h5cpp and pninexus libraries

DESY HDF5 meeting 2023

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Deutsches Elektronen-Synchrotron

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PETRA III Beamlines

Description

h5cpp: c++ library which wraps the hdf5 library

- uses c++ class objects to wrap pointers and hid's,

  we avoid `new`, `delete` and `close()`
- maps native c++ datatypes to hdf5 datatypes

  making use of c++ traits, `create()` and `get()` methods
- maps native std c++ containers to hdf5 dataspaces

  making use of c++ traits, `create()` and `get()` methods

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pninexus: c++ library which adds DESY/NeXus functionality 

- XML builder: `create_from_string(...)`, `create_from_file(...)`, ...
- NeXus specific: `create_file(...)`, `get_objects(...)`, ...
- maps non-std c++ dataspaces and datatypes to hdf5 dataspaces and datatypes with c++ traits

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pninexus: c++ library which adds DESY/NeXus functionality 

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- NeXus specific: `create_file(...)`, `get_objects(...)`, ...
- maps non-std c++ dataspaces and datatypes to hdf5 dataspaces and datatypes with c++ traits

python-pninexus: simple boost python bindings 

- maps numpy objects to hdf5 datatypes and dataspaces with c++ traits

NeXus format and HDF5

- NeXus is a set of rules how data must be organized

within a particular format in order to become a valid file.

NeXus International Advisory Committee at https://www.nexusformat.org

- Every NeXus file written by us is also a valid HDF5 file!

Hierarchical Data Format v5: file format that supports large, complex, heterogeneous data

NeXus

Layer 3: application definitions

Layer 2: base classes

Layer 1: nxgroup, nxfield, nxattribute, nxlink, types

- scalar and multidimensional data within a single file
- data within the file in a tree like manager
- additional attributes can be attached to objects in a file
  storing metadata which might be required for later analysis

Usage

Tango Servers:

Lambda, AGIPD, PCO,
FireBird, Varex,
Vimba, DALSA, Andor,
PiLC, Express3, ...

Yuelong, Yu, Teresa Nunez,
Johannes Blume, Jan Garrevoet, ...

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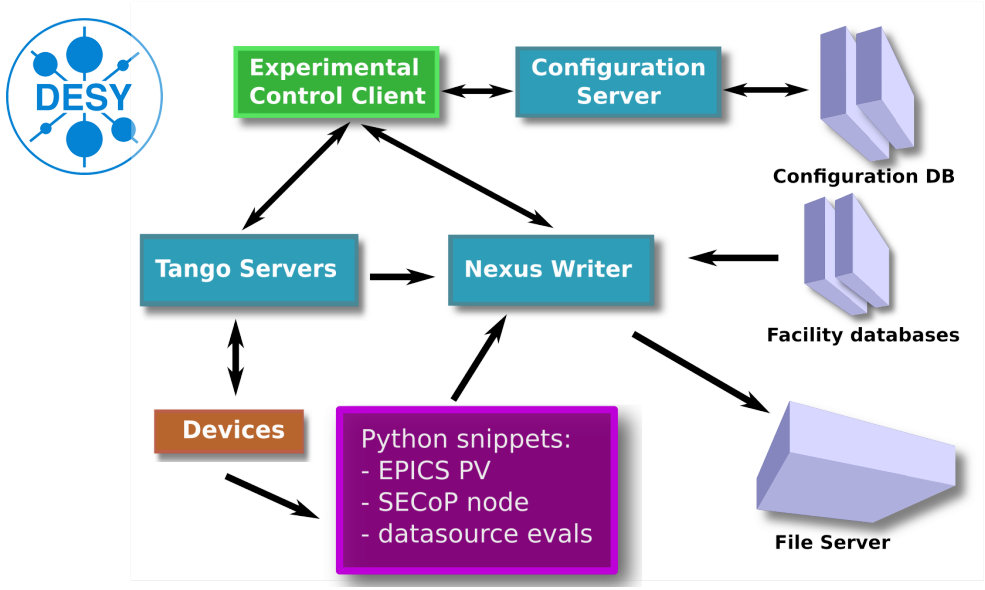
NeXus Metadata Framework:



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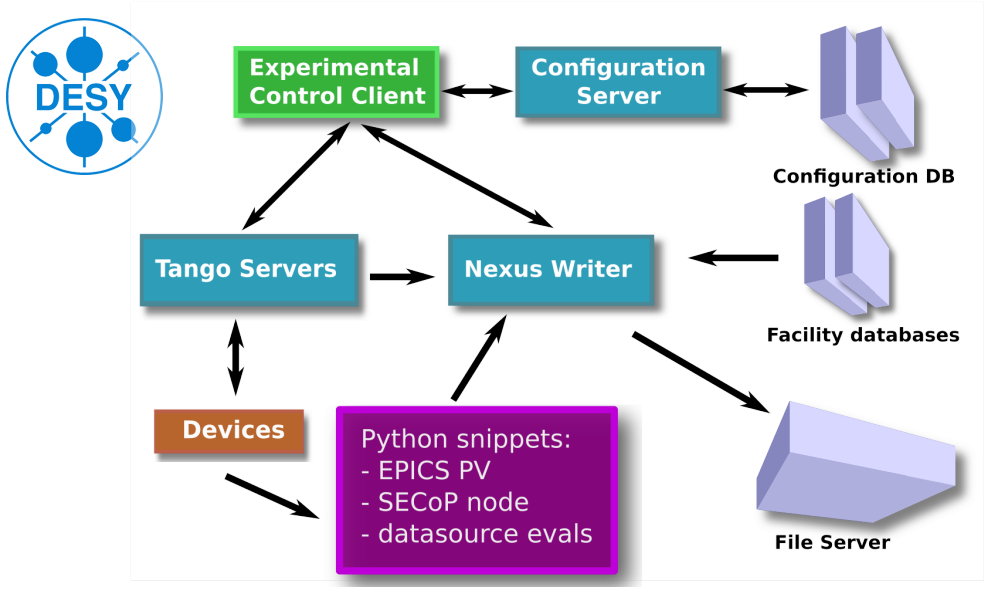
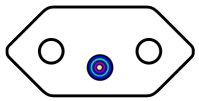


PLUG2: Online XPCS Analysis

Vijay Kartik



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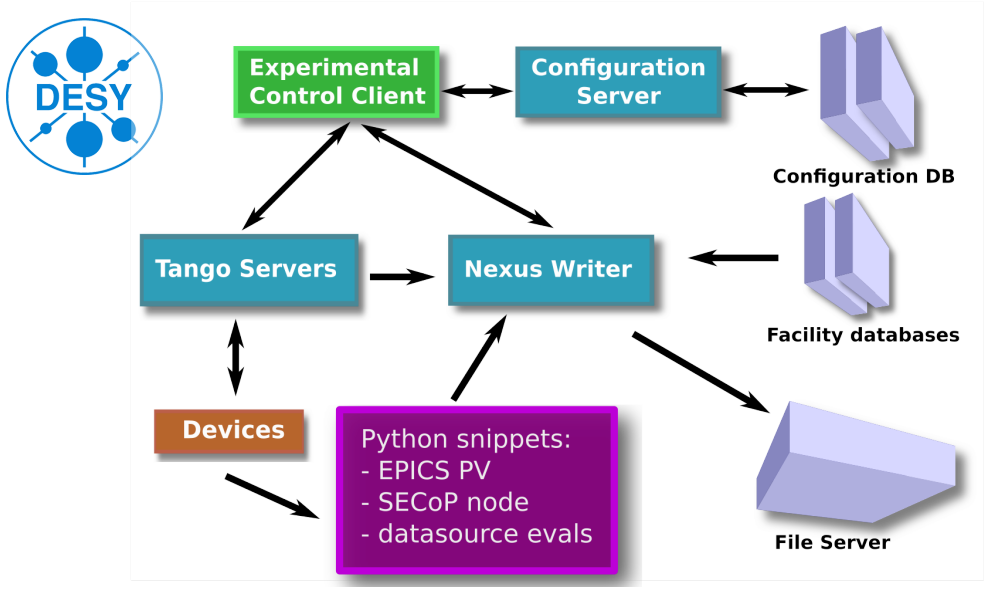

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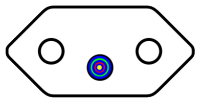

European Spallation Source:

Kafka-to-NeXus, ...

ess EUROPEAN SPALLATION SOURCE

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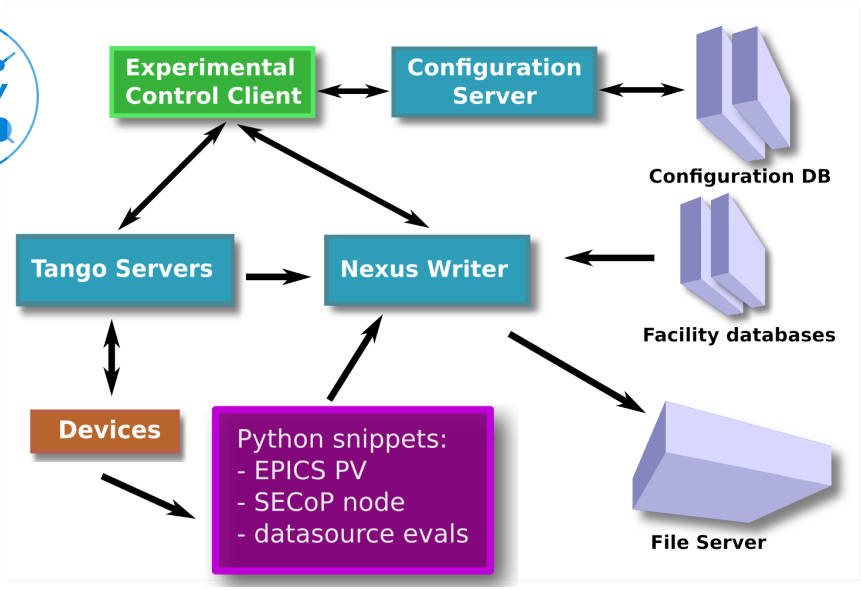

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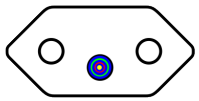

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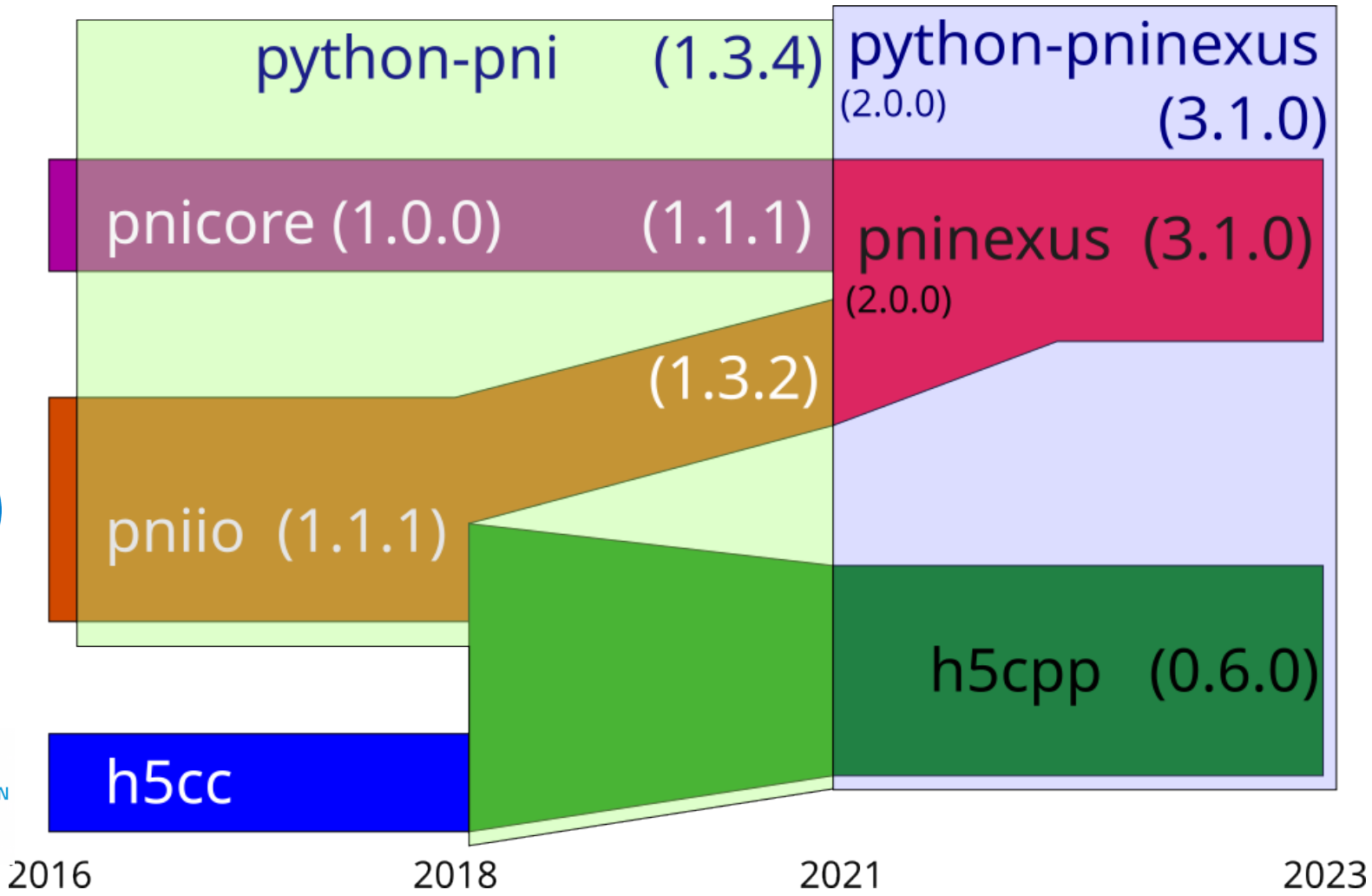
ESS EUROPEAN SPALLATION SOURCE

Other facilities and also outside science

h5cc, pniio + pnicore ⇒ h5cpp + pninexus

c++ wrapping libraries of hdf5 and their python bindings



Eugen Wintersberger (DESY), Martin Shetty (ESS), Jan Kotanski (DESY), Matthew D Jones (STFC/ESS), Alfonso Mukai (ESS), Jonas Nilsson (ESS), Sebastian Koenig (NC), Yuelong Yu (DESY), Andrew Marshall (UK), Shiv Upadhyay (WA), ...

Installation from sources

- libh5cpp from github

```
git clone https://github.com/ess-dmsc/h5cpp.git
cd h5cpp && mkdir build && cd build
cmake -DCMAKE_INSTALL_PREFIX=/opt/h5cpp -DCMAKE_BUILD_TYPE=Release
\
  -DH5CPP_CONAN=DISABLE -DH5CPP_DISABLE_TESTS=True \
  -DH5CPP_WITH_BOOST=False ../

make install -j4 && cd ../../
```

- libpninexus from github

```
git clone https://github.com/pni-libraries/libpninexus.git
cd libpninexus && mkdir build && cd build
cmake -DCMAKE_INSTALL_PREFIX=/opt/pninexus \
  -Dh5cpp_DIR=/opt/h5cpp/lib/cmake/h5cpp-0.6 \
  -DPNINEXUS_CONAN=DISABLE -DCMAKE_BUILD_TYPE=Release ../

make install -j4
```

- python-pninexus from github

```
git clone https://github.com/pni-libraries/python-pninexus.git
H5CPP_LOCAL_PATH=/opt/h5cpp PNINEXUS_LOCAL_PATH=/opt/pninexus \

  python3 setup.py install
```

details instructions on their github CI or documentation

Debian packages from our HDRI repository

- add the HDRI repository

```
curl -s http://repos.pni-hdri.de/debian_repo.pub.gpg | gpg \
  --import --no-default-keyring \
  --keyring gnupg-ring:/etc/apt/trusted.gpg.d/debian-hdri-repo.gpg
chmod 644 /etc/apt/trusted.gpg.d/debian-hdri-repo.gpg
cd /etc/apt/sources.list.d
wget http://repos.pni-hdri.de/bookworm-pni-hdri.list

apt-get update
```

- install h5cpp

```
apt-get install libh5cpp0.6.0 libh5cpp0.6.0-dev \
  libh5cpp0.6.0-doc libh5cpp0.6.0-dbg
```

- install pninexus

```
apt-get install libpninexus3.1.0 libpninexus3.1.0-dev \
  libpninexus3.1.0-doc libpninexus3.1.0-dbg
```

- install python-pninexus

```
apt-get install python3-pninexus
```

Also for buster, bullseye debian and focal, jammy, lunar ubuntu.

Using h5cpp with cmake

minimal CMakeLists.txt file

```
# project name
project(h5cpp_create_dataset)

# cmake required version
cmake_minimum_required(VERSION 3.13...3.20)
# we use c++17 standard
set(CMAKE_CXX_STANDARD 17)

# find h5cpp
find_package(H5CPP REQUIRED)

# define executable and its content
add_executable(h5cpp_create_dataset h5cpp_create_dataset.cpp)
# link h5cpp::h5cpp and std::filesystem
target_link_libraries(h5cpp_create_dataset PRIVATE h5cpp::h5cpp stdc++fs)
```

from https://gitlab.desy.de/h5cpp-pninexus-examples/h5cpp_create_dataset.git

Create a dataset with h5cpp: tree structure

```cpp
#include <h5cpp/hdf5.hpp>

int main()
{
  using namespace hdf5;

  // create a file
  file::File f = file::create("myscan_00123.nxs", file::AccessFlags::Truncate);

  // create an entry group
  node::Group root_group = f.root();

  // create a root group attribute
  root_group.attributes.create<std::string>("default").write("entry");

  // create an entry group
  node::Group entry_group = root_group.create_group("entry");

  entry_group.create_dataset("title",
                             datatype::get<std::string>(),
                             dataspace::Scalar()).write("My scan");

  // create entry group attributes
  entry_group.attributes.create<std::string>("NX_class").write("NXentry");
  entry_group.attributes.create<std::string>("default").write("data");

  // create an data group
  node::Group data_group = entry_group.create_group("data");

  // create a data group attributes
  data_group.attributes.create<std::string>("NX_class").write("NXdata");
  data_group.attributes.create<std::string>("signal").write("counter");
  data_group.attributes.create<std::string>("axes").write("x");
```

Create a dataset with h5cpp: write data

```
    // create a counter dataset
    using int_type = std::vector<int>;
    int_type counter_data {0, 1, 2, 4, 6, 5, 1, 0};
    node::Dataset cdataset = data_group.create_dataset("counter",
                                                       datatype::get<int_type>(),
                                                       dataspace::create(counter_data));
    // set units attribute
    cdataset.attributes.create<std::string>("units").write("counts");

    // write to counter dataset
    cdataset.write(counter_data);

    // create a motor dataset
    using float_type = std::vector<double>;
    float_type x_data {2.01, 2.98, 4.01, 4.99, 6.00, 7.1, 8.2, 9.1};
    node::Dataset xdataset = data_group.create_dataset("x",
                                                       datatype::get<float_type>(),
                                                       dataspace::create(x_data));
    // set units attribute
    xdataset.attributes.create<std::string>("units").write("mm");

    // write to x dataset
    xdataset.write(x_data);
}
```

Create a dataset with h5cpp: view in NeXpy

Compiling:

mkdir build
cd build
cmake ../
make

Executing:

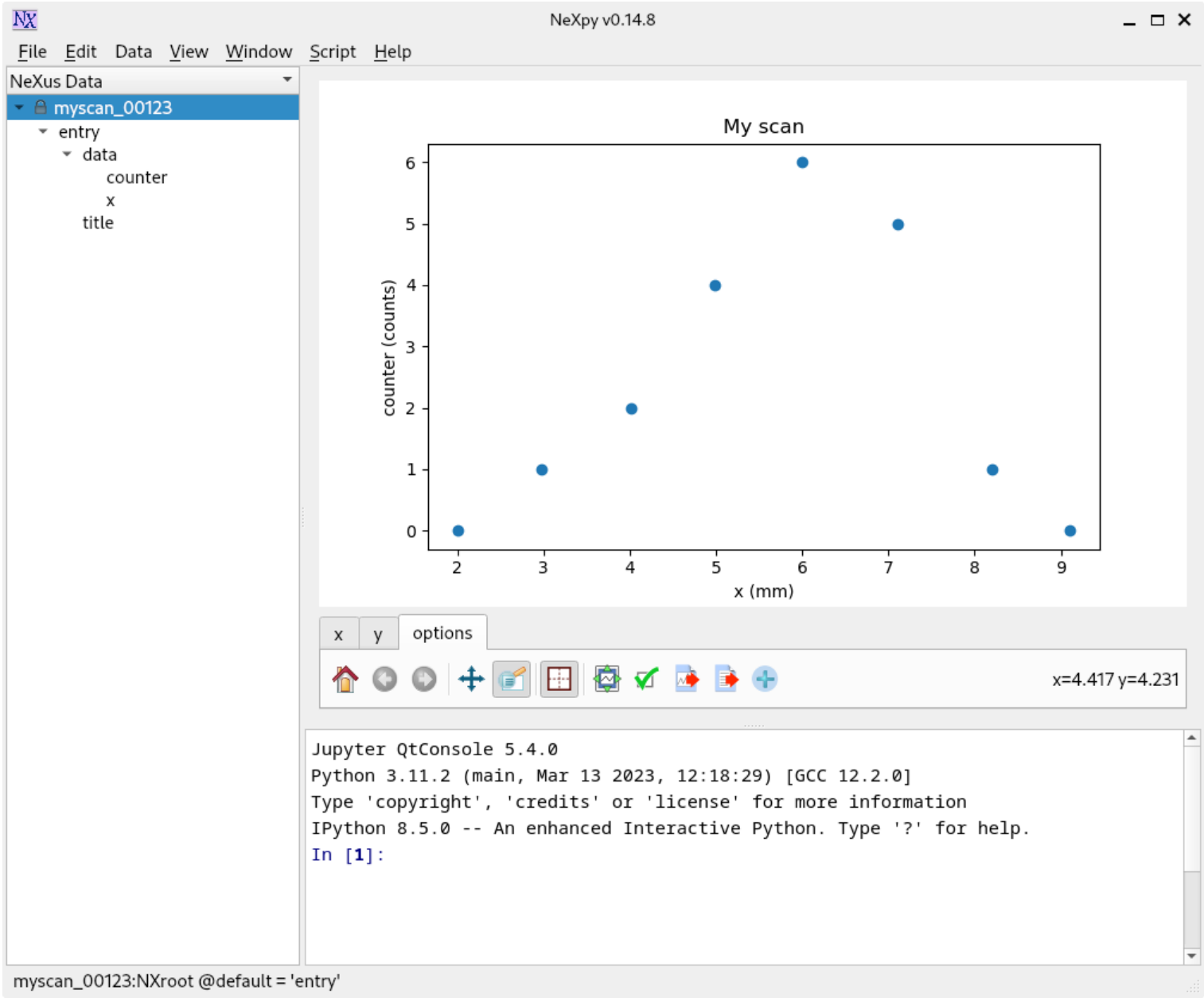
./h5cpp_create_dataset

View in NeXpy:

default plot

units

title

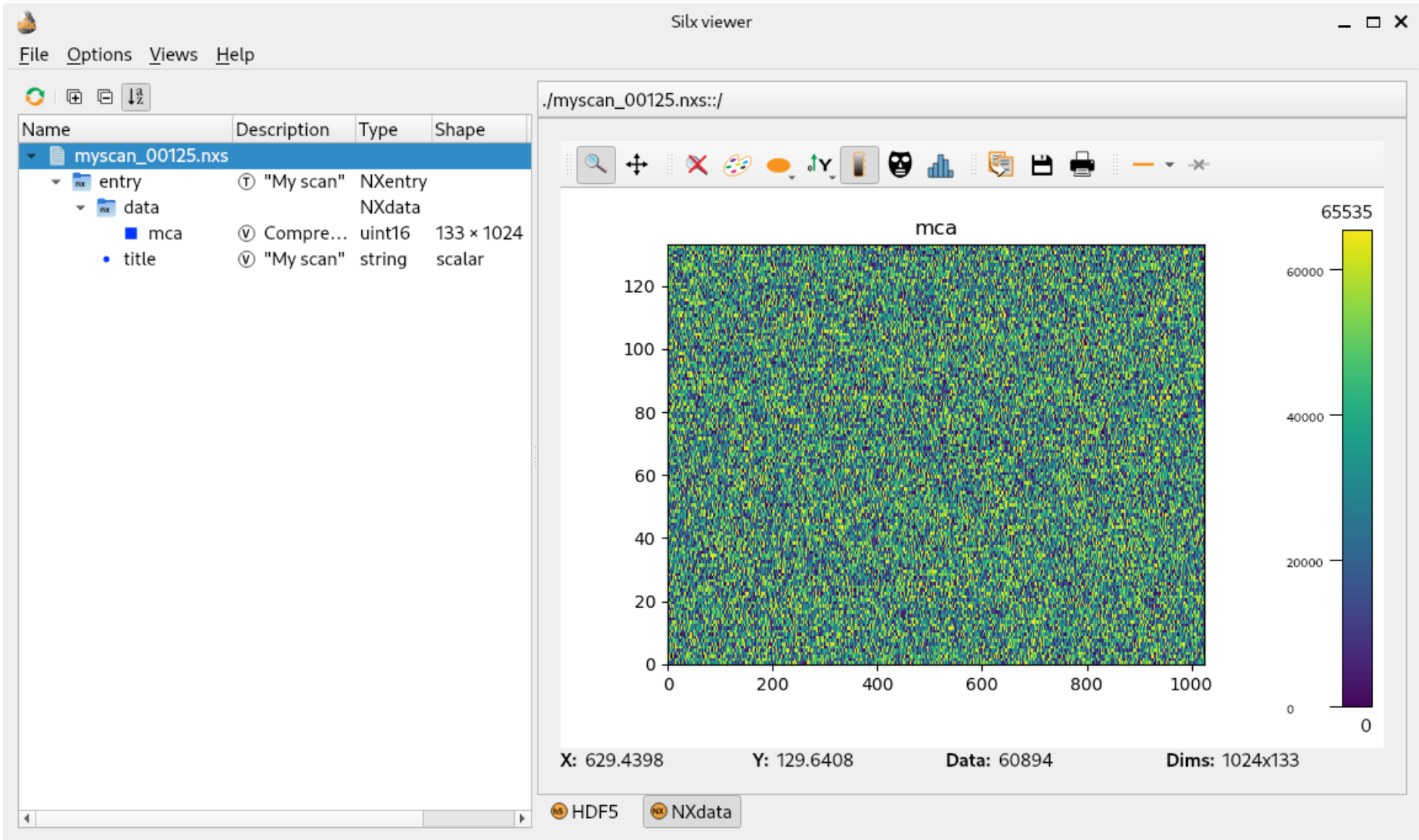


Append data with h5cpp

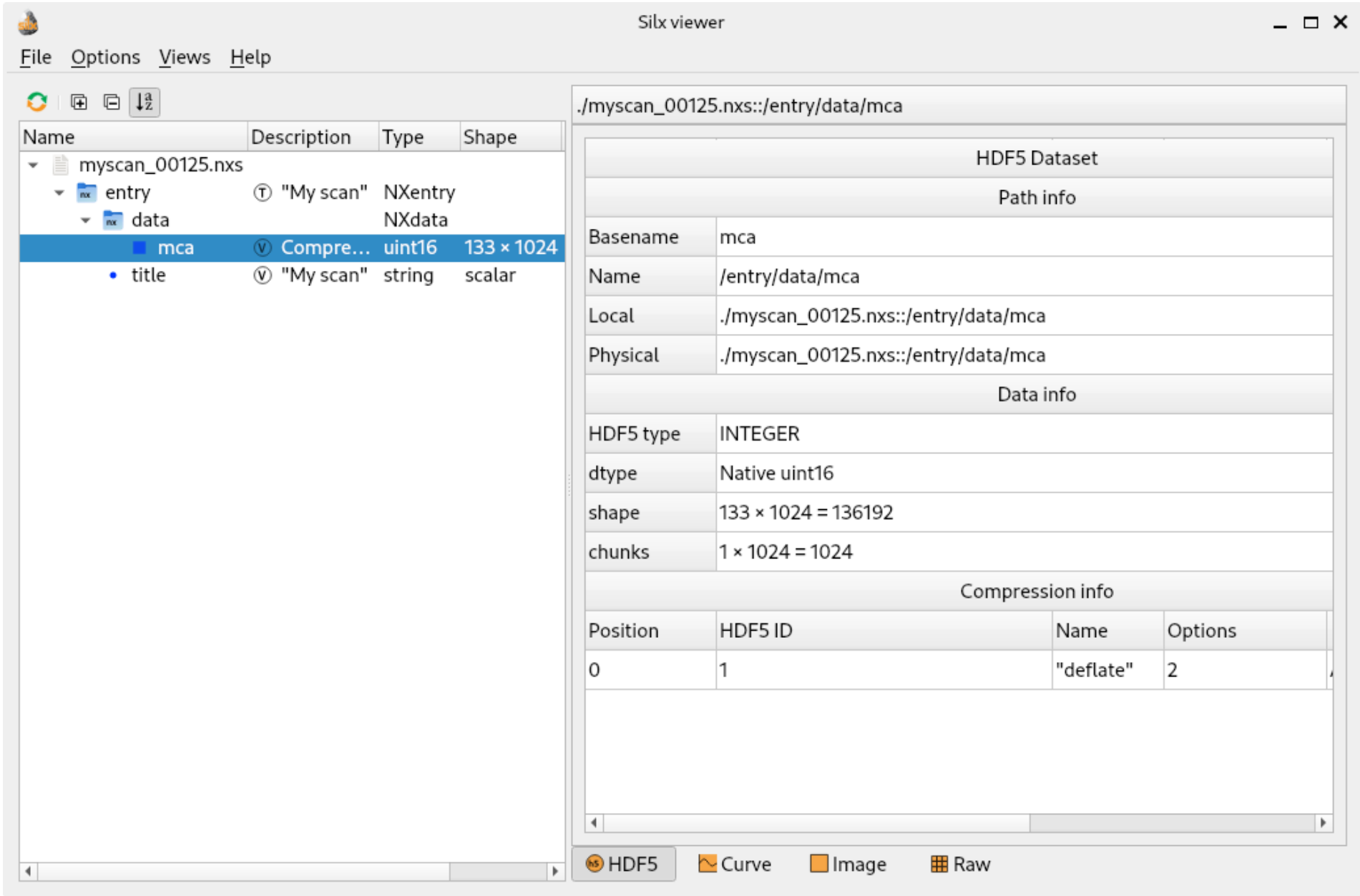
```
    const long long unsigned int xdim = 1024;
    const long long unsigned int nframe = 133;

    std::vector<unsigned short int> mca_data(xdim);

    // define our chunk size
    property::DatasetCreationList dcpl;
    dcpl.layout(property::DatasetLayout::Chunked);
    dcpl.chunk({1, xdim});

    // compression filter
    filter::Deflate filter(2u);
    filter(dcpl);

    // create a dataset
    using hdf5::dataspace::Simple;
    node::Dataset dataset =
        data_group.create_dataset("mca", datatype::get<unsigned short int>(),
                                  Simple({0, xdim}, {Simple::unlimited, Simple::unlimited}),
                                  dcpl);

    // define hyperslab of the chunk size
    dataspace::Hyperslab framespace{{0, 0}, {1, xdim}};

    for (long long unsigned int i = 0; i != nframe; i++) {
        // generate test data
        std::generate(mca_data.begin(), mca_data.end(), std::rand);

        // extend dataset, update hyperslab offset, write data
        dataset.extent(0, 1);
        framespace.offset({i, 0});
        dataset.write(mca_data, framespace);
    }
}
```

// from https://gitlab.desy.de/h5cpp-pninexus-examples/h5cpp_append_dataset.git

Append data with h5cpp: default plot



Append data with h5cpp: chunked dataset



Using pninexus with cmake

minimal CMakeLists.txt file

```
# project name
project(pninexus_from_xml)

# cmake required version
cmake_minimum_required(VERSION 3.13...3.20)
# we use c++17 standard
set(CMAKE_CXX_STANDARD 17)

# find h5cpp and pninexus
find_package(H5CPP REQUIRED)
find_package(PNINEXUS REQUIRED)

# define executable and its content
add_executable(pninexus_from_xml pninexus_from_xml.cpp)
# link h5cpp::h5cpp pninexus and std::filesystem
target_link_libraries(pninexus_from_xml PRIVATE h5cpp::h5cpp  pninexus stdc++fs)
```

from https://gitlab.desy.de/h5cpp-pninexus-examples/pninexus_from_xml.git

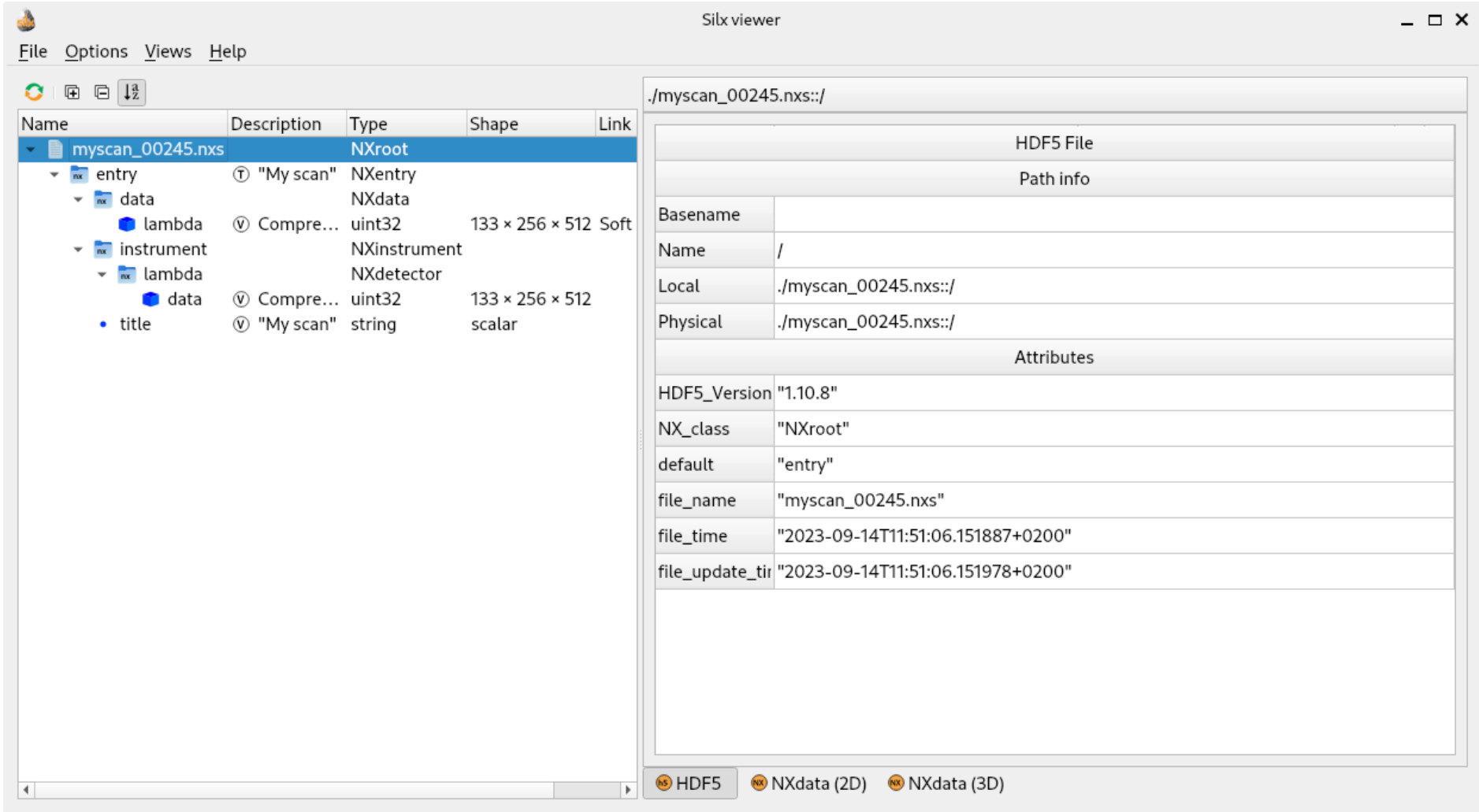
NeXus from xml: xml configuration

```
#include <h5cpp/hdf5.hpp>
#include <pni/nexus.hpp>

int main()
{
  using namespace hdf5;
  using namespace pni;

  const long long unsigned int xdim = 256;
  const long long unsigned int ydim = 512;
  const long long unsigned int nframe = 133;


  // NeXus configuration
  std::ostringstream xmlcnf;
  xmlcnf << "<attribute name=\"default\" type=\"string\">entry</attribute>"
         << "<group name=\"entry\" type=\"NXentry\">"
         << "  <attribute name=\"default\" type=\"string\">data</attribute>"
         << "  <field name=\"title\" type=\"string\">My scan</field>"
         << "  <group name=\"instrument\" type=\"NXinstrument\">"
         << "    <group name=\"lambda\" type=\"NXdetector\">"
         << "      <field name=\"data\" type=\"uint32\">"
         << "        <dimensions rank=\"3\">"
         << "          <dim value=\"0\" index=\"1\" />"
         << "          <dim value=\"" << xdim << "\" index=\"2\" />"
         << "          <dim value=\"" << ydim << "\" index=\"3\" />"
         << "        </dimensions>"
         << "        <strategy compression=\"true\" rate=\"2\" shuffle=\"false\" />"
         << "      </field>"
         << "    </group>"
         << "  </group>"
         << "  <group name=\"data\" type=\"NXdata\">"
         << "    <attribute name=\"signal\" type=\"string\">lambda</attribute>"
         << "    <link name=\"lambda\" target=\"/entry/instrument/lambda/data\" />"
         << "  </group>"
         << "</group>";
```

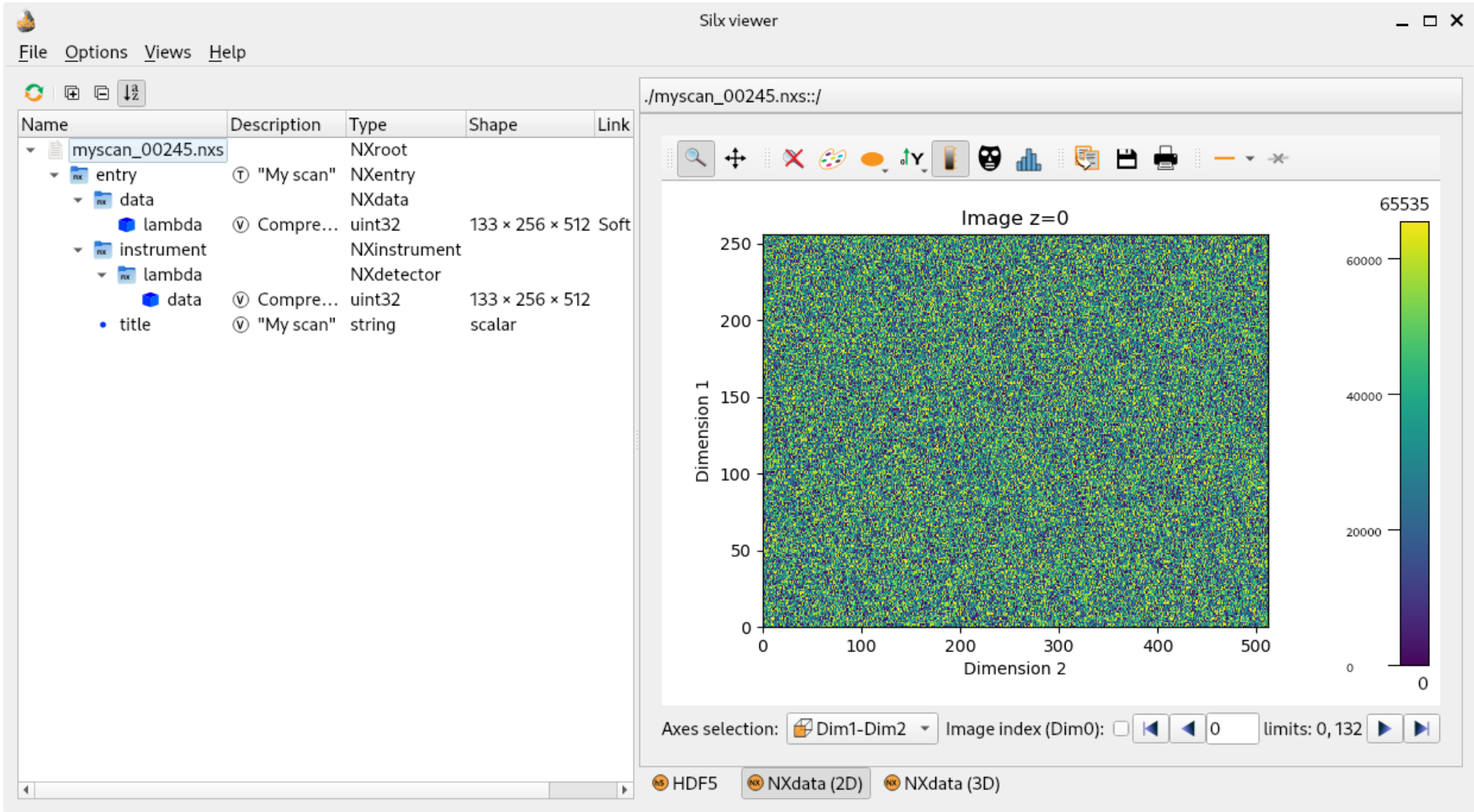
NeXus from xml: create a file and write data

```
  // create a file
  file::File f =
    nexus::create_file("myscan_00245.nxs", file::AccessFlags::Truncate);

  // create metadata from the xml string
  nexus::xml::create_from_string(f.root(), xmlcnf.str());
  node::Dataset dataset =
    node::get_dataset(f.root(), "/entry/instrument/lambda/data");

  // detector image buffer
  std::vector<unsigned short int> det_data(xdim * ydim);

  // hyperslab of the chunk size
  dataspace::Hyperslab framespace{{0, 0, 0}, {1, xdim, ydim}};

  for (long long unsigned int i = 0; i != nframe; i++) {
    // generate test data
    std::generate(det_data.begin(), det_data.end(), std::rand);

    // extend dataset, update hyperslab offset, write data
    dataset.extent(0, 1);
    framespace.offset({i, 0, 0});
    dataset.write(det_data, framespace);
  }
}
```

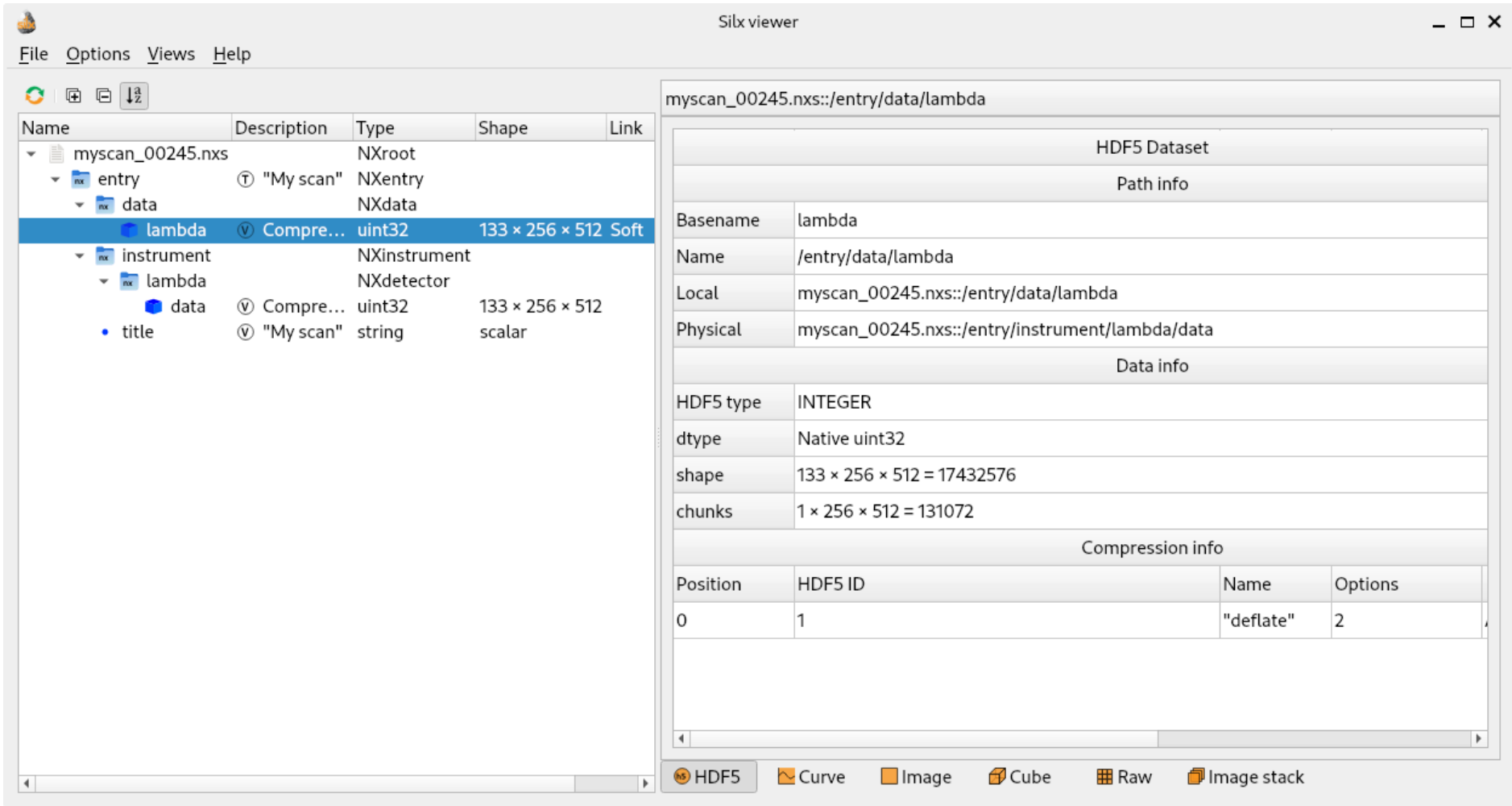
NeXus from xml: root attributes



NeXus from xml: default plot



NeXus from xml: chunked dataset



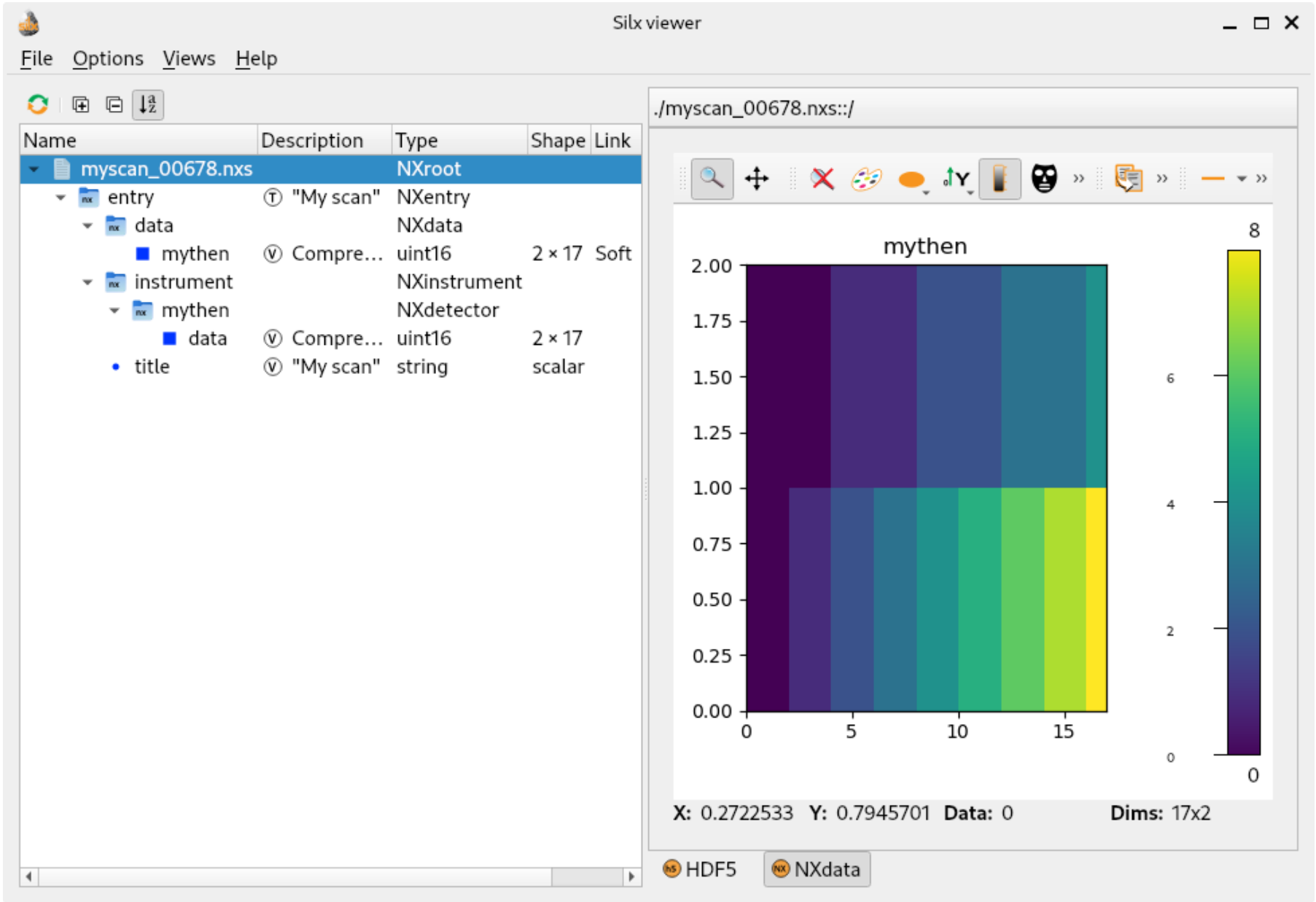
python bindings: xml configuration

```
import numpy

from pninexus import h5cpp
from pninexus import nexus

xml_config = """
<attribute name="default" type="string">entry</attribute>
<group name="entry" type="NXentry">
  <attribute name="default" type="string">data</attribute>
  <field name="title" type="string">My scan</field>
  <group name="instrument" type="NXinstrument">
    <group name="mythen" type="NXdetector">
      <field name="data" type="uint16">
        <dimensions rank="2">
          <dim value="0" index="1" />
          <dim value="17" index="2" />
        </dimensions>
        <strategy compression="true" rate="2" shuffle="false" />
      </field>
    </group>
  </group>
  <group name="data" type="NXdata">
    <attribute name="signal" type="string">mythen</attribute>
    <link name="mythen" target="/entry/instrument/mythen/data" />
  </group>
</group>
"""
```

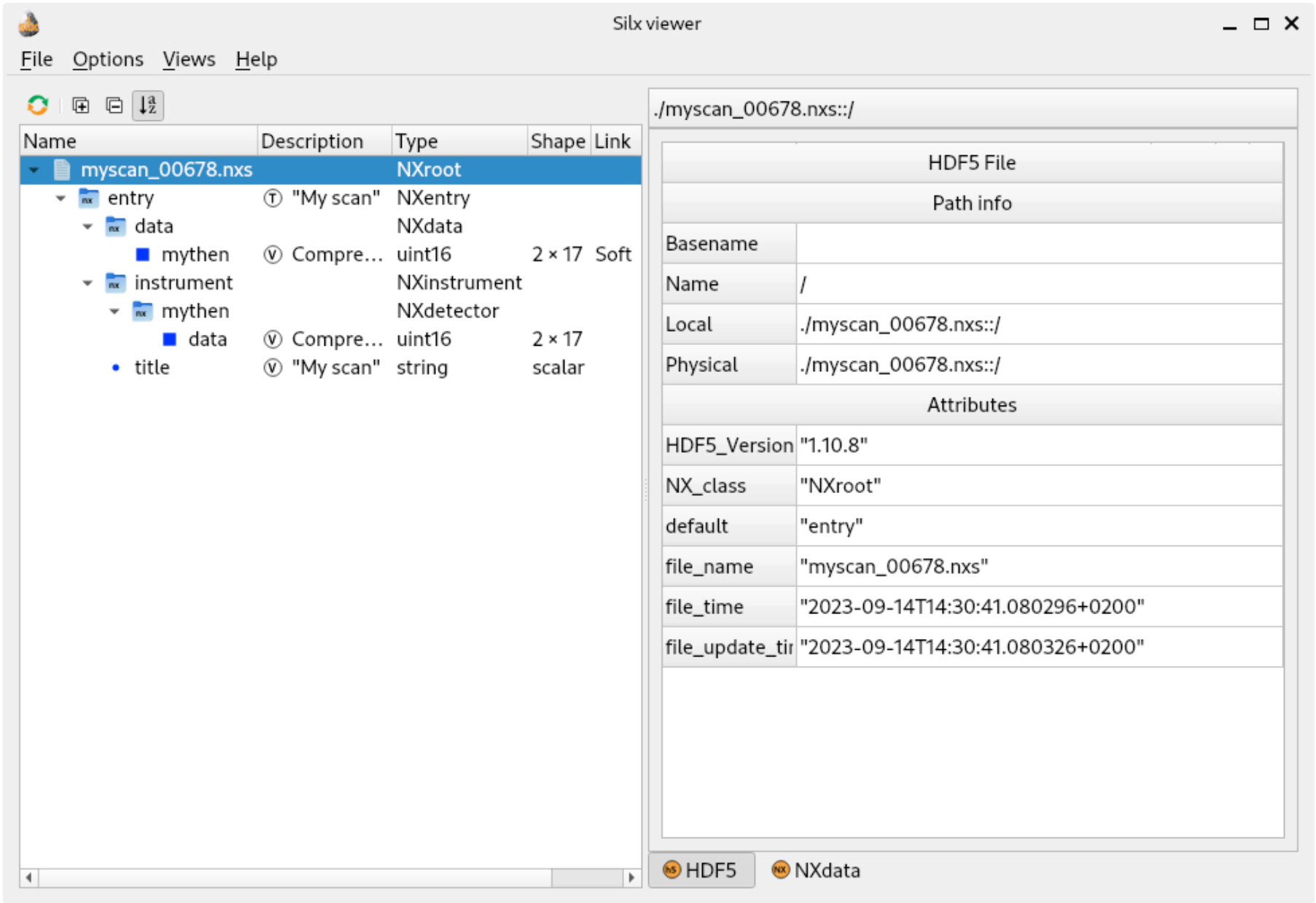
python bindings: white chunks directly

```
# create nexus file
mfile = nexus.create_file("myscan_00678.nxs", h5cpp.file.AccessFlags.TRUNCATE)
root = mfile.root()

# create nexus file structure
nexus.create_from_string(root, xml_config)

# get dataset directly
dataset = root.get_dataset(h5cpp.Path("/entry/instrument/mythen/data"))

# get datasets by group types (optional)
datasets = nexus.get_objects(root,
    nexus.Path.from_string(":NXentry/:NXinstrument/:NXdetector/data"))
if datasets:
    dataset = datasets[0]

# compressed detector frames
frame1 = numpy.array(
    [24184, 49677, 4609, 12288, 49156, 6832, 65478, 44127,
     151, 40580, 42322, 55254, 14696, 2563, 16640], dtype="uint16")
frame2 = numpy.array(
    [24184, 24675, 128, 1606, 25608, 32866, 26176, 2054, 24932, 0,
     20993, 7424], dtype="uint16")
frames = [frame1, frame2]

# write first direct
for i in range(len(frames)):
    dataset.extent(0, 1)
    dataset.write_chunk(frames[i], [i, 0])
```

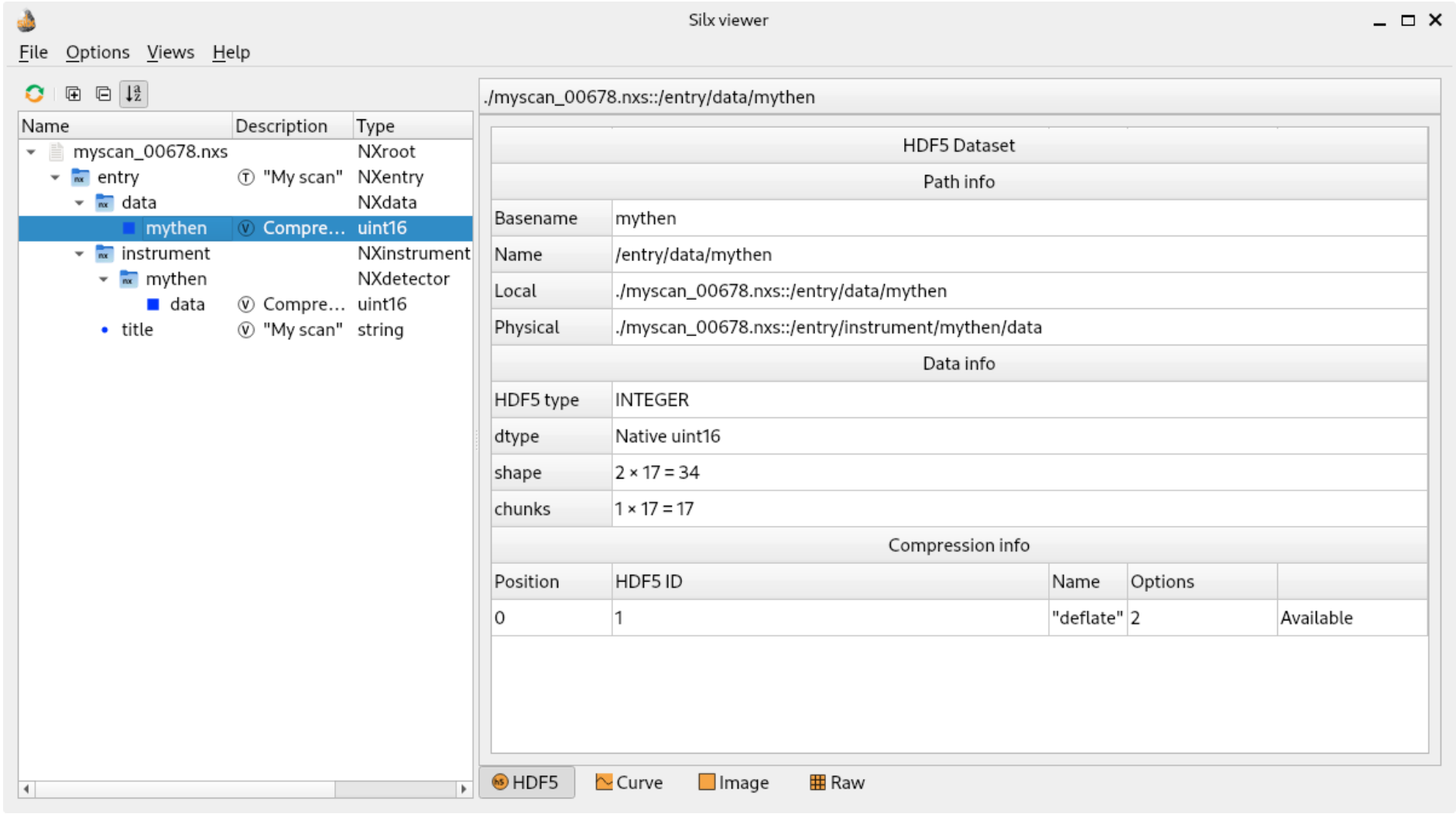
python bindings: default plot



python bindings: root attributes



python bindings: dataset details



Summary

- The h5cpp and pninexus libraries simplify our work with the HDF5 library: SWMR, external filters, direct chunk access, VDS, user datatypes/dataspaces with c++ traits, ...
- They are widely used also outside the science (h5cpp)
- We test them on: Linux (h5cpp, pninexus), Windows (h5cpp, pninexus) and MacOS (h5cpp)
- Open Source Projects:
  https://github.com/ess-dmsc/h5cpp.git
  https://github.com/pni-libraries/libpninexus.git
  https://github.com/pni-libraries/python-pninexus.git
- Debian/Ubuntu packages are available in our HDRI repository

...

Summary

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Thank You !