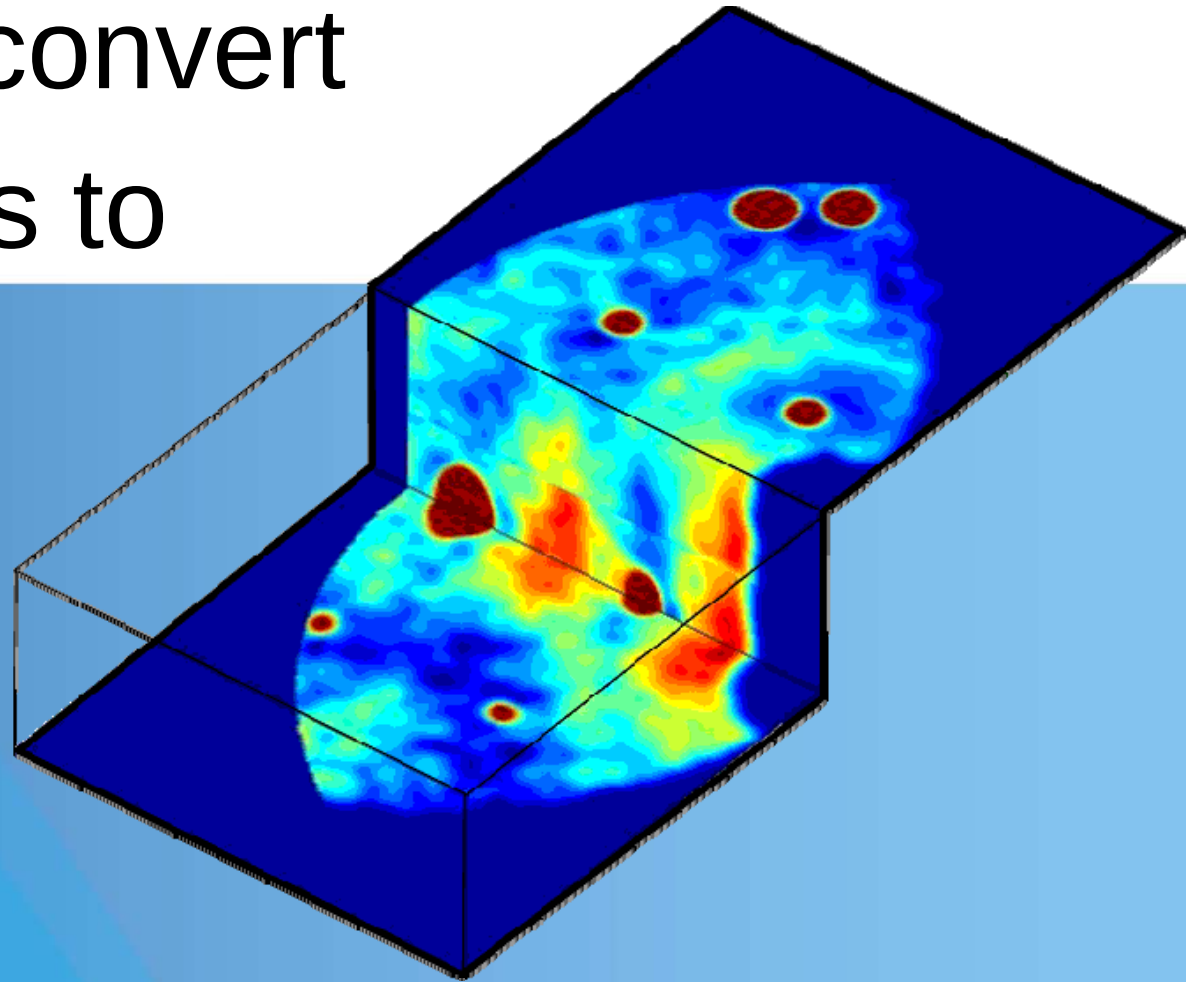


How-to convert data sets to **NeXus**



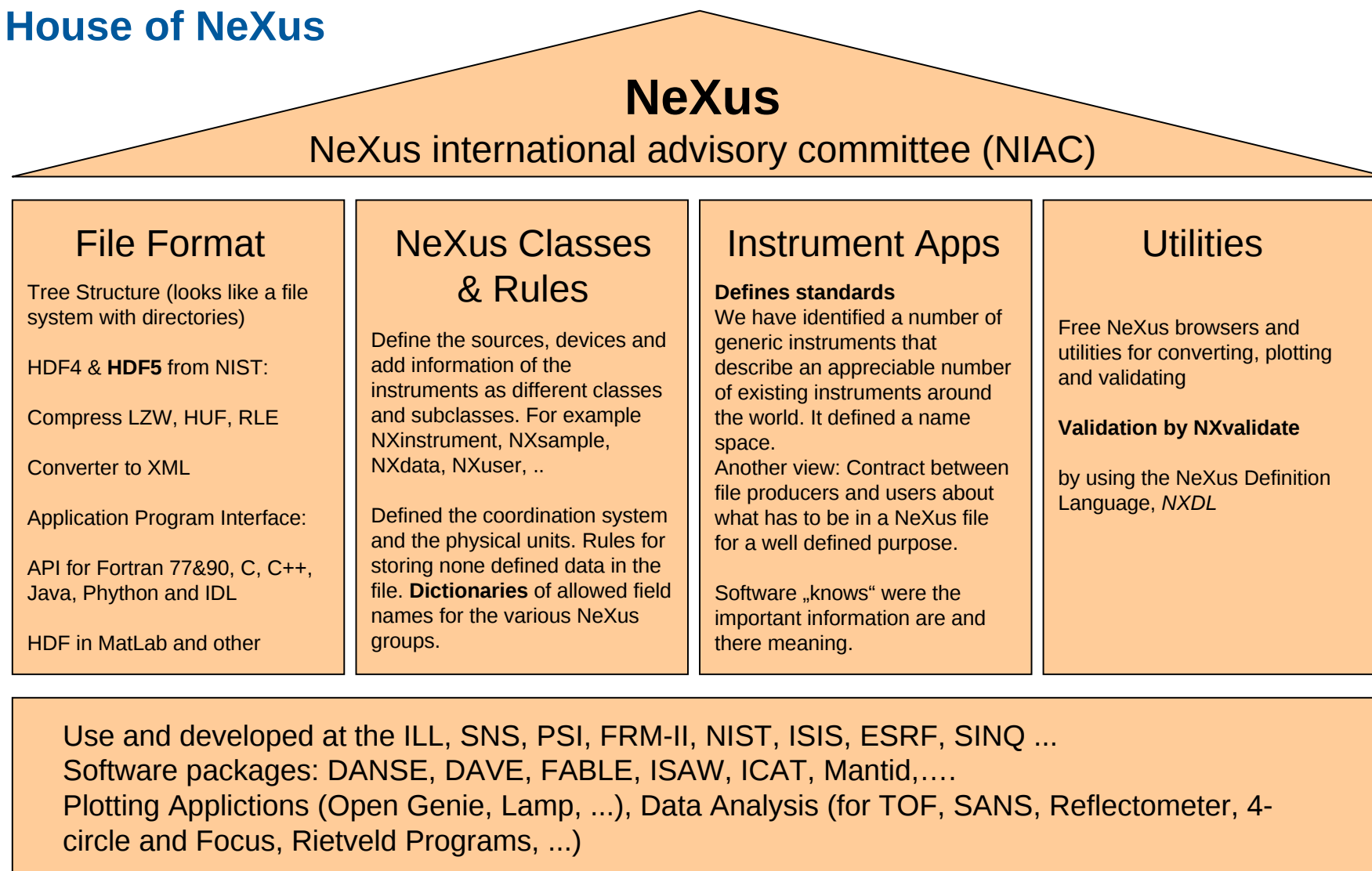
Jens-Uwe Hoffmann
Dept. Complex Magnetic Materials

Few slides provided by
Mark Krönnicke, PSI

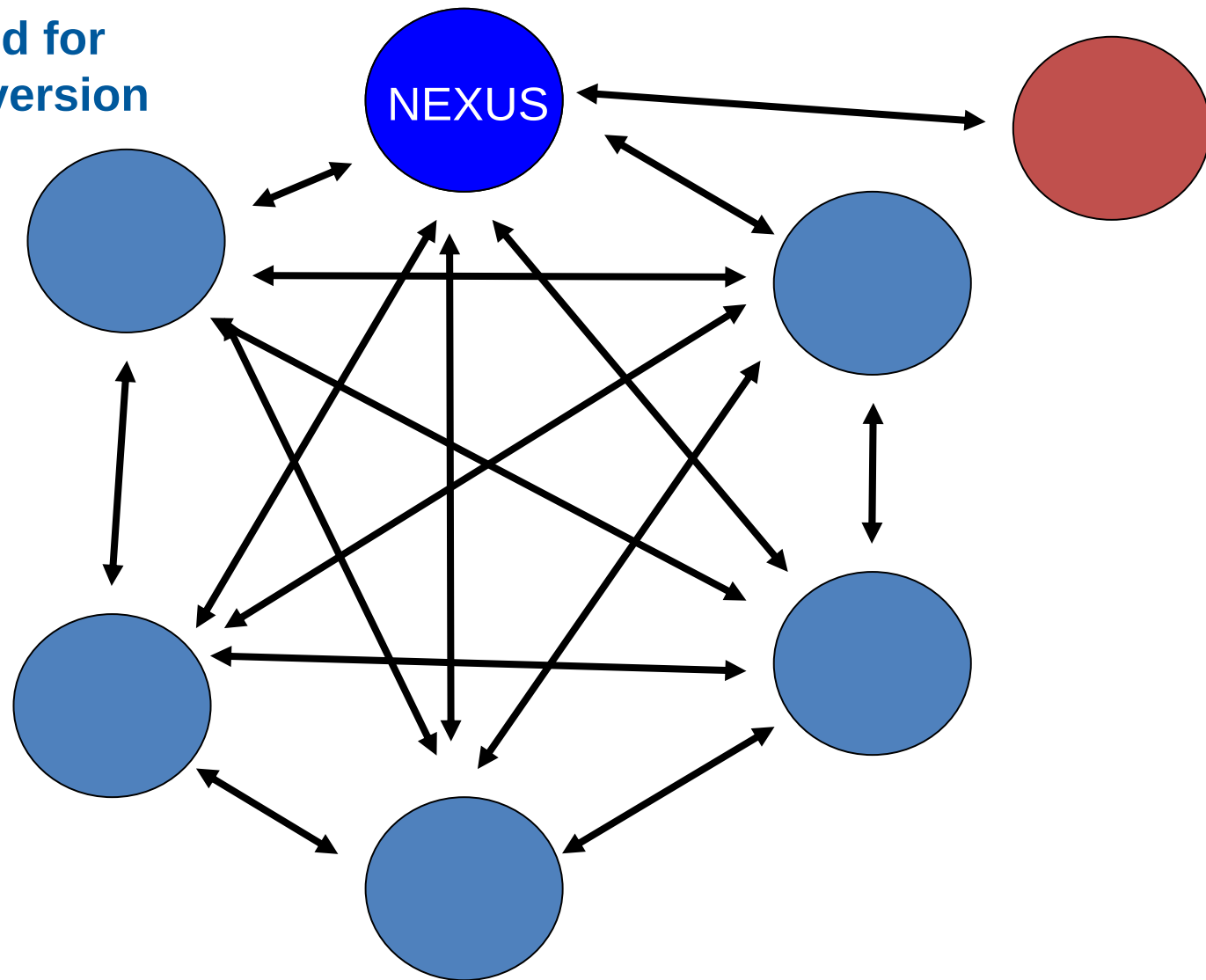
Time table of NeXus at HZB

- Design datacollector – diploma thesis J. Gasse (2006)
- Implemented caress & root format (2006)
- Flat-Cone Diffractometer E2 (since 2007)
- Starting Tests (2010)
 - Powder Diffractometer E6
 - Single Crystal Diffractometer E4
- Regularly storing E6 data (now)
- Discussion about BESSY ASCII data (now)
- Start testing for all thermal neutron instruments data (soon)
- New instruments in the neutron guide hall (HDR, planed)

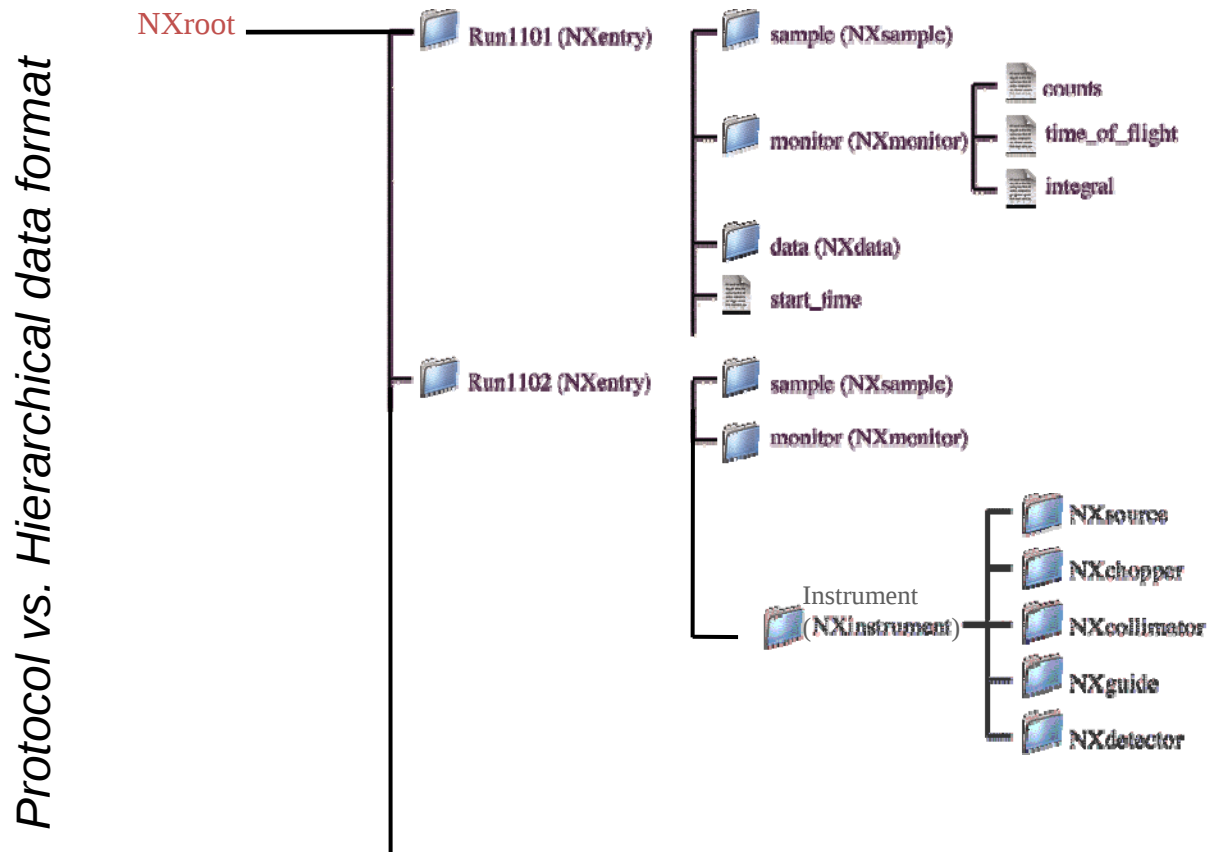
House of NeXus



Reduced need for data set conversion



Principle Structure



Each class is defined in the new NeXus Definition Language (NXDL) file.

Nexus Raw Data File Structure

```
entry:NXentry
  sample:NXsample
  instrument:NXinstrument
    source:NXsource
    velocity_selector:NXvelocity_selector
    detector:NXdetector
      data[xsize,ysize], signal=1 (1)
  control:NXmonitor
    data
  data:NXdata
    link to (1)
```

NeXus Precessed Data File Structure

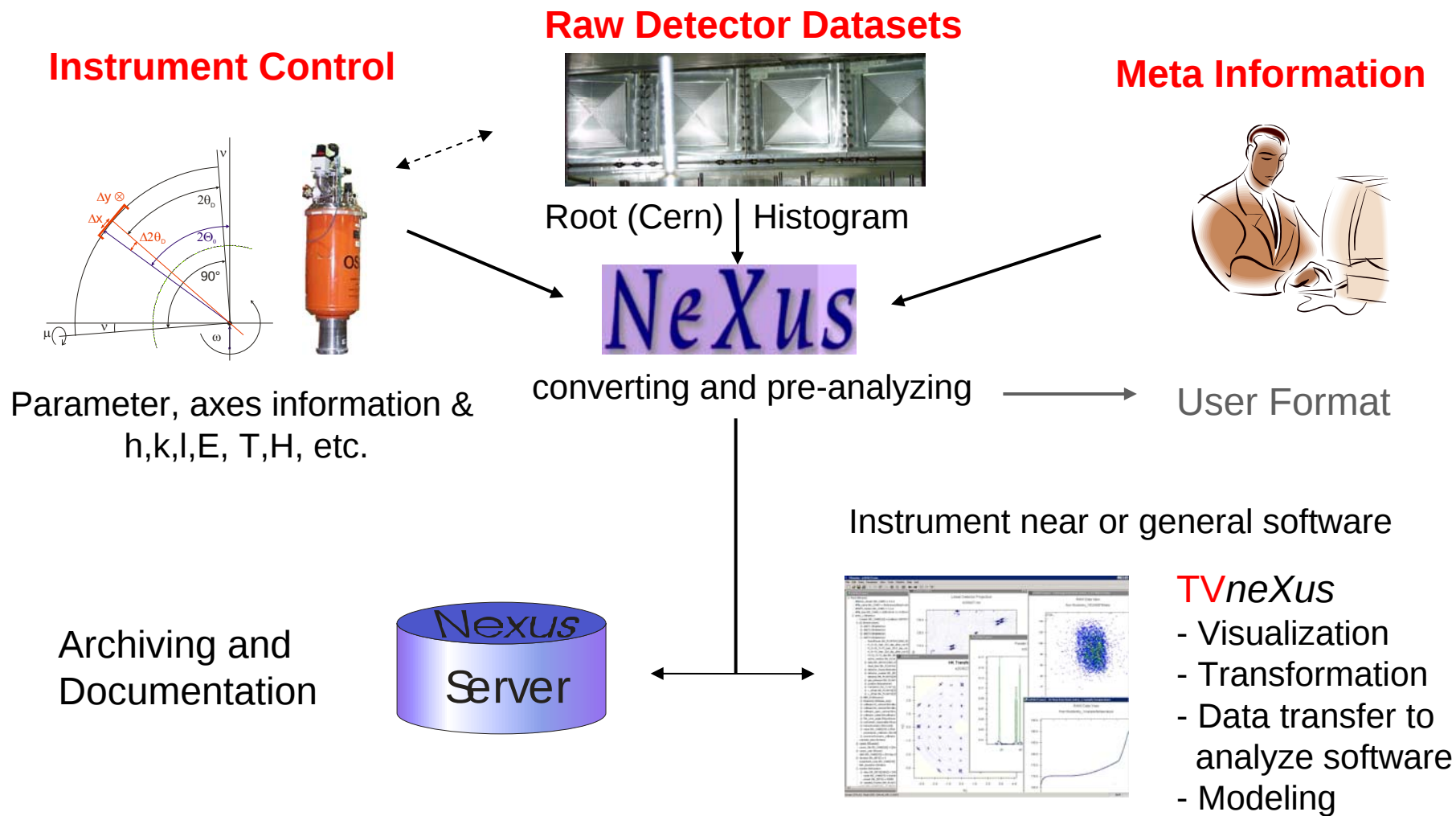
```
entry:NXentry
  sample:NXsample
  processing_name:NXprocess
    program
    version
  parameters:NXparameter
  raw_file
data:NXdata
  data[nx,ny,nz], signal=1
```

Archiving

NXentry

Name	Type	Description	Attributes
title	NX_CHAR	Extended title for entry	
experiment_identifier	NX_CHAR[]	Unique identifier for the experiment, defined by the facility, possibly linked to the proposals	
experiment_description	NX_CHAR	Brief summary of the experiment, including key objectives.	
experiment_documentation	NXNote	Description of the full experiment (document in pdf, latex, ...)	
collection_identifier	NX_CHAR	User or Data Acquisition defined group of NeXus files or NXentry	
collection_description	NX_CHAR	Brief summary of the collection, including grouping criteria.	
entry_identifier	NX_CHAR	unique identifier for the measurement, defined by the facility.	
definition	NX_CHAR	Name of entry DTD	version="{DTD version number}" URL="{URL of DTD file}"
definition_local	NX_CHAR	Name of entry DTD	version="{DTD version number}" URL="{URL of DTD file}"
start_time	ISO 8601	Starting time of measurement	
end_time	ISO 8601	Ending time of measurement	
duration	NX_INT	Duration of measurement	units="seconds"
collection_time	NX_FLOAT	Time transpired actually collecting data i.e. taking out time when collection was suspended due to e.g. temperature out of range	units="seconds"
run_cycle	NX_CHAR[]		
program_name	NX_CHAR	Name of program used to generate this file	version="{Program version number}" configuration="{configuration of the program}"
revision	NX_CHAR	Revision id of the file due to re-calibration, reprocessing, new analysis, new instrument definition format, ...	comment=""
notes	NX_CHAR	Notes describing entry	
thumbnail	NXnote	An small image that is representative of the entry. {An example of this is a 640x480 jpeg image automatically produced by a low resolution plot of the NXdata.}	mime_type="{image/*}"
NXcharacterizations	NX_CHAR		
{user}	NXuser		
{sample}	NXsample		
{Name of instrument}	NXinstrument		
{Name of monitor}	NXmonitor		
{Name of data block}	NXdata		
{Name of the process}	NXprocess		

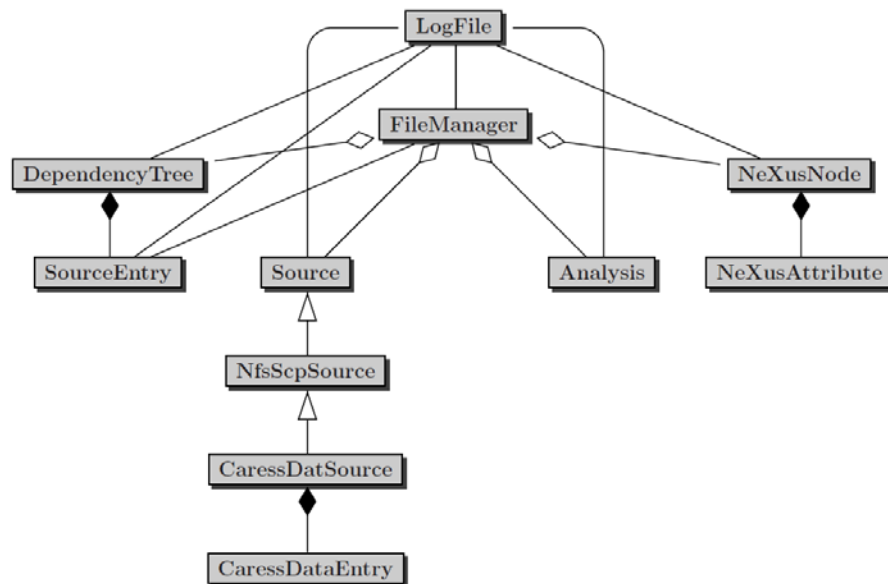
Data Sources



Design of the data collector software

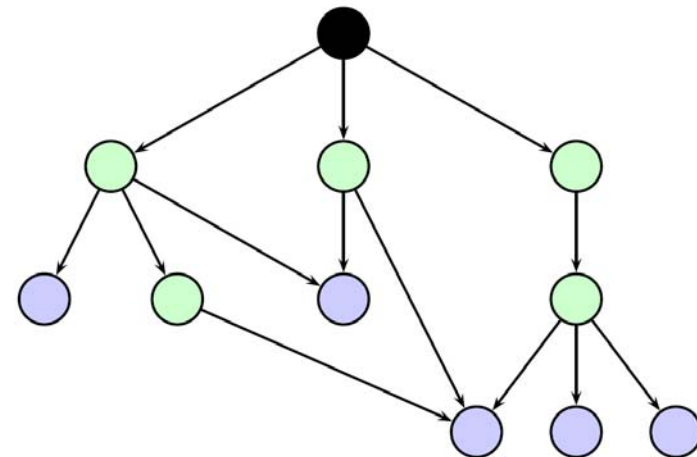
Class schema of data collector

Object oriented concept



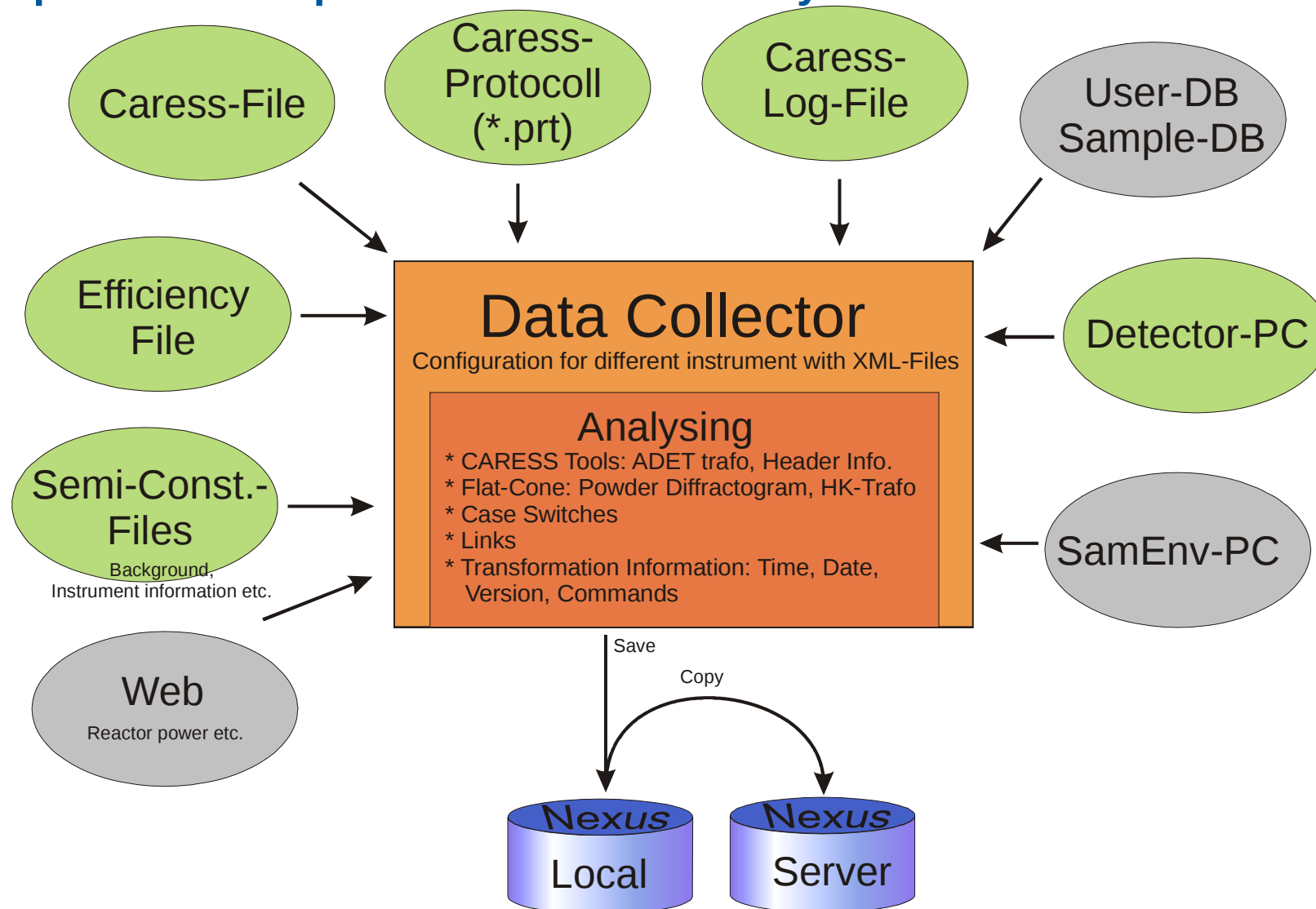
Multi-trees for thread management

Order of executing.



Diploma thesis: [Jörg Gasse](#), „Konzeptionierung und Erstellung einer Software zur Serialisierung und automatisierten Analyse von komplexen Daten aus unterschiedlichen Quellen“, 2006

Implemented Import Filter and Pre-Analysis Classes



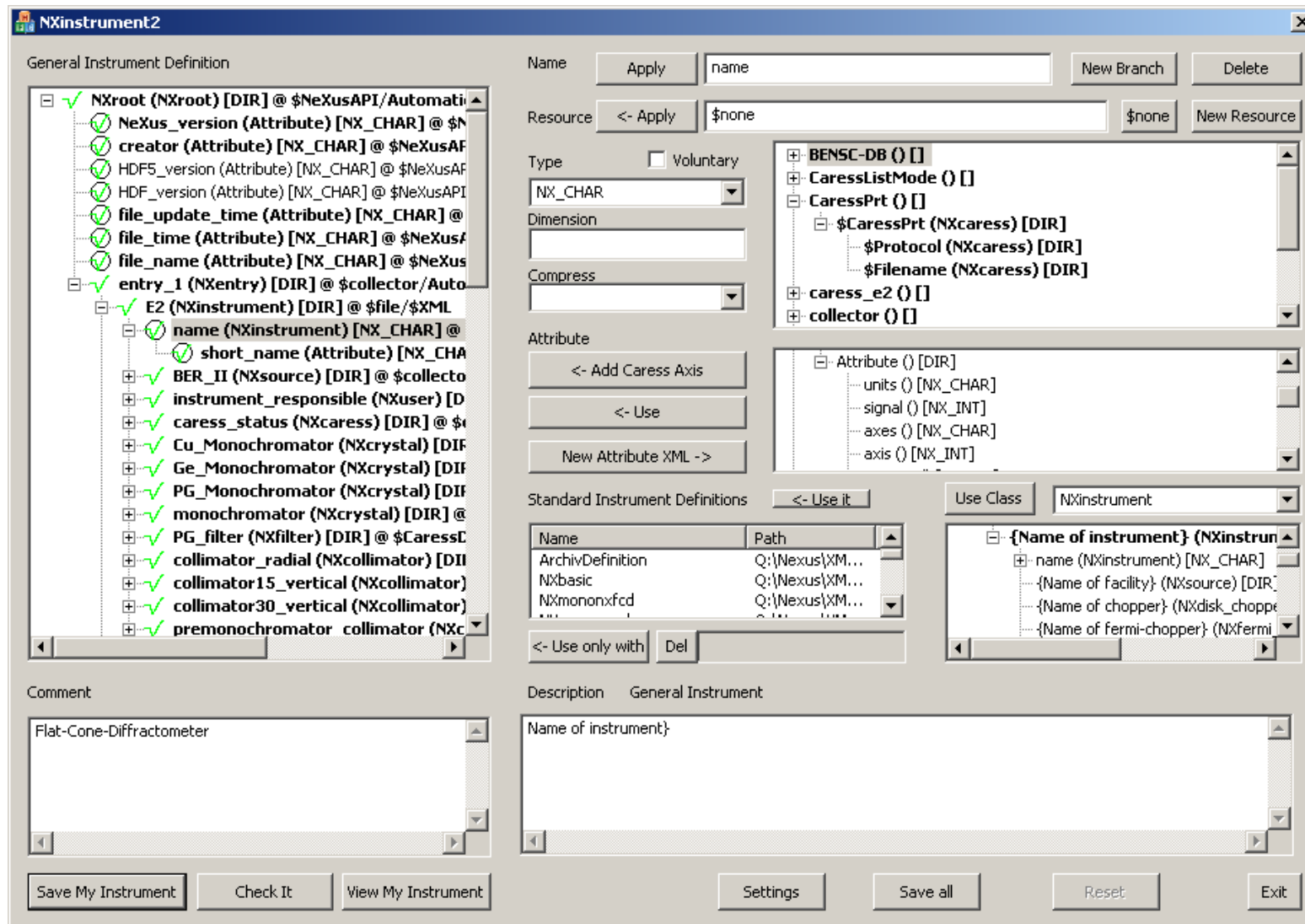
Example Source-File

```
<?xml version="1.0" encoding="utf-8" ?>
<SourceConfig>
  <Options>
    <LogFile enabled="true" append="false" />
    <ScreenLog enabled="true" />
    <Threads>
      <General>10</General>
      <DataAquisition>1</DataAquisition>
      <DataTransfer>1</DataTransfer>
      <Analyses>5</Analyses>
    </Threads>
    <NeXusFile>/hmi/caress/data/data/e2.nxs</NeXusFile>
    <TempDirectory>/hmi/caress/data</TempDirectory>
  </Options>
  <Sources>
    <Source medium="nfs" type="$CaressDat" name="1">
      <Dependencies>
        <Dependency type="command line">
          <Parameter number="0" wildcard="*" />
        </Dependency>
      </Dependencies>
      <Path>/hmi/caress/data/caress/*.dat</Path>
    </Source>
  </Sources>
</SourceConfig>
```

Example of a NeXus configuration file (XML DTD)

```
<CARDirectory nameDef = "caress" sourceDef = "$collector/Automatic" >
  {current state of the instrument at the beginning of the scan}
  <Link nameDef = "test" typeDef = "NX_INT" sourceDef = "$Link/entry_1/E6/ADET2/rawdata">
    {Link-Testverzeichnis nach entry_1/E6/ADET2/rawdata}
  </Link>
  <NXpositioner nameDef = "Two_Theta" sourceDef = "$collector/Automatic">
    {Positioner of TTHS}
    <data sourceDef = "$CaressDat/MASTER1V/TTHS">
      {Position of TTHS}
    </data>
  </NXpositioner>
  <CARDirectory nameDef = "READ" sourceDef = "$CaressDat/$Header/READ">
    {Header READ - Anfangsstatus}
  </CARDirectory>
</CARDirectory>
```

Configuration tool



How-to convert data sets to NeXus

NeXus Homepage: www.nexusformat.org

NeXus

NXentry Class

URL: <http://www.nexus.anl.gov/classes/xml/NXentry.xml>
Editor: NIAC
\$Id: NXentry.xml,v 1.2 2005/07/19 04:10:26 rio Exp \$

Template of the top-level NeXus group which contains all the data and associated information that comprise a single measurement. It is mandatory that there is at least one group of this type in the NeXus file.

Name	title	definition
start_time	ISO8601	Starting time of measurement
end_time	ISO8601	Ending time of measurement
duration	NX_INT	Duration of measurement
experiment_identifier	NX_CHAR[]	
run_number	NX_INT	Number of run or scan stored in this entry
run_cycle	NX_CHAR[]	
program_name	NX_CHAR	Name of program used to generate this file
command_line	NX_CHAR	Name of command line used to generate this file
notes	NX_CHAR	Notes describing entry
thumbnail	NXnote	An small image that is representative of the entry. An example of this is a 640x480 jpeg image automatically produced by a low resolution plot of the NXdata.
NXcharacterizations		
NXuser		
NXsample		
NXinstrument		
NXmonitor		
NXdata		

[Download NXentry.xml]

Home Introduction Design Classes Instruments API Utilities FAQ

New HZB NeXus web page coming soon....