

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

Release 2011-08

http://nexusformat.org

# **CONTENTS**

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.

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# Part I

## **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.

NeXus: a common	data format for	neutron, x-ray	, and muon scie	ence, Release 2	2011-08

# 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"
                                           @long_name = "strip detector 1-D array"
6
                                           @signal = 1
                                  bins:[0, 1, 2, ... 1023]
8
                                           @long_name = "bin index numbers"
9
                 sample:NXsample
10
                         name = "zeolite"
11
12
                 data:NXdata
                         data --> /entry/instrument/detector/data
13
                         bins --> /entry/instrument/detector/bins
14
```

#### 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.)

#### 1.1 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.

This manual is also available in a PDF version.

## Part II

# **Contents**

### **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*.

#### 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* to help people understand what is in the data files.
- 2. A set of *data storage objects* (base classes and application definitions) to allow the development of more portable analysis software.
- 3. A set of *subroutines* (utilities) to make it easy to read and write NeXus data files.
- 4. *Scientific Community* to provide 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.

In addition, NeXus relies on a set of low-level file formats to actually store NeXus files on physical media. Each of these components are described in more detail in *Fileformat*.

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* (\*volume1/introduction:introduction-napi). (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 Design .

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*.

#### A Set of Design Principles

NeXus data files contain four types of entity: data groups, data fields, attributes, and links. See *Design-Groups* for more details.

- 1. **Data Groups** *Data groups* are like folders that can contain a number of fields and/or other groups.
- 2. **Data Fields** *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** Extra information required to describe a particular group or field, such as the data units, can be stored as a data attribute.
- 4. **Links** Links are used to reference the plottable data from NXdata when the data is provided in other groups such as NXmonitor or NXdetector.

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 represented as a tree structure.

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.

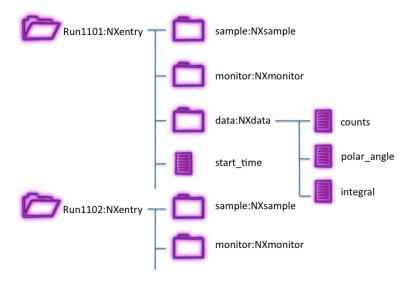


Figure 2.1: Example of a NeXus data file

#### **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 (*Design*).

**Note:** NXentry and NXdata are the only two classes **required** in a valid NeXus data file.

NXentry (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** (**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** 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** 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.

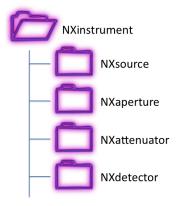


Figure 2.2: NXinstrument excerpt

#### 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.)

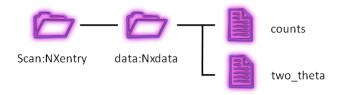


Figure 2.3: Simple Data File Example

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: introduction.rst 869 2011-08-17 23:19:06Z 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*).

#### 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**

**Note: TODO:** Show how these work together.

- NIAC
- NeXus Wiki
- •

#### 2.1.2 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. <sup>1</sup>

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. <sup>2</sup> 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 example of *fig.simple-example*, 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");
                    NXopengroup (fileID, "data", "NXdata");
10
                    /* somehow, we already have arrays tth and counts, each length n*/
11
                      NXmakedata (fileID, "two theta", NX FLOAT32, 1, &n);
12
                      NXopendata (fileID, "two_theta");
13
                            NXputdata (fileID, tth);
14
                            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
23
           return;
24
```

<sup>&</sup>lt;sup>1</sup> http://download.nexusformat.org

<sup>&</sup>lt;sup>2</sup> http://svn.nexusformat.org/code/trunk/doc/api/NeXusIntern.pdf

- [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* (\*volume1/introduction:ex-simple-write) above.

#### Reading a simple NeXus file

```
NXopen ('NXfile.nxs', NXACC_READ, &fileID);
1
      NXopengroup (fileID, "Scan", "NXentry");
2
            NXopengroup (fileID, "data", "NXdata");
3
              NXopendata (fileID, "two_theta");
4
                    NXgetinfo (fileID, &rank, dims, &datatype);
5
                    NXmalloc ((void **) &tth, rank, dims, datatype);
                    NXgetdata (fileID, tth);
7
              NXclosedata (fileID);
8
            NXclosegroup (fileID);
9
10
      NXclosegroup (fileID);
   NXclose (fileID);
11
```

#### 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* (\*volume1/introduction:introduction-napi)). 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* (\*volume1/introduction:exnxbrowse-lrmecs) 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
13
    NX Data : title[44] (NX_CHAR)
    NX Data : analysis[7] (NX_CHAR)
14
    NX Data : start_time[24] (NX_CHAR)
15
    NX Data : end_time[24] (NX_CHAR)
16
    NX Data : run number (NX INT32)
17
    NX Group : sample (NXsample)
18
    NX Group : LRMECS (NXinstrument)
19
    NX Group : monitor1 (NXmonitor)
20
    NX Group: monitor2 (NXmonitor)
21
    NX Group : data (NXdata)
22
  NX/Histogram1> read title
23
   title[44] (NX CHAR) = MqB2 PDOS 43.37q 8K 120meV E0@240Hz T0@120Hz
  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
```

- 42 NX/Histogram1> close
- 43 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 <sup>3</sup> provides an example of how to write a NeXus reader. The test programs included in the NeXus API (*NAPI: The NeXus Application Programming Interface* (\*volume1/introduction:introduction-napi)) may also be useful to study.

<sup>&</sup>lt;sup>3</sup> https://svn.nexusformat.org/code/trunk/applications/NXbrowse/NXbrowse.c



CHAPTER THREE

# NEXUS: REFERENCE DOCUMENTATION

Contents:



**CHAPTER** 

**FOUR** 

### **CHEATSHEET**

This is a cheat sheet and will be removed later.

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

#### 4.1 Symbols to mark Sections

#### **Sidebar Title**

#### **Optional Sidebar Subtitle**

This is a demo of a sidebar. Subsequent indented lines comprise the body of the sidebar, and are interpreted as body elements.

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.

$$\tilde{I}(Q) = \frac{2}{l_o} \int_0^\infty I(\sqrt{(q^2 + l^2)}) dl$$
 (4.1)

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

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

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# Part III Indices and tables

- genindex
- search

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