: literal_block.

Two colons ('::') at the end of a paragraph signifies that all following **indented** text blocks comprise a literal block. No markup processing is done within a literal block. It is left as-is, and is typically rendered in a monospaced typeface:

```
This is a typical paragraph. A literal block follows::

for a in [5,4,3,2,1]: # this is program code, formatted as-is print a print "it's..."

# a literal block continues until the indentation ends

This text has returned to the indentation of the first paragraph, is outside of the literal block, and therefore treated as an ordinary paragraph.
```

When '::' is immediately preceded by whitespace, both colons will be removed from the output. When text immediately preceds the '::', *one* colon will be removed from the output, leaving only one (i.e., '::' will be replaced by ':'). When '::' is alone on a line, it will be completely removed from the output; no empty paragraph will remain.

In other words, these are all equivalent:

1. Minimized:

```
Paragraph::
Literal block
```

2. Partly expanded:

```
Paragraph: ::

Literal block

3. Fully expanded:

Paragraph:
::
```

Literal block

The minimum leading whitespace will be removed from each line of the literal block. Other than that, all whitespace (including line breaks) is preserved. Blank lines are required before and after a literal block, but these blank lines are not included as part of the literal block.

Syntax diagram:

14.4.7 Block Quotes

DTD element: block_quote.

A text block that is indented relative to the preceding text, without markup indicating it to be a literal block, is a block quote. All markup processing (for body elements and inline markup) continues within the block quote:

```
This is an ordinary paragraph, introducing a block quote:

"It is my business to know things. That is my trade."

--Sherlock Holmes
```

Blank lines are required before and after a block quote, but these blank lines are not included as part of the block quote.

Syntax diagram:

14.4.8 **Tables**

DTD elements: table, tgroup, colspec, thead, tbody, row, entry.

Tables are described with a visual outline made up of the characters '-', '=', 'l', and '+'. The hyphen ('-') is used for horizontal lines (row separators). The equals sign ('=') may be used to separate optional header rows from the table body. The vertical bar ('l') is used for vertical lines (column separators). The plus sign ('+') is used for intersections of horizontal and vertical lines.

Each cell contains zero or more body elements. Example:

As with other body elements, blank lines are required before and after tables. Tables' left edges should align with the left edge of preceding text blocks; otherwise, the table is considered to be part of a block quote.

14.4.9 Comment Blocks

A comment block is a text block:

- whose first line begins with '.. ' (the 'comment start'),
- whose second and subsequent lines are indented relative to the first, and
- which ends with an unindented line.

Comments are analogous to bullet lists, with '..' as the bullet. Blank lines are required between comment blocks and other elements, but are optional between comment blocks where unambiguous.

The comment block syntax is used for comments, directives, footnotes, and hyperlink targets.

Comments

DTD element: comment.

Arbitrary text may follow the comment start and will be processed as a comment element, possibly being removed from the processed output. The only restriction on comments is that they not use the same syntax as directives, footnotes, or hyperlink targets.

Syntax diagram:

Directives

DTD element: directive.

Directives are indicated by a comment start followed by a single word (the directive type, regular expression '[a-zA-Z][a-zA-Z0-9_-]*'), two colons, and whitespace. Two colons are used for these reasons:

• To avoid clashes with common comment text like:

```
.. Danger: modify at your own risk!
```

• If an implementation of reStructuredText does not recognize a directive (i.e., the directive-handler is not installed), the entire directive block (including the directive itself) will be treated as a literal block, and a warning generated. Thus '::' is a natural choice.

Directive names are case-insensitive. Actions taken in response to directives and the interpretation of data in the directive block or subsequent text block(s) are directive-dependent.

No directives have been defined by the core reStructuredText specification. The following are only examples of *possible uses* of directives.

Directives can be used as an extension mechanism for reStructuredText. For example, here's how a graphic could be placed:

```
.. graphic:: mylogo.png
```

A figure (a graphic with a caption) could be placed like this:

```
.. figure:: larch.png
The larch.
```

Directives can also be used as pragmas, to modify the behavior of the parser, such as to experiment with alternate syntax.

Syntax diagram:

Hyperlink Targets

DTD element: target.

Hyperlink targets consist of a comment start ('... '), an underscore, the hyperlink name (no trailing underscore), a colon, whitespace, and a link block. Hyperlink targets go together with indirect hyperlinks (page 178) and internal hyperlinks (page 179). Internal hyperlink targets have empty link blocks; they point to the next element. Indirect hyperlink targets have an absolute or relative URI in their link blocks.

If a hyperlink name contains colons, either:

• the phrase must be enclosed in backquotes:

```
.. _'FAQTS: Computers: Programming: Languages: Python':
http://python.faqts.com/
```

• or the colon(s) must be backslash-escaped in the link target:

```
.. _Chapter One\: 'Tadpole Days':
It's not easy being green...
```

Whitespace is normalized within hyperlink names, which are case-insensitive.

Syntax diagram:

Footnotes

DTD elements: footnote, label.

Footnotes are similar to hyperlink targets: a comment start, an underscore, open square bracket, footnote label, close square bracket, and whitespace. To differentiate footnotes from hyperlink targets:

- the square brackets are used,
- the footnote label may not contain whitespace,
- no colon appears after the close bracket.

Footnotes may occur anywhere in the document, not necessarily at the end. Where or how they appear in the processed output depends on the output formatter. Here is a footnote, referred to in Footnote References (page 179):

```
.. _[GVR2001] Python Documentation, van Rossum, Drake, et al., http://www.python.org/doc/
```

Syntax diagram:

14.5 Inline Markup

Inline markup is the markup of text within a text block. Inline markup cannot be nested.

There are six inline markup constructs. Four of the constructs (emphasis (page 176), strong emphasis (page 177), interpreted text (page 177), and inline literals (page 177)) use start-strings and end-strings to indicate the markup. The indirect hyperlinks (page 178) construct (shared by internal hyperlinks (page 179)) uses an end-string only. Standalone hyperlinks (page 178) are interpreted implicitly, and use no extra markup.

The inline markup start-string and end-string recognition rules are as follows:

- 1. Inline markup start-strings must be immediately preceded by whitespace and zero or more of single or double quotes, '(', '[', or '{'.
- 2. Inline markup start-strings must be immediately followed by non-whitespace.
- 3. Inline markup end-strings must be immediately preceded by non-whitespace.
- 4. Inline markup end-strings must be immediately followed by zero or more of single or double quotes, '.', ',', ':', ';', '!', '?', '-', ')', ']', or '}', followed by whitespace.
- 5. If an inline markup start-string is immediately preceded by a single or double quote, '(', '[', or '{', it must not be immediately followed by the corresponding single or double quote, ')', ']', or '}'.
- 6. An inline markup end-string must be separated by at least one character from the start-string.
- 7. Except for the end-string of inline literals (page 177), an unescaped backslash preceding a start-string or end-string will disable markup recognition. See escaping mechanism (page 166) above for details.

For example, none of the following are recognized as inline markup start-strings: '*', "*", "*", "(*)', '(*', '[*]', '{*}', '*', '', etc.

14.5.1 Emphasis

DTD element: emphasis.

Text enclosed by single asterisk characters (start-string = end-string = '*') is emphasized:

```
This is *emphasized text*.
```

Emphasized text is typically displayed in italics.

14.5.2 Strong Emphasis

DTD element: strong.

Text enclosed by double-asterisks (start-string = end-string = '**') is emphasized strongly:

```
This is **strong text**.
```

Strongly emphasized text is typically displayed in boldface.

14.5.3 Interpreted Text

DTD element: interpreted.

Text enclosed by single backquote characters (start-string = end-string = ") is interpreted:

```
This is 'interpreted text'.
```

The semantics of interpreted text are domain-dependent. It can be used as implicit or explicit descriptive markup (such as for program identifiers, as in the Python Extensions to reStructuredText), for cross-reference interpretation (such as index entries), or for other applications where context can be inferred. The role of the interpreted text may be inferred implicitly. The role of the interpreted text may also be indicated explicitly, either a prefix (role + colon + space) or a suffix (space + colon + role), depending on which reads better:

```
'role: interpreted text'
'interpreted text :role'
```

14.5.4 Inline Literals

DTD element: literal.

Text enclosed by double-backquotes (start-string = end-string = "") is treated as inline literals:

```
This text is an example of ''inline literals''.
```

Inline literals may contain any characters except two adjacent backquotes in an end-string context (according to the recognition rules above). No markup interpretation (including backslash-escape interpretation) is done within inline literals. Line breaks are *not* preserved; other whitespace is not guaranteed to be preserved.

Inline literals are useful for short code snippets. For example:

```
The regular expression ''[+-]?(\d+(\.\d*)?|\.\d+)'' matches non-exponential floating-point numbers.
```

14.5.5 Hyperlinks

Hyperlinks are indicated by a trailing underscore, '_', except for standalone hyperlinks (page 178) which are recognized independently.

Standalone Hyperlinks

DTD element: link.

An absolute URI (page 178) within a text block is treated as a general external hyperlink with the URI itself as the link's text (start-string = end-string = '', the empty string). For example:

```
See http://www.python.org for info.
```

would be marked up in HTML as:

```
See <A HREF="http://www.python.org">http://www.python.org</A> for info.
```

Uniform Resource Identifier: URIs are a general form of URLs (Uniform Resource Locators). For the syntax of URIs see RFC2396.

Indirect Hyperlinks

DTD element: link.

Indirect hyperlinks consist of two parts. In the text body, there is a source link, a name with a trailing underscore (start-string = ', end-string = ', end-s

```
See the Python_ home page for info.
```

Somewhere else in the document is a target link containing a URI (see Hyperlink Targets (page 175) for a full description):

```
.. _Python: http://www.python.org
```

After processing into HTML, this should be expressed as:

```
See the <A HREF="http://www.python.org">Python</A> home page for info.
```

See the Python home page for info.

Phrase-links (a hyperlink whose name is a phrase, two or more space-separated words) can be expressed by enclosing the phrase in backquotes and treating the backquoted text as a link name:

```
Want to learn about 'my favorite programming language'_?
.. _my favorite programming language: http://www.python.org
```

Want to learn about my favorite programming language?

Whitespace is normalized within hyperlink names, which are case-insensitive.

Internal Hyperlinks

DTD element: link.

Internal hyperlinks connect one point to another within a document. They are identical to indirect hyperlinks (start-string = '', end-string =

```
Clicking on this internal hyperlink will take us to the target_ below.
.. _target:
The hyperlink target above points to this paragraph.
```

Clicking on this internal hyperlink will take us to the target (page 179) below. The hyperlink target above points to this paragraph.

Footnote References

DTD element: footnote_reference.

Footnote references consist of a square-bracketed label (no whitespace), with a trailing underscore (start-string = '[', end-string = ']_'):

```
Please refer to the fine manual [GVR2001]_.
```

See Footnotes (page 175) for the footnote itself.

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