Developing a NeXus Instrument Definition for Muon Users

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Introduction

Despite having been originated by the Neutron and X-ray communities, the flexibility of the NeXus data format [1] makes it equally suitable for storing data collected during muon experiments. Importantly, it provides the community with an excellent basis for defining a common data exchange format, enabling analysis codes to be shared between the four worldwide muon facilities. Its use also opens up the possibility of sharing software beyond the muon community, immediately giving access to the many tools already in existence for manipulating NeXus and HDF based files.

A rudimentary NeXus Instrument Definition was defined by ISIS in 2001 [2], required by a move of the data acquisition software from VMS to Microsoft Windows and inspired by a conference discussion considering the need for a common muon data format [3]. The need to revise this definition has arisen for several reasons. Firstly, for a successful common data exchange format, there was a need to properly consider the requirements of the other muon sources and to be able to include metadata for the wide range of specialist muon experiments now run. Secondly, there was a need to incorporate new ideas and standards being set down by the NeXus International Advisory Committee (NIAC). Finally, there was a desire to bring the muon definition closer to those published on the NIAC website [4], making it easier to manipulate data files using standard tools designed for NeXus and HDF files.

Accordingly, a revised definition has been prepared. In particular, the new definition includes improved support for multi-period data (where the experiment state/stimulus is switched at regular intervals), provides support and guidance for including information relating to more complex experiments involving, for example, RF or laser stimuli and introducing a convenient method for organising the large number of sample environment log files that are generated during a typical experiment. The opportunity has been taken to ensure appropriate entries are defined to enable comprehensive metadata to be included to properly describe the experiment, spectrometer and beamline. The latter is becoming increasingly important to link with the instrument simulation codes that are now being used for experiment analysis [5]. Finally, the ability to store diagnostic logs to describe spectrometer performance during measurements is particularly useful, and the format for this data has now been formalised.

A Revised Instrument Definition for Muon data

A complete listing of the definition can be found in the report 'NeXus Instrument Definitions for muon data' [5]. Key features are as follows:

- **Improved support for multi-period data**

Experiments at pulsed muon sources, in particular, might involve the application of external stimuli such as laser light, radio frequency excitation or an electric field. Stimuli are typically switched after a defined number of accelerator pulses, and experiments typically cycle through all combinations of these stimuli generating a separate dataset for each combination (or acquisition period). Thus, an

experiment that uses a single stimulus will collect data in two interleaved acquisition periods, generating two datasets.

It is advantageous to keep each period datasets within a single data file, and therefore the array storing the raw counts has been generalised to a 3D array (histogram number, time and period number being the axes). Additional information about the periods is also stored. All entries are linked from NXdata to provide a complete account of the setup for experiment data acquisition from the single group (see Figure 1).

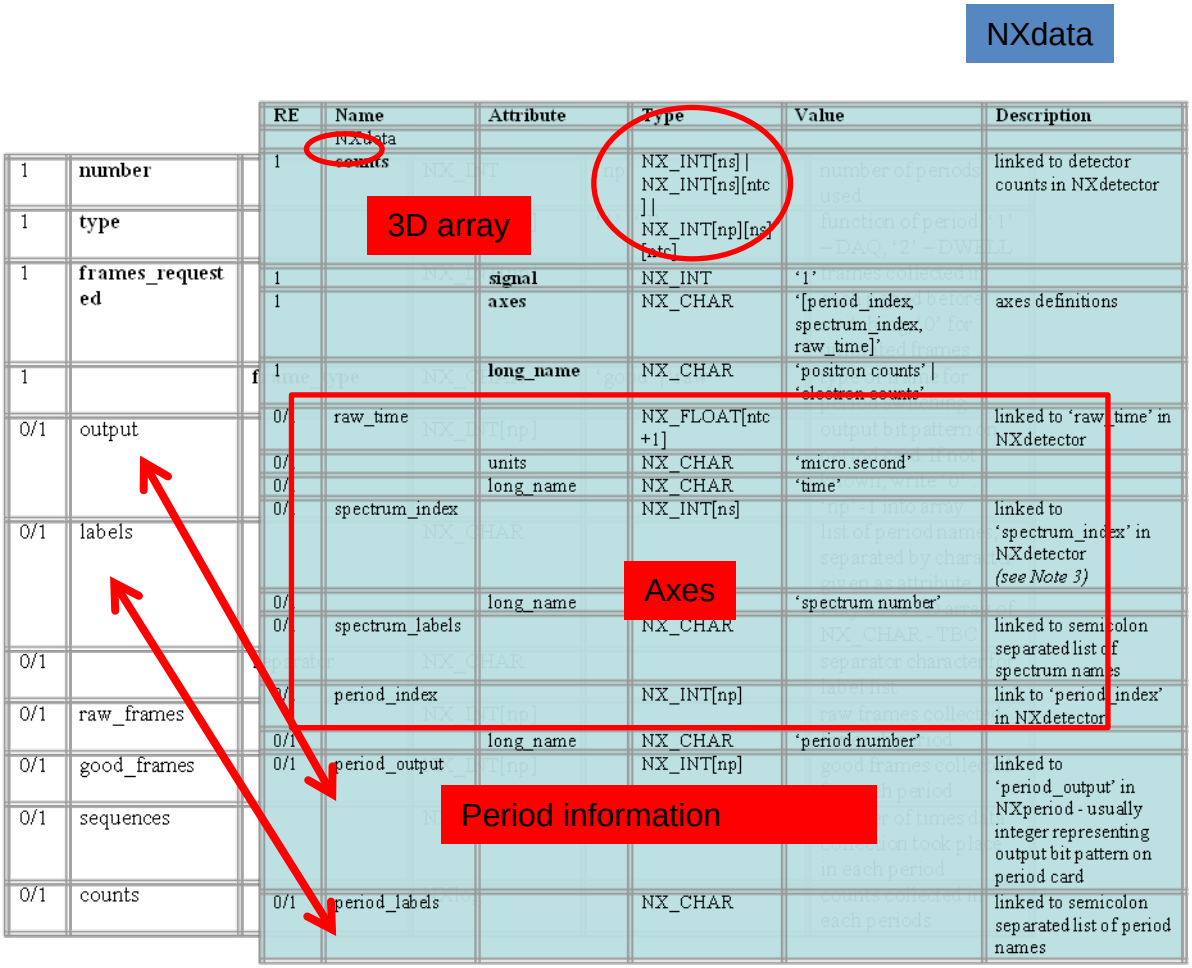

Figure 1: Histogram counts and period information linked from NXdata. A 3D array is used to enable multi-period data to be stored

- **Improved Metadata**

The opportunity has been taken to define a comprehensive dictionary of metadata, enabling facilities to use the definition to create an understandable description of muon experiments. With standardised metadata, it's easy for read routines to query a data file for specific experiment information, and those browsing the file can immediately understand the contents. Clearly, not all entries will be relevant to any particular experiment; however, the NeXus format is flexible in that only those appropriate need be included, with an error flagged by the API if a non-existent entry is accessed.

In particular, metadata has been defined to enable a complete description of the operating parameters of the muon beamline to be included within the data file (Figure 2). The metadata enables the beam setup to be confirmed and has been designed to link with standard beam simulation codes (such as TURTLE or TRANSPORT) to allow beam transport and the final beam spot to be modelled. This facility will become increasingly important as simulation codes such as 'musrSIM' [5] (based on GEANT) are exploited to model the experiment setup.

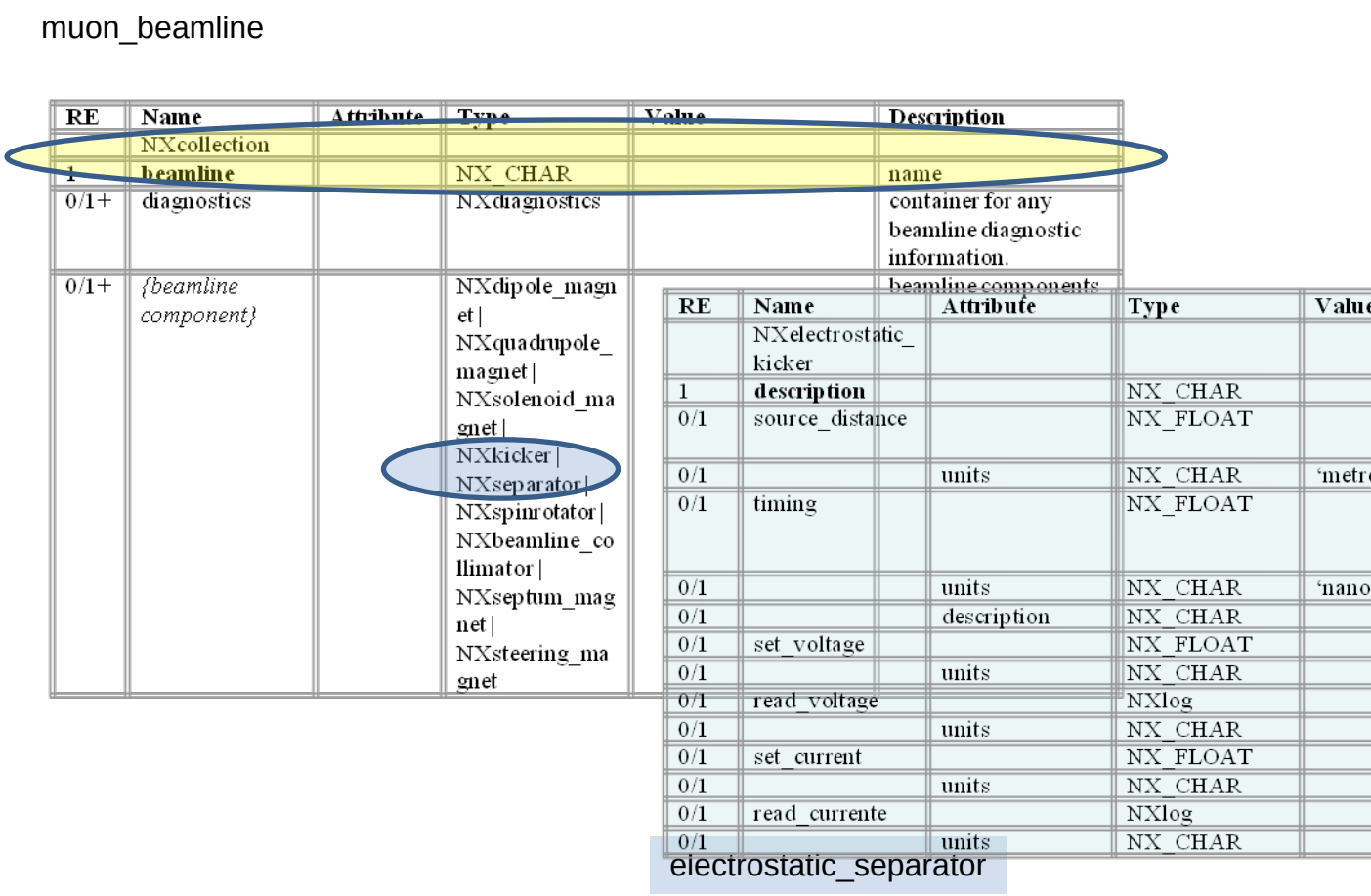

Figure 2: Beamline parameters can be stored to confirm setup and to use as input to beam transport simulations

- **Improved support for diagnostic information**

Facility experiments typically run unattended for long periods of time. While a modern equipment is very reliable, things do still go wrong. Container classes have therefore been defined to make it easy to log and store time stamped acquisition parameters, such as the activity of the acquisition electronics or sample environment kit, enabling a detailed reconstruction of the progress of the experiment to be made.

runlogs (NXcollection)

RE	Name	Attribute	Type	Value	Description
	NXcollection				
To contain action and acquisition logs arising from activities of the data acquisition electronics (DAE) during the run – entries will be facility specific.					

selogs (NXcollection)

RE	Name	Attribute	Type	Valu
	NXcollection			
To contain sample environment logs arising from activities of the experin facility specific.				

Figure 3: Container classes enable diagnostic information to be captured.

- **Guidance for extending the definition**

Muon experiments are becoming increasingly complex, with new methods (such as low energy μSR) or novel techniques (such as electric fields, humidity, laser light and radio frequency stimulation) frequently being applied. While a comprehensive dictionary of metadata is now available, it is clearly impossible to anticipate all future requirements. Therefore, the new definition comes with recommendations as to how to extend the metadata dictionary for new techniques in a consistent manner. New entries should be named using a unique prefix, with multiple instances of a device being numbered. Figure 4 shows part of a definition for an extension of the Instrument Definition for a radio frequency experiment.

RE	Name	Attribute	Type	Value	Description
	rf_frequency		NX_FLOAT32	rffrquency	
		units	NX_CHAR	'MHz'	
		hardware	NX_CHAR	'marconi'	
		display_name	NX_CHAR	name displayed on DAE software	at , typically SECI block name
		software	NX_CHAR	version of driver used to collect data	at , typically VIname and version
	rf_delay		NX_FLOAT32	rfdelay	relative to extract
		units	NX_CHAR	'us'	
		hardware	NX_CHAR	'stanford'	
		display_name	NX_CHAR	name displayed on DAE software	at , typically SECI block name
		software	NX_CHAR	version of driver used to collect data	at , typically VIname and version

Figure 4: Prefixed names are suggested when extending the Instrument Definition for new techniques. An example radio frequency definition is shown.

A Common Exchange Format for Muon data

In the revised definition only a minimal set of entries are marked as being 'essential' for a well formed muon data file. The entries have been chosen to provide the raw counts and minimal

metadata required to carry through a basic analysis of the dataset. The 'essential' entries have been chosen following detailed discussions between ISIS and PSI, and together they could form a definition of a Common Exchange Format for data files within the muon community. The required set of entries has deliberately been kept small to ensure meaningful information can be written for each entry regardless of the facility or muon technique being used.

As an example of the utility of this Common Exchange Format, Figure 5 shows ISIS data read and analysed in the PSI analysis program, 'musrfit' and, conversely, PSI data displayed in the Mantid analysis software developed at ISIS. If required, data files have been converted to the Common Exchange Format, with appropriate read routines being included in the software packages.

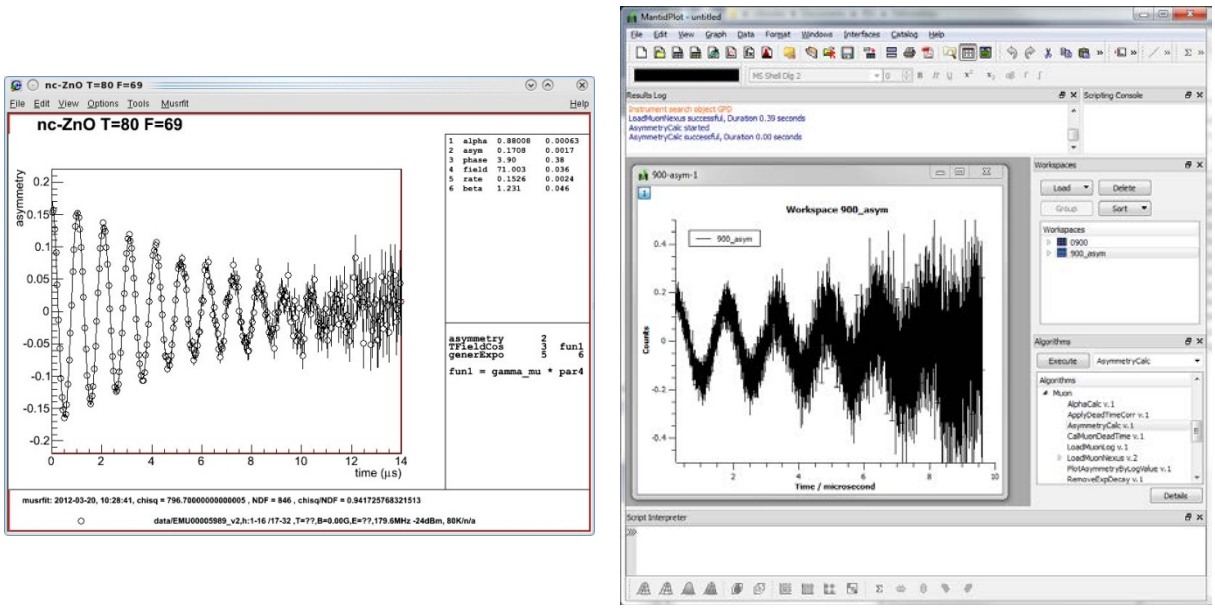

Figure 5: (left) ISIS data read and analysed in the PSI analysis program 'musrfit'and (right) PSI data displayed using the Mantid analysis software developed at ISIS.

Data File Validation

A particular advantage of the NeXus data format is the ability to validate data files against a standard formulated using the NeXus Definition Language (NXDL) to check conformance. A Java program ('NXvalidate') intended to simplify the progress of validation against an NXDL-based definition is currently being developed by the NeXus software development team, and an early version of the utility is distributed with the latest NeXus Distribution kit [1]. At present the validation tool requires a flat NXDL file (as opposed to presenting the NeXus groups as a tree), but with this restriction an effective validation of NeXus data files is now possible.

The ability to validate muon data files intending to conform to the Common Exchange Format is particularly useful, and a suitable NXDL definition (Appendix 1) has been developed and the validation tested. The process of using 'NXvalidate' to check conformance of a muon data file is shown in Figure 6.

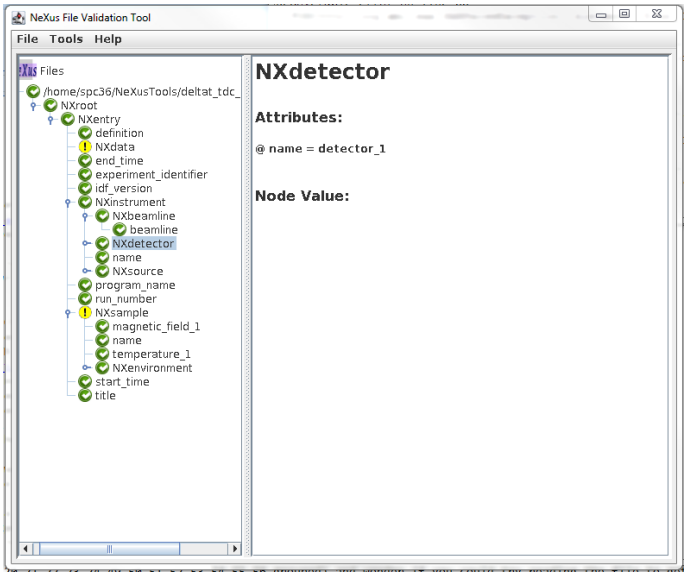

Figure 6: The Java tool 'NXvalidate' enables NeXus data files to be validated against a standard NXDL definition.

Summary

Significant progress has been made during the lifetime of the JRA in developing the NeXus data format for the muon community. Agreement between ISIS and PSI has been reached on a common Instrument Definition that contains a comprehensive dictionary of metadata for properly describing muon experiments. Within this definition, a subset of essential entries has been agreed that is suitable for use by the worldwide muon community as a Common Exchange Format. The utility of this exchange format has been demonstrated with PSI data being viewed with ISIS analysis codes and vice versa. The standard definition has been formulated as an NXDL file and the NeXus validation tool ('NXvalidate') used to demonstrate validation of muon NeXus data files, an effective way of ensuring they conform to and can be read as a Muon Common Exchange file.

References

[1] See http://www.nexusformat.org/
[2] D. Flannery, S.P. Cottrell, P.J.C King, Physica B 326 (2003) 238
[3] T.M. Riseman, Physica B 289-290 (2000) 722
[4] See http://trac.nexusformat.org/definitions/browser/trunk/applications?rev=574#
[5] See http://nmi3.eu/about-nmi3/joint-research-activities/muons/publications.html

Appendix 1: NXDL definition for the muon Common Exchange Format

```
<?xml version="1.0" encoding="UTF-8"?>
<definitions>

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# $Author: Pete Jemian $
# $Revision: 866 $
# $HeadURL: https://svn.nexusformat.org/definitions/trunk/base_classes/NXroot.nxdl.xml $
# $Id: NXroot.nxdl.xml 866 2011-07-19 12:46:16Z Pete Jemian $
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      xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
      xsi:schemaLocation="http://definition.nexusformat.org/nxdl/3.1 ../nxdl.xsd"
      name="NXroot"
      version="1.0"
      svnid="$Id: NXroot.nxdl.xml 866 2011-07-19 12:46:16Z Pete Jemian $"
      type="group" extends="NXobject">
    <doc>Definition of the root NeXus group.</doc>
    <attribute name="NX_class">
      <doc>
        The root of any NeXus data file is an NXroot class
        (no other choice is allowed for a valid NeXus data file).
        This attribute cements that definition.
      </doc>
      <enumeration>
        <item value="NXroot"></item>
      </enumeration>
    </attribute>
    <attribute name="file_time">
      <doc>Date and time file was originally created</doc>
    </attribute>
    <attribute name="file_name">
      <doc>File name of original NeXus file</doc>
    </attribute>
    <attribute name="file_update_time">
      <doc>Date and time of last file change at close</doc>
    </attribute>
    <attribute name="NeXus_version">
      <doc>Version of NeXus API used in writing the file</doc>
    </attribute>
    <attribute name="HDF_version">
      <doc>Version of NeXus API used in writing the file</doc>
    </attribute>
    <attribute name="HDF5_Version">
      <doc>
        Version of NeXus API used in writing the file.
        Note this attribute is spelled with uppercase "V",
        different than other version attributes.
      </doc>
    </attribute>
    <attribute name="XML_version">
      <doc>Version of NeXus API used in writing the file</doc>
    </attribute>
    <attribute name="creator">
      <doc>facility or program where file originated</doc>
    </attribute>
    <group type="NXentry" minOccurs="1" >
      <doc>entries</doc>
    </group>
```

```
  </definition>

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      name="NXentry"
      version="1.0"
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      type="group" extends="NXobject">
    <doc>Definition of the NXentry NeXus group.</doc>

    <field name="idf_version" type="NX_INT">
      <doc>ISIS Muon IDF_Version, '2'</doc>
    </field>

    <field name="run_number" type="NX_INT">
      <doc>Unique number of run</doc>
    </field>

    <field name="program_name" type="NX_CHAR">
      <doc>Name of program that generated the file></doc>
    </field>

    <field name="title">
      <doc>Extended title for entry</doc>
    </field>

    <field name="experiment_identifier">
      <doc>Unique identifier for the experiment, defined by the facility, possibly linked to the proposals</doc>
    </field>

    <field name="definition" type="NX_CHAR">
      <doc>
        muon definitions should use the prefix 'muon',
        ISIS uses muonTD (= muon time differential)
      </doc>
      <enumeration>
        <item value="muonTD"></item>
      </enumeration>
    </field>

    <field name="start_time" type="NX_DATE_TIME">
      <doc>Starting time of measurement</doc>
    </field>

    <field name="end_time" type="NX_DATE_TIME">
      <doc>Ending time of measurement</doc>
    </field>

    <group type="NXinstrument"/>
    <group type="NXdata"/>
</definition>

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      name="NXinstrument"
      version="1.0"
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      type="group" extends="NXobject">
    <doc>Definition of the NXinstrument NeXus group.</doc>

      <field name="name" type="NX_CHAR">
        <doc>instrument name</doc>
      </field>

      <group type="NXsource"/>
      <group type="NXbeamline"/>
      <group type="NXdetector" name="detector_1"/>
  </definition>

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      version="1.0"
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      type="group" extends="NXobject">

    <doc>Definition of the NXsource NeXus group.</doc>

    <field name="name" type="NX_CHAR">
      <doc>facility name</doc>
```

```
    </field>

    <field name="type" type="NX_CHAR">
      <doc>type of facility</doc>
      <enumeration>
        <item value="pulsed muon source"></item>
        <item value="continuous muon source"></item>
        <item value="continuous decay channel muon source"></item>
        <item value="low energy muon source"></item>
      </enumeration>
    </field>

    <field name="probe" type="NX_CHAR">
      <doc>type of probe</doc>
      <enumeration>
        <item value="positive muons"></item>
        <item value="negative muons"></item>
      </enumeration>
    </field>

    </definition>

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      name="NXbeamline"
      version="1.0"
      svnid="$Id: NXroot.nxdl.xml 866 2011-07-19 12:46:16Z Pete Jemian $"
      type="group" extends="NXobject">

    <field name="beamline" type="NX_CHAR">
      <doc>name of beamline</doc>
    </field>
  </definition>

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      name="NXdetector"
      version="1.0"
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      type="group" extends="NXobject">

    <symbols>
      <doc>These symbols will be used below to coordinate datasets with the same shape.</doc>
      <symbol name="np">
        <doc>number of periods used in data acquistion</doc>
      </symbol>
      <symbol name="ns">
        <doc>number of spectra</doc>
      </symbol>
      <symbol name="ntc">
        <doc>number of time channels</doc>
      </symbol>
    </symbols>

    <field name="description">
      <doc>name/manufacturer/model/etc. information</doc>
    </field>

    <field type="NX_INT" name="counts">

      <dimensions rank="3">
        <dim index="1" value="np" />
        <dim index="2" value="ns" />
        <dim index="3" value="ntc" />
      </dimensions>

      <attribute name="signal" type="NX_POSINT">
        <enumeration>
          <item value="1"/>
        </enumeration>
      </attribute>

      <attribute name="axes">
        <doc>[period_index,spectrum_index,raw_time]</doc>
      </attribute>

      <attribute name="long_name">
        <doc>Title of measurement</doc>
      </attribute>

      <field name="period_index" type="NX_INT">
        <doc>period number, axis description</doc>
        <dimensions rank="1">
          <dim index="1" value="np"></dim>
        </dimensions>
      </field>

      <field name="spectrum_index" type="NX_INT">
        <doc>spectrum index, axis description</doc>
        <dimensions rank="1">
          <dim index="1" value="ns"></dim>
        </dimensions>
      </field>

      <field name="raw_time" type="NX_FLOAT">
        <doc>raw_time, axis description</doc>
        <dimensions rank="1">
          <dim index="1" value="ntc"></dim>
        </dimensions>
      </field>

    </field>
  </definition>

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########### SVN repository information ####################
# $Date: 2011-07-19 13:46:16 +0100 (Tue, 19 Jul 2011) $
# $Author: Pete Jemian $
# $Revision: 866 $
# $HeadURL: https://svn.nexusformat.org/definitions/trunk/base_classes/NXroot.nxdl.xml $
# $Id: NXroot.nxdl.xml 866 2011-07-19 12:46:16Z Pete Jemian $
########### SVN repository information ####################
-->
  <definition xmlns="http://definition.nexusformat.org/nxdl/3.1" category="application"
      xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
      xsi:schemaLocation="http://definition.nexusformat.org/nxdl/3.1 ../nxdl.xsd"
      name="NXdata"
      version="1.0"
      svnid="$Id: NXroot.nxdl.xml 866 2011-07-19 12:46:16Z Pete Jemian $"
      type="group" extends="NXobject">

    <link name="counts" target="/NXentry/NXinstrument/NXdetector/counts"></link>
    <link name="raw_time" target="/NXentry/NXinstrument/NXdetector/raw_time"></link>
    <link name="spectrum_index" target="/NXentry/NXinstrument/NXdetector/spectrum_index"></link>
    <link name="period_index" target="/NXentry/NXinstrument/NXdetector/period_index"></link>

  </definition>
</definitions>
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