Sharing data between facilities: using the NeXus time-of-flight powder diffractometer file format - NOBUGS2002/036

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NeXus is an international standard data format intended to reduce the need for redundant software development efforts in the neutron and x-ray scattering communities. As the NeXus standard matures it is starting to be used at laboratories for storing raw data. The Manuel Lujan Jr. Neutron Scattering Center (MLNSC) at Los Alamos National Laboratory and the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory have been working with NeXus in an effort to share data and software. MLNSC is now writing files compliant with NeXus and the Integrated Spectral Analysis Workbench (ISAW) software from IPNS is being used with this data. Problems can arise if the standard is interpreted in different ways and information that belongs in the file is not accounted for in the standard. This paper will discuss an inter-laboratory collaboration in relation to a maturing data standard.

I. INTRODUCTION

Using an international standard file format for data storage is very appealing. Rather than having to write, or track down, a conversion utility one can directly use a variety of software packages. For scattering data the clear choice is to use NeXus. NeXus is a binary file format built on top of the Hierarchical Data Format (HDF) library. The binary format allows for more efficient data storage while the hierarchical nature of HDF allows for intelligent grouping of information to describe what is in the file.

The early development of NeXus concentrated on providing a powerful application program interface (API) implemented in C with wrappers for FORTRAN 77/90, IDL, and Java. The variety of supported languages simplifies the work for those who do want to read or write NeXus files directly. More recently the focus turned to standardizing the organization of the data and associated information. Originally, the NeXus standard provided a mechanism for storing information in the file, but did not spell out a detailed policy for using that mechanism. Instrument definitions were incomplete and did not provide enough information to generate truly portable data files. This was the main problem when the authors began to collaborate.

NeXus was starting to define what constituted a generic compliant file. Each file contains multiple NX-entries, and each NXentry is of the form seen in Fig. 1. The key to NeXus is that while very little information is required, if it is to be included in the file it has to be included in the manner specified by the standard.

The Integrated Spectral Analysis Workbench (ISAW) was designed to visualize and analyze data taken at time-of-flight neutron sources. In order to appeal to a broader community it looked to support the NeXus format. The data acquisition system (DAS) team at the Manuel Lujan Jr. Neutron Scattering Center (MLNSC) was working on an upgrade of their system which included moving to a more widely used file format to reduce some of the work involved in analyzing data. Immediately the two groups tried to share files and found that, while the data could be written by one system and loaded into the other, much information was lost due to organizational differences. To solve this problem the authors decided to specify what needed to be included in a time-of-flight neutron powder diffractometer (TOFNPD) file. While this is a conceptually simple instrument, information such as detector position is needed by many other instruments. This paper will discuss several of the decisions made during a meeting at Los Alamos National Laboratory concerning the description of detectors.

II. IDENTIFYING DETECTOR PIXELS

In NeXus, data is stored as a multidimensional rectangular array inside the NXdata object as seen in Fig. 1.
FIG. 2: Schematic of an simple tube detector (a), LPSD (b), and area detector (c) split into its component pixels.

III. DESCRIBING DETECTORS

Arguably the most important information, after the data, is a description of the detector configuration. The detector’s position is needed for corrections to wavelength (\(\lambda\)), d-spacing, and momentum transfer (\(Q\)) as well as data corrections such as inelastic scattering. The solid angle covered is needed to normalize the spectra for measurement area effects. Other information is useful for diagnostics such as physical size (length, width, and depth), orientation, electronics configuration, and type (such as 3He or scintillator). Some information about the detector is redundant as well. For example if the size and orientation is known then the solid angle covered is straightforward to calculate and does not need to be explicitly included. This section will discuss some of the properties of a detector.

A. Specifying Position

Due to the differences in preferred coordinate systems and the variety of naming conventions, specifying a detector position is more difficult than one would expect. While the choice of spherical coordinates is fairly straightforward, the decision of what to call the angles, and what to reference them from, was a long topic of discussion. With diffraction experiments the beam direction is always special since things such as the Bragg angle are with respect to it. Due to this symmetry the preferred coordinate system is spherical with the pole coinciding with the beam direction. This is shown in Fig. 3 with the azimuthal angle being zero at the horizontal plane of the instrument. The zero point for the azimuthal angle was chosen to be in the horizontal plane, to coincide with the location of detectors on many diffractometers and to be consistent with the traditional labeling of detector position. The angles labeled in the figure are some of the standard choices used with spherical coordinates. The one way that the group could speak and not have any inconsistencies was discussing the angle \(\alpha\) as the polar angle and \(\beta\) as the azimuthal angle. Other possibilities for \(\alpha\) were Bragg angle, \(2\theta\), \(\theta\), and \(\phi\). \(\beta\) was also possibly \(\theta\) or \(\phi\). All greek labels are used in most mathematics texts, (except \(2\theta\)) however, their interpretations vary greatly. For this reason we decided that the most precise way to refer to the angles were as polar_angle and azimuthal_angle.

B. Specifying Orientation and Size

Another important correction in data analysis is to normalize the detectors by the solid angle they cover. Therefore, the information needed is either the solid angle itself, or the physical size (length, width, and depth) and orientation of the detector so the solid angle can be calculated. In Fig. 4 a couple of the ways of determining...
FIG. 4: Schematic of specifying the orientation of a detector with various possible frames of reference. The labels \( d_0 \), \( d_1 \), and \( d_2 \) are described in the main text.

the detector orientation are shown. \( d_0 \) is the coordinates of the center of the instrument, shown for clarity. The second frame of reference, \( d_1 \), is parallel to \( d_0 \) but shifted to the position of the detector. \( d_2 \) is coincident with the major symmetry axes of the detector. Looking at this picture the simplest description of the orientation is the Euler angles to rotate \( d_1 \) to \( d_2 \).

IV. SUMMARY

This paper reviewed the results of discussions concerning storing data in a NeXus file. We described the format for the data itself as well as specifying the layout of the detectors that measured the data.

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\[ \text{Nexus homepage, http://www.neutron.anl.gov/nexus/}. \]
\[ \text{Hierarchical data format homepage, http://hdf.ncsa.uiuc.edu/}. \]
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