

NeXus Validation

Mark Könnecke Paul Scherrer Institute NFDI NeXus Workshop



- NeXus Application Definitions define standards
- How can I check if my file fulfills the requirements of an application definition?
- How can I check if additional fields match NeXus base class fields?
- —> cnxvalidate



What do you need?

- cnxvalidate from: <u>https://github.com/nexusformat/cnxvalidate</u>
 - Written in ANSII-C against the HDF5, XML2 libraries
 - Needs to be compiled
 - Comes with a test suite
- A copy of the NeXus application definitions from: <u>https://github.com/nexusformat/definitions</u>
 - Checking out the right version takes care of application definition versioning



- nxvalidate -l <appdefdir> <nexusfile>
 - Locates application definition in NXentry/ NXsubentries
 - Recursively compares the file with the application definition
 - Complains about conflicts



More Command Line Options

- -a <appdef>
- -p <path in NeXus file>
- -t, all output
- -d, trace what nxvalidate does
- -b, warn about additional base class fields found
- -u, warn about fields and groups NeXus does not know about
- -o, warn about optional fields missing
- -e, more whitespace in output
- -r, check file level attributes
- -x, validate depends_on chains



What does nxvalidate test?

- The file structure
- That all required groups and fields from the application definition are present
- That additional and optional fields conform to base classes
- That dimensions, number types and units match the application definition
- That attributes required by the application definition are present and well formed
- That attributes in general follow NeXus standards
- Verifies that depends_on fields are well formed
- That NeXus links point to valid data items
- A lot more, read the source code :-)



- As all software it has bugs..., report on github
- It does not check all group attribute data
- When using string arrays in the axes attribute, not checked
- Units attributes are checked against the application definitions but not against general validity.

Nxvalidate Example Run

NeXus

baer:20223344 konnecke\$ ~/src/cnxvalidate/build/nxvalidate -l ~/src/nexus_definitions hrpt2022n000040.hdf message="Missing required global HDF5_Version attribute" sev=error dataPath=/ dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Required group missing" nxdlPath=/NXentry/NXinstrument/NXdetector sev=error dataPath=/entry1/HRPT da taFile=hrpt2022n000040.hdf 2 errors and 26 warnings found when validating hrpt2022n000040.hdf baer:20223344 konnecke\$ baer:20223344 konnecke\$ baer:20223344 konnecke\$ ~/src/cnxvalidate/build/nxvalidate -l ~/src/nexus_definitions -buo hrpt2022n000040.hdf message="Missing required global HDF5_Version attribute" sev=error dataPath=/ dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Required group missing" nxdlPath=/NXentry/NXinstrument/NXdetector sev=error dataPath=/entry1/HRPT da taFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Unknown group HRPT-CERCA-Detector of class NXpsd found" nxdlPath=/NXentry/NXinstrument sev=warnundef dataPath=/entry1/HRPT/HRPT-CERCA-Detector dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Additional base class group Kollimator1 of type NXcollimator found" nxdlPath=/NXentry/NXinstrument s ev=warnbase dataPath=/entry1/HRPT/Kollimator1 dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Additional base class group Monochromator of type NXmonochromator found" nxdlPath=/NXentry/NXinstrum ent sev=warnbase dataPath=/entry1/HRPT/Monochromator dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Unknown group beam_reduction of class NXslit found" nxdlPath=/NXentry/NXinstrument sev=warnundef dat aPath=/entry1/HRPT/beam_reduction dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Unknown group exit_slit of class NXslit found" nxdlPath=/NXentry/NXinstrument sev=warnundef dataPath =/entry1/HRPT/exit_slit dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Unknown dataset sample_changer_position found" nxdlPath=/NXentry/NXsample sev=warnundef dataPath=/en try1/sample/sample_changer_position dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Unknown dataset sample_mur found" nxdlPath=/NXentry/NXsample sev=warnundef dataPath=/entry1/sample/s ample_mur dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Unknown dataset sample_name found" nxdlPath=/NXentry/NXsample sev=warnundef dataPath=/entry1/sample/ sample_name dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Unknown dataset sample_rotation_state found" nxdlPath=/NXentry/NXsample sev=warnundef dataPath=/entr y1/sample/sample_rotation_state dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Unknown dataset sample_table_rotation found" nxdlPath=/NXentry/NXsample sev=warnundef dataPath=/entr y1/sample/sample_table_rotation dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Additional base class dataset temperature found" nxdlPath=/NXentry/NXsample sev=warnbase dataPath=/e ntry1/sample/temperature dataFile=hrpt2022n000040.hdf definition=NXmonopd.nxdl.xml message="Additional base class group temperature_log of type NXlog found" nxdlPath=/NXentry/NXsample sev=warn base dataPath=/entry1/sample/temperature_log dataFile=hrpt2022n000040.hdf



- 1. Include <nxvalidate.h>
- 2. Create a reporting function
- 3. Create a validation context
- 4. Validate
- 5. Delete validation context
- See nxvmain.c as an example



- More fine grained then application definitions
- Use features field in NXentry, NXsubentry to enumerate features supported by the entry
- Write and register code to test for the feature
- See: <u>https://github.com/nexusformat/features</u>
- Not official yet but you may ask for it...



- NeXus has a powerful validation tool in the form of cnxvalidate.
- <u>https://github.com/nexusformat/cnxvalidate</u>
- Questions, comments, virtual rotten tomatoes....