The Scientific Data Exchange Reference Guide

Includes x-ray tomography, x-ray fluorescence microscopy, and

x-ray photon correlation

http://www.aps.anl.gov/DataExchange

Version 0.0.12

April 6, 2012

Table 1: Version history

Version	Date	Notes
v000	Nov 15, 2011	FdC: First version of the Data Exchange file format for full field x-ray imaging and tomography based on the definition from https://confluence.aps.anl.gov/.
v001	Dec 23, 2011	FdC: Added sample and instrument class to meet APS (2-BM, 13-BM, 32-ID) and SLS (Tomcat) meta data requirements and definitions.
v002	Jan 5, 2012	FdC: Merged with the Coherent X-ray Imaging Data Bank file format CXI from http://cxidb.org/cxi.html. Converted the document using the same diagram definition set by Filipe Maia in "CXI file format" and modified to fit the Data Exchange definitions.
v003	Jan 15, 2012	NS: Added Provenance Class
v004	Feb 6, 2012	FdC: Added measurement class and moved sample and instrument under it to meet ESRF request to allow for multiple tomography measurements to be stored in the same file (relevant for nano CT raster scans and similar).
v005	Feb 19, 2012	FdC: Clean up 2FXi vs Data Exchange and moved to version control.
v006	Feb 21, 2012	FdC/FM (SLS): explained more clearly that the 3D array dimension order (rotation, ccd y, ccd x) is a default but not mandatory. Affected sections 3.4, **??**, 4.4.1, **??**.
v007	Feb 22, 2012	FdC/YP: added more info in the reconstruction and algorithm classes. Affected section **??** and table **??**.
v008	Feb 25, 2012	FdC: Expanded Data Exchange and Detector definition to add fluorescence, photon correlation. Affected section 2.2, **??**, **??**, **??**, **??**, 4.3.2.5, **??**.
v009	Feb 26, 2012	NS: Expanded Data Exchange and Detector definition for XPCS. Affected section **??**, **??**, **??**.

Table 1: Version history

Version	Date	Notes
v010	Mar 1, 2012	NS: Expanded Data Sample, Source, and Shutter definitions as well as Detector and other definitions for XPCS. Affected section 4.3.1, 4.3.2.2, 4.3.2.1, **??**, **??**, **??**, **??**
v011	Mar 2, 2012	FdC: Split into technique specific the ”instrument” definitions. Affected section **??**, **??**, **??**
v012	Mar 5, 2012	NS: Added sample thickness. Expanded XPCS definition. Affected section 4.3.1, **??**
v013	Apr 5, 2012	CS: Restructuring document into sections included into main document(s)

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1 Introduction

For various reasons, many x-ray techniques developed at synchrotron facilities around the world, are unable to directly compare results due to their inability to exchange data and software tools. The aim of Data Exchange is to define a simple file format offering few basic rules and allowing each community to extend and add technique specific components. The goal is to provide simplicity and extensibility in defining data, meta data and provenance information in a simple way that can be easily adopted by various x-ray techniques.

The Data Exchange format is implemented using Hierarchical Data Format 5 (HDF5), which offers platform-independent binary data storage with optional compression, hierarchical data ordering, and self-describing tags so that one can examine a HDF5 file's contents with no knowledge of how the file writing program was coded.

The aim and the scope of Data Exchange is very similar to the Coherent X-ray Imaging Data Bank file format (CXI), so whenever possible we will use the same conventions, name tags and reference system. This document is using the same diagram definition set by Filipe R. N. C. Maia in ”CXI file format” (`http://cxidb.org/cxi.html`) and has been modified to fit the Data Exchange definitions.

2 The Design of Data Exchange

The core principle of Data Exchange is that it must be simple enough that it is not necessary to use a support library beyond core HDF5. The simplicity of Data Exchange read and write is achieved using basic HDF5 calls, making it easy for anyone to either look at an example file using h5dump or HDFView, or to look at example code in language X, and then create their own read and write routines in language Y.

The simplest Data Exchange file provides information and exchange definition sufficient to share a multidimensional data array as simply as possible. In its simplest implementation Data Exchange implements only one ”exchange” group. The ”exchange” definition is designed to allow for simple exchange of images, spectra, and other forms of beamline detector data with a minimum of fields. This definition is essentially a technique-agnostic format for exchanging data with others. Data Exchange is also designed to be extended to include technique-specific data and metadata information. This is achieved by providing optional, but clearly defined, metadata components to the base definition.

2.1 HDF5

The HDF5 format is the basis of Data Exchange format. Data Exchange, like CXI, is not really a completely new file format but simply a set of rules designed to create HDF5 files with a common structure and to allow a uniform and consistent interpretation of such files.

HDF5 was chosen as the basis because it is a widely used high performance scientific data format which many programs can already, at least partially, read and write. It also brings with it the almost automatic fulfillment of the Data Exchange requirements, i.e. simplicity, flexibility and extensibility. HDF5 version 1.8 or higher is required as previous versions don't support all features required by Data Exchange.

2.1.1 Data types

Data Exchange uses the same CXI convention for data types as defined at `http://cxidb.org/cxi.html` using HDF5 native datatypes. The data should be saved in the same format as it was created/acquired. For example CCD images acquired as 16 bit integers should be saved using the `H5T_NATIVE_SHORT` HDF5 type. In this way all cross platform big-little endian issues reading and writing files are eliminated.

2.2 Data Exchange Definition

While HDF5 gives great flexibility in data storage, straightforward file readability and exchange requires adhering to an agreed-upon naming and organizational convention. To achieve this goal, Data Exchange adopts a layered approach by defining a set of *mandatory* and `optional` fields. The general rules of a Data Exchange file is that must contain the following members:

implements - A colon separated list in the root level of the HDF5 file that shows which components are present in the file. All groups listed in the *implements* string attribute are placed in the HDF5 file at the same level as *implements* and *version*. In a Data Exchange file the only *mandatory* implements is *exchange*. A more general Data Exchange file also contain `measurement` and `provenance` information, if so these will be declared in implements as "*exchange*: `measurement`: `provenance`"

Table 2: Data Exchange general rules

Member	Type	Example
implements	string	"exchange:measurement:provenance"
version	string	"1.0.1"
exchange	Exchange group	
`measurement`	Measurement group	
`provenance`	Provenance group	

version - Located in the root level of the HDF5 file, identifies the Data Exchange version in use.

exchange - Mandatory group containing one or more arrays that represent the most basic version of the data, such as raw or normalized optical density maps or a elemental signal map. *Exchange_N* is used when more than one arrays or processing step are saved in the file. The *exchange* implementation for specific techniques is defined later (x-ray micro tomography in section **??**, x-ray fluorescence in section **??**) .

`measurement` - Optional group containing the measurement made on the sample. `Measurement` contains information about the `sample` and the `instrument`. `Measurement_`*N* is used when more than one measurement is stored in the same file.

`provenance` - Optional group containing information about the status of each processing step.

In a Data Exchange file each data field has a unit defined using the `units` attribute. `Units` is not mandatory, if omitted the default unit as defined in Appendix A.1 is used.

3 Data Exchange by example

3.1 Diagram color code

The diagrams of the Data Exchange file follow the same color conventions used by the CXI and reported in Figure 1

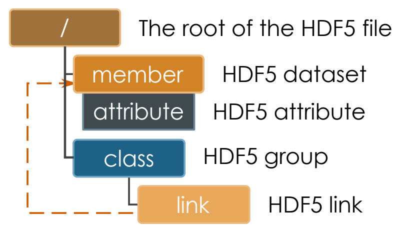

Figure 1: Explanation of the color code used in the diagrams

3.2 Data Exchange for Full Field X-ray Imaging

The data file format for full field x-ray imaging (2FXi) is defined as the Data Exchange implementation to store all experimental data collected during full field x-ray imaging and tomography experiments as well as to capture infrastructure meta data and data provenance by recording how the data were acquired, processed and transferred.

The 2FXi file format complies with the Data Exchange file format defined in Section 2.2, adding, as required by the Data Exchange definition, the technique-specific groups for full field x-ray imaging and tomography.

The goal of Data Exchange implementation for x-ray full field imaging is to provide simplicity and extensibility in defining data, meta data and provenance information for x-ray imaging, micro and nano tomography.

3.3 A minimal Data Exchange file for Imaging

Figures 2 shows a diagram a minimal Data Exchange file to store a single projection image. As no units are specified the data is assumed to be in “counts” with the axes (x, y) in pixels.

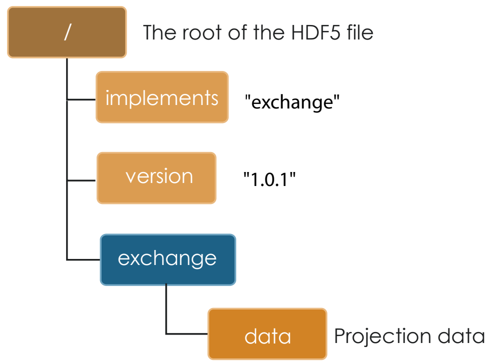

Figure 2: Diagram of a minimal Data Exchange file for a single image.

3.4 A minimal Data Exchange file for tomography

A tomographic data set consists of a series of projections, dark and white field images. The dark and white fields must have the same projection image dimensions and can be collected at any time before, after or during the projection data collection. The angular position of the tomographic rotation axis is used to keep track of when the dark and white images are collected. 2FXi saves projection images, dark and white images in three 3D arrays as shown in Figure 3 and 4 using, by default, the natural HDF5 order of the a multidimensional array (rotation axis, ccd y, ccd x), i.e. with the fastest changing dimension being the last dimension, and the slowest changing dimension being the first dimension. If using the default dimension order, the axes attribute (see Table 4) "theta:y:x" can be omitted. The `axes` attribute is mandatory if the 3D arrays use a different axes order. This could be the case when, for example, the arrays are optimized for sinogram read (`axes` = "y:theta:x"). As no units are specified the data is assumed to be in "counts" with the axes (x, y) in pixels.

3.5 A typical Data Exchange file for tomography

A series of tomographic data sets are typically collected changing the instrument status (energy, detector or optics position) or changing the sample status (position, environment etc.). Figure 5, 6 and 7 show the content of 2FXi files changing the sample temperature, the x-ray source energy and detector-sample distance.

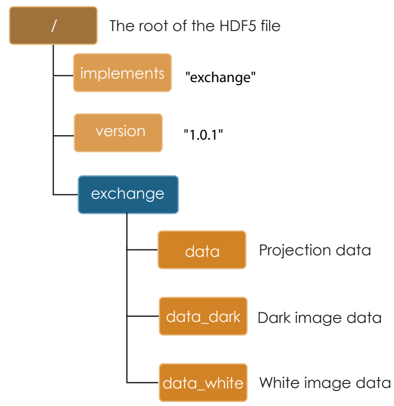

Figure 3: Diagram of a minimal Data Exchange file for a single tomographic data set including raw projections, dark and white fields. Since the positions of the rotation axis for each projection, dark and white images are not specified is assumed that the raw projections are taken at equally spaced angular intervals between 0 and 180 degree, with white and dark field collected at the same time before or after the projection data collection.

3.5.1 Sample Temperature Scan

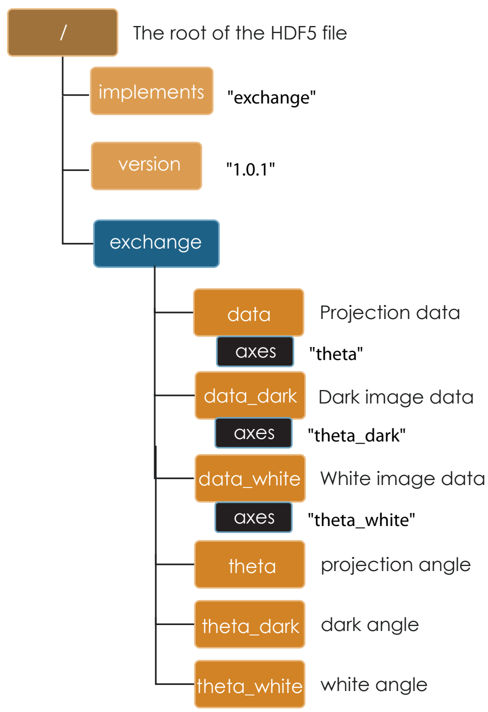

Figure 4: Diagram of a minimal Data Exchange file for a single tomographic data set including raw projections, dark and white fields. In this case the attribute `axes` indicates the presence of theta vectors containing the positions of the rotation axis for each projection, dark and white images.

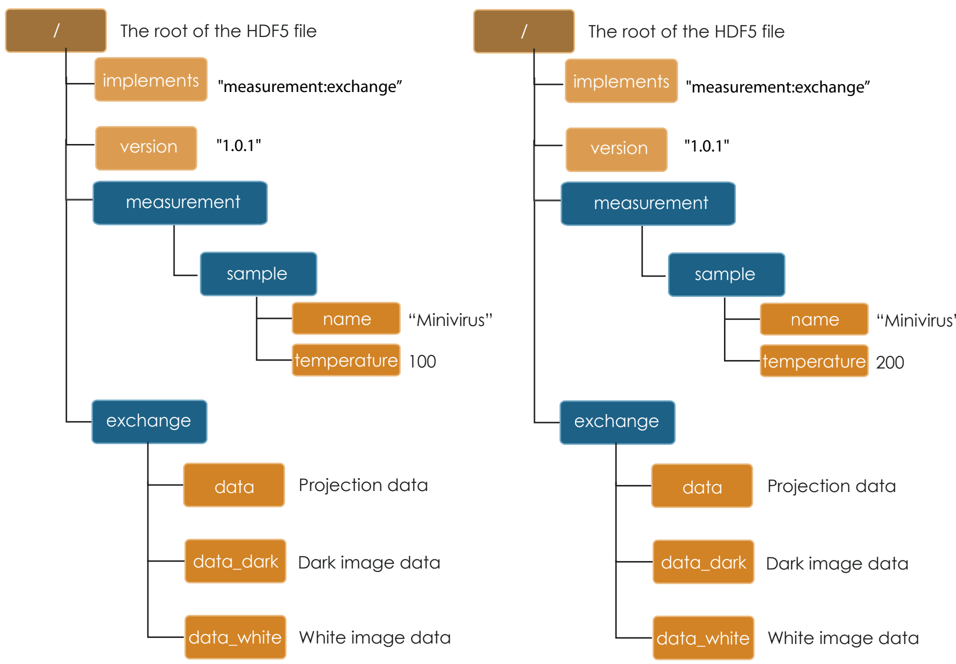

Figure 5: Diagram of two tomographic data sets taken at two different sample temperatures (100 and 200 K). To store the temperature in °C is necessary to add the attribute `units = "celsius"` to the `temperature` tag.

3.5.2 X-ray Energy Scan

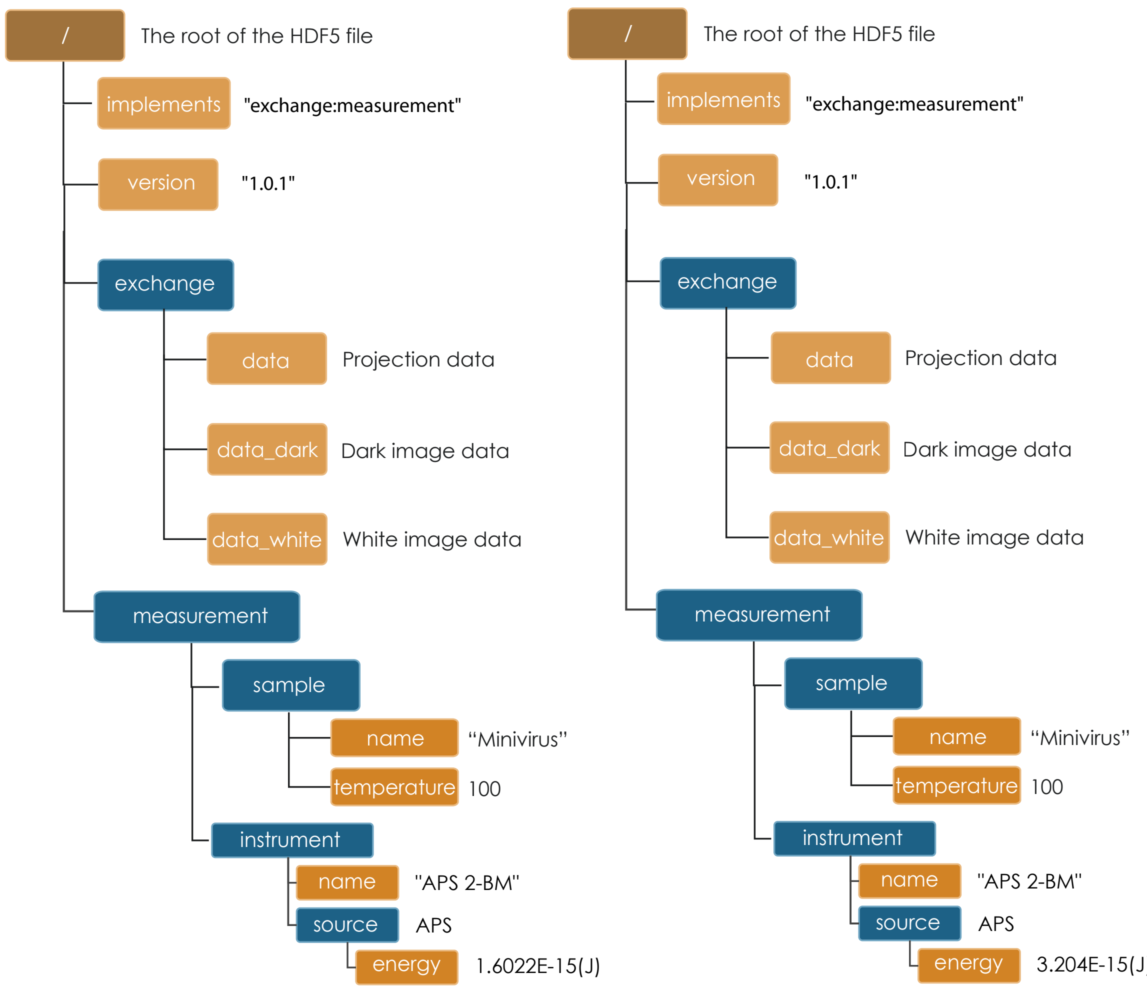

Figure 6: Diagram of two tomographic data sets taken at two different energy (10 and 20 keV). To store the temperature in keV is necessary to add the attribute `units = "keV"` to the `energy` tag.

3.5.3 Detector-sample Distance Scan

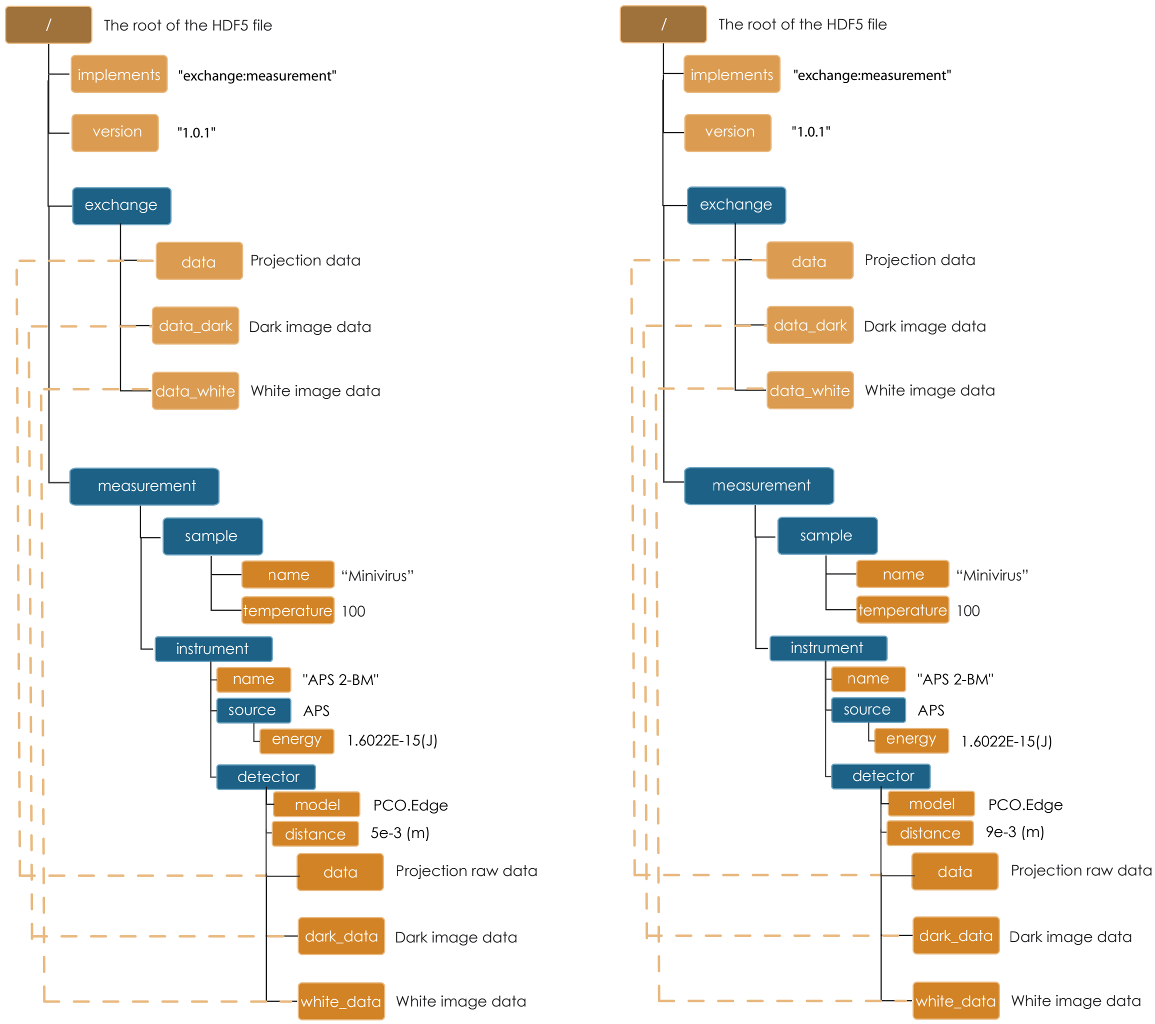

Figure 7: Diagram of two tomographic data sets collected with two different detector-sample distances (5 and 9 mm).

3.5.4 Series of Tomographic Measurements

A series of tomographic measurements, when relevant, can be stored in the same 2FXi file appending $\_N$ to the measurement tag. For example in nano tomography experiments the detector field of view is often smaller than the sample. To collect a complete tomographic data set is necessary to raster the sample across the field of view moving its x and y location. Figure 8 shows a 2FXi file from a nano tomography experiment when the sample rasters through the filed of view. The details of how the *exchange* arrays for a raster nano tomography scan are generated will be discussed in more details in Section 4.4.

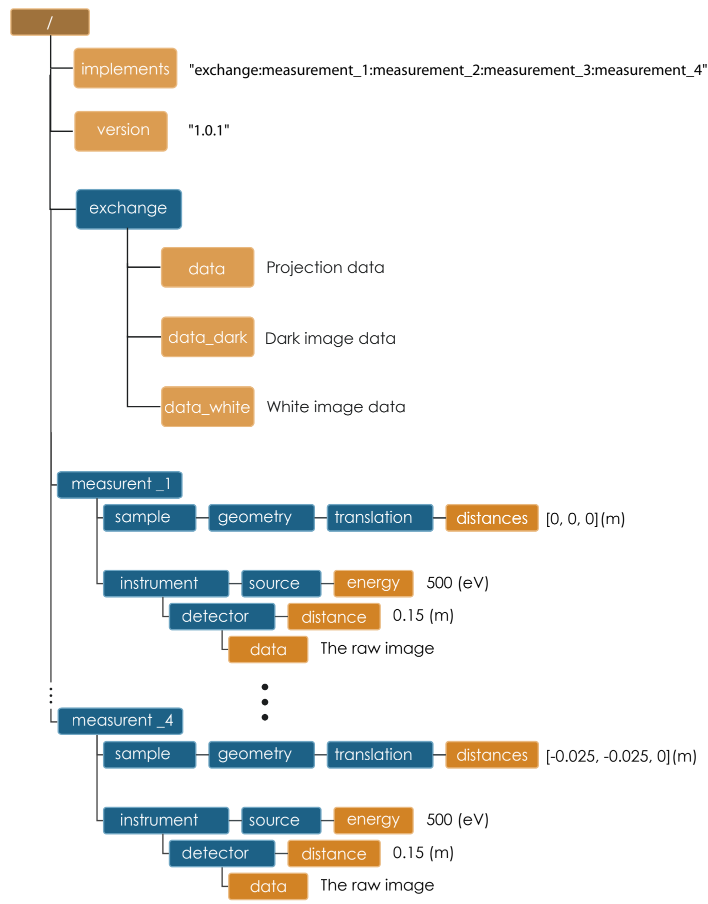

Figure 8: Diagram of a 2FXi file with 4 tomographic data sets from a nano tomography experiment.

4 Data Exchange Entries - Core Reference

4.1 Top level (root)

This node represents the top level of the HDF5 file and holds some general information about the file.

Table 3: Data Exchange top level entries

Member	Type	Example
implements	string	"exchange:measurement:provenance"
version	string	"1.0.1"
exchange_N	Exchange group	
measurement_N	Measurement group	
provenance	Provenance group	

implements - A colon separated list that shows which components are present in the file. The only *mandatory* component is *exchange*. A more general Data Exchange file also contains measurement and provenance information, if so these will be declared in implements as "exchange:measurement:provenance"

version - Data Exchange format version.

exchange_N - The data taken from measurements or processing.

measurement_N - Each measurement made on the sample.

provenance - The Provenance class describes all process steps that have been applied to the data.

4.2 Exchange Group

This class is a general placeholder for the most important information in a Data Exchange file and contains one or more arrays representing the most basic version of the data.

4.2.1 3D array data attributes

Table 4: data attributes

Member	Type	Example
description	string	"transmission"
units	string	"counts"
axes	string	"theta:y:x"

Table 5: x, y, theta, theta_dark, theta_white attribute

Member	Type	Example
units	string	"μm", "degree"

4.3 Measurement

This class holds sample and instrument information.

Table 6: Data Exchange top level entries

Member	Type	Example
sample	Sample class	
instrument	Instrument class	

sample - The sample measured.

instrument - The instrument used to collect this data.

4.3.1 Sample

This class holds basic information about the sample, its geometry, properties, the sample owner (user) and sample proposal information.

Table 7: Sample class members

Member	Type	Example
name	string	"cells sample 1"
description	string	"malaria cells"
preparation_date	string ISO 8601	"2011 07 15T15 10Z"
chemical_formula	string abbr. CIF format	"(Cd 2+)3, 2(H2 O)"
mass	float	0.25
concentration	float	0.4
environment	string	"air"
temperature	float	25.4
temperature_set	float	26.0
pressure	float	101325
thickness	float	0.001
position	string	"2D" APS robot coord.
geometry	Geometry group	
ids	Experiment identifier group	
experimenter	Experimenter identifier group	

name - Descriptive name of the sample.

description - Description of the sample.

preparation_date - Date and time the sample was prepared.

chemical_formula - Sample chemical formula using the CIF format.

mass - Mass of the sample.

concentration - Mass/volume.

environment - Sample environment.

temperature - Sample temperature.

temperature_set - Sample temperature set point.

pressure - Sample pressure.

thickness - Sample thickness.

position - Sample position in the sample changer/robot.

geometry - Sample center of mass position and orientation.

ids - Facility experiment identifiers.

experimenter - Experimenter identifiers.

4.3.1.1 Geometry

This class holds the general position and orientation of a component.

Table 8: Geometry class members

Member	Type	Quantity
translation	Translation class	
orientation	Orientation class	

orientation - The rotation of the object with respect to the coordinate system.

translation - The position of the object with respect to the origin.

Only one orientation and one translation is permitted in each geometry class.

The position of the origin of the object should be explicitly defined for each object. If it is not defined it should be assumed to be the center of the object.

4.3.1.1.1 Translation

This is the description for the general spatial location of a component - it is used by the Geometry class

Table 9: Translation class members

Member	Type	Example
distances	3 floats	0, 0.001, 0

distances - The x, y and z components of the translation of the origin of the object relative to the origin of the global coordinate system (the place where the X-ray beam meets the sample when the sample is first aligned in the beam). If distances does not have the attribute units set then the units are in meters (see table 22)

4.3.1.1.2 Orientation

This is the description for a general orientation of a component - it is used by the Geometry class.

Table 10: Orientation class members

Member	Type	Quantity
value	6 floats	unitless

value - Dot products between the local and the global unit vectors.

The orientation information is stored as direction cosines. The direction cosines will be between the local coordinate directions and the global coordinate directions. The unit vectors in both the local and global coordinates are right-handed and orthonormal.

Calling the local unit vectors (x', y', z') and the reference unit vectors (x, y, z) the six numbers will be $[x' \cdot x, x' \cdot y, x' \cdot z, y' \cdot x, y' \cdot y, y' \cdot z]$ where "$\cdot$" is the scalar dot product (cosine of the angle between the unit vectors).

Notice that this corresponds to the first two rows of the rotation matrix that transforms from the global orientation to the local orientation. The third row can be recovered by using the fact that the basis vectors are orthonormal.

Table 11: Experiment identifier class

Member	Type	Example
proposal	string	"1234"
activity	string	"9876"
safety	string	"9876"

4.3.1.2 Experiment identifier

proposal - Proposal reference number. For the APS this is the General User Proposal number.

activity - Proposal scheduler id. For the APS this is the beamline scheduler activity id.

safety - Safety reference document. For the APS this is the Experiment Safety Approval Form number.

Table 12: Experimenter identifier class

Member	Type	Example
name	string	"John Doe"
role	string	"Project PI"
affiliation	string	"University of California, Berkeley"
address	string	"EPS UC Berkeley CA 94720 4767 USA"
phone	string	"+1 123 456 0000"
email	string	"johndoe@berkeley.edu"
facility_user_id	string	"a123456"

4.3.1.3 Experimenter identifier

name - User name.

role - User role.

affiliation - User affiliation.

address - User address.

phone - User phone number.

email - User e-mail address

facility_user_id - User badge number

4.3.2 Instrument

The instrument group stores all relevant beamline components status at the beginning of the tomographic measurement.

Table 13: Instrument group members

Member	Type	Example
name	string	"XSD/2-BM"
source	Source group	
shutter_N	Shutter group	
attenuator_N	Attenuator group	
monochromator	Monochromator group	
interferometer	Interferometer group	
detector_N	Detector group	
sample_stack	Sample Stack group	
acquisition	Acquisition group	

name - Name of the instrument.

source - The source used by the instrument.

shutter_N - The shutter(s) used by the instrument.

attenuator_N - The attenuators that are part of the instrument.

monochromator - The monochromator used by the instrument.

detector_N - The detectors that compose the instrument.

4.3.2.1 Source

Class describing the light source being used.

Table 14: Source class members

Member	Type	Example
name	string	"APS"
datetime		
beamline	string	"2-BM"
distance	float	-48.5
current	float	0.094
energy	float	4.807e-15
pulse_energy	float	1.602e-15
pulse_width	float	15e-11
mode	string	"TOPUP"
beam_intensity_incident	float	55.93
beam_intensity_transmitted	float	100.0

name - Name of the facility.

datetime - Date and time source was measured.

beamline - Name of the beamline.

distance - The source distance (m) from the sample.

current - Electron beam current (A).

energy - Characteristic photon energy of the source (J). For an APS bending magnet this is 30 keV or 4.807e-15 J.

pulse_energy - Sum of the energy of all the photons in the pulse (J).

pulse_width - Duration of the pulse (s).

source - Beam mode: TOPUP.

beam_intensity_incident - Incident beam intensity in (photons per s).

beam_intensity_transmitted - Transmitted beam intensity (photons per s).

4.3.2.2 Shutter

Class describing the light source being used.

Table 15: Source class members

Member	Type	Example
name	string	"Front End Shutter 1"
distance	float	-48.5
status	string	"OPEN"

name - Shutter name.

distance - Shutter distance (m) from the sample.

status - "OPEN" or "CLOSED" or "NORMAL"

4.3.2.3 Attenuator

This class describes a beamline attenuator(s) used during data collection. If more than one attenuators are used they will be named as attenuator_1, attenuator_2 etc.

Table 16: Attenuator class members

Member	Type	Example
distance	float	-35.7
thickness	float	1e-3
attenuator_transmission	float	unit-less
type	string	Al

distance - The Attenuator distance (m) from the sample. Negative distances represent beamline components that are before the sample while positive distances represent components that are after the sample. In this case the filter is located 35.7 m upstream of the sample.

thickness - Thickness of attenuator along beam direction.

attenuator_transmission - The nominal amount of the beam that gets through (transmitted intensity)/(incident intensity).

type - Type or composition of attenuator.

4.3.2.4 Monochromator

Define a monochromator used in the instrument.

type - Multilayer type.

Table 17: Monochromator class members

Member	Type	Example
type	string	"Multilayer"
energy	float	1.602e-15
energy_error	float	1.602e-17
mono_stripe	string	"Ru/C"

energy - Peak of the spectrum that the monochromator selects. Since units is not defined this field is in J and corresponds to 10 keV.

energy_error - Standard deviation of the spectrum that the monochromator selects. Since units is not defined this field is in J.

mono_stripe - Type of multilayer coating or crystal.

4.3.2.5 Detector This class holds information about the detector used during the experiment. If more than one detector are used they will be all listed as detector_N. In x-ray fluorescence ....

Table 18: X-ray fluorescence detector class members

Member	Type	Example
manufacturer	string	"CooKe Corporation"
model	string	"pco dimax"
serial_number	string	"1234XW2"

manufacturer - The detector manufacturer.

model - The detector model.

serial_number - The detector serial number .

4.4 Provenance

The documentation of all transformations, analyses and interpretations of data is called data provenance. Maintaining this history allows for reproducible data. The Data Exchange format tracks provenance using the Provenance class. The index value attached to the process class denotes the execution order of the processes. The Process class uses references to other classes that describe the analysis in detail. The Provenance class describes all process steps that have been applied to the data.

Table 19: Provenance class members

Member	Type	Example
process_N	Process class	

process_N - A process applied to the data.

4.4.1 Process

The process class holds basic information about a process. It is a generic container for recording the status of a process, and maintaining references to detailed process information.

Table 20: Process class members

Member	Type	Example
status	string	"SUCCESS"
reference	string	"/reconstruction"
message	string	"Full reconstruction."

status - Current process status. May be one of the following: QUEUED, RUNNING, FAILED, or SUCCESS.

reference - Path to a process description group. The process description group contains all metadata to perform or run the specific process.

message - A process specific message generated by the process. It may be a confirmation that the process was successful, or a detailed error message, for example.

Table 21: Process class examples

process_1		
	status	"SUCCESS"
	reference	"/sinogram"
	message	"modify axes from "theta:y:x" to "y:theta:x"
process_2		
	status	"SUCCESS"
	reference	"/ring_removal"
	message	"RIng removal algorithm."
process_3		
	status	"SUCCESS"
	reference	"/reconstruction"
	message	"Full reconstruction."
process_4		
	status	"RUNNING"
	reference	"/gridftp"
	message	"cluster to remote user data transfer"
process_5		
	status	"RUNNING"
	reference	"/export"
	message	"reconstructed data conversion"

4.4.2 Process description

The process description group defined in the reference tag in each process steps contains all parameters, including input and output datasets to execute a specific process steps and it should be placed at the root of the HDF5 file.

5 Code examples

All the code examples as well as the resulting Data Exchange files are available from http://www.aps.anl.gov/DataExchange/.

5.1 Creating a minimal Data Exchange file

Include code here

The resulting file should be equivalent to the one in Fig. 2.

5.2 Creating a minimal Data Exchange file for tomography

Include code here

The resulting file should be equivalent to the one in Fig. 4.

5.3 Creating a typical Data Exchange file for tomography

Include code here

The resulting file should be equivalent to the one in Fig. 5.

A Appendix

A.1 Default units for Data Exchange entries

The default units for Data Exchange entries follow the CXI entries definition, i.e. are SI based units (see table 22) unless the ”units” attribute is specified. Data Exchange prefers not to use ”units” and use the default SI based units whenever possible.

Table 22: SI (and common derived) base units for different quantities

Quantity	Units	Abbreviation
length	meter	m
mass	kilogram	kg
time	second	s
electric current	ampere	A
temperature	kelvin	K
amount of substance	mole	mol
luminous intensity	candela	cd
frequency	hertz	Hz
force	newton	N
pressure	pascal	Pa
energy	joule	J
power	watt	W
electric potential	volt	V
capacitance	farad	F
electric resistance	ohm	Ω
absorbed dose	gray	Gy
area	square meter	m^2
volume	cubic meter	m^3

A.1.1 Angles

Angles are always defined in degrees *not* in radians.

A.1.2 Dates

Dates are always specified according to the ISO 8601. This means for example “1996-07-31T21:15:22+0600”. Note the “T” separating the data from the time and the “+0600” timezone specification.

A.2 Geometry

A.2.1 Coordinate System

The Data Exchange uses the same CXI coordinate system. This is a right handed system with the z axis parallel to the X-ray beam, with the positive z direction pointing away from the light source, in the downstream direction. The y axis is vertical with the positive direction pointing up, while the x axis is horizontal completing the right handed system (see Fig. 9). The origin of the coordinate system is defined by the point where the X-ray beam meets the sample.

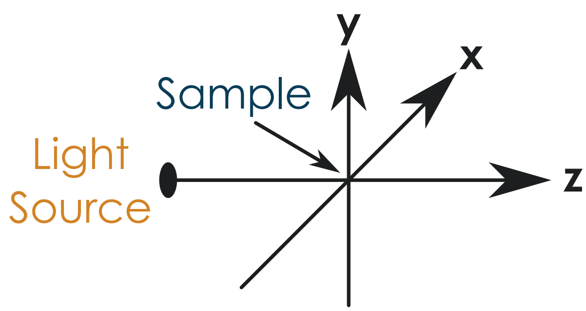

Figure 9: The coordinate system used by CXI. The intersection of the X-ray beam with the sample define the origin of the system. The z axis is parallel to the beam and points downstream.

A.2.2 The local coordinate system of objects

For many detectors their location and orientation is crucial to interpret results. Translations and rotations are used to define the absolute position of each object. But to be able to apply these transformations we need to know what is the origin of the local coordinate system of each object. Unless otherwise specified the origin should be assumed to be the geometrical center of the object in question. The default orientation of the object should have the longest axis of the object aligned with the x axis, the second longest with the y axis and the shortest with the z axis.