The Scientific Data Exchange Introductory Guide

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

Version 0.0.13

April 11, 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 2.3, **??**, **??**, **??**, **??**, 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). Other edits.

Contents

1 Introduction

This document is a guide to the basic design principles and core guidelines for the Data Exchange file format. Briefly, Data Exchange is a set of guidelines for storing scientific data and metadata in a Hierarchical Data Format 5 (HDF5) file (http://www.hdfgroup.org/HDF5). The design guidelines for Data Exchange provide a starting point to which one may add custom data and metadata to solve particular problems.

This reference guide describes the basic design principles, examples of their application, a core reference for guidelines common to most uses, and coding examples.

2 The Design of Data Exchange

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 a similar diagram definition set by Filipe R. N. C. Maia in "CXI file format" (http://cxidb.org/cxi.html), with a few minor modifications for Data Exchange definitions.

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 sufficient to share a multidimensional data array. In this simplest form, 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 the Data Exchange format. Data Exchange, like CXI, is not a completely new file format, but simply a set of rules designed to create HDF5 files with a common structure 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.

2.2 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.

2.3 Root Level Structure

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 structure of a Data Exchange file is shown in table 2. The most basic file must have an "implements" string, and an "exchange" group at the root level/group of the HDF5 file. Optional "measurement" and "provenance" groups are also defined. Beyond this, additional groups may be added to meet individual needs, with guidelines suggesting the best structure.

implements

Mandatory scalar string dataset in the root of the HDF5 file whose value is a colon separated list that shows which components are present in the file. All components listed in the *implements* string are to be groups placed in the HDF5 file at the root level/group.

Table 2: Data Exchange Top Level Members

Member	Type	Example
implements	string dataset	"exchange:measurement:provenance"
exchange	group	
`measurement`	group	
`provenance`	group	

In a minimal Data Exchange file, the only mandatory item in this list is *exchange*. A more general Data Exchange file also contain `measurement` and possibly `provenance`, in which case the implements string would be: "*exchange*: `measurement`: `provenance`"

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 core dataset or derived datasets are saved in the file. The *exchange* implementation for specific techniques are defined in separate sections in the Reference Guide.

`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 dataset 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.

The detailed rules about how to store datasets within the exchange group are best shown through examples in the next section. Detailed reference information can be found in the Data Exchange Core Reference section.

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

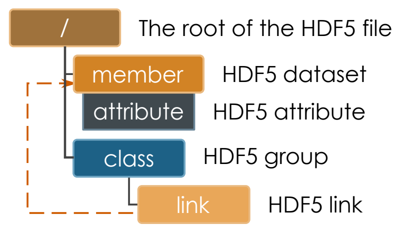

Figure 1: Explanation of the color code used in the diagrams

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 2.3, 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.

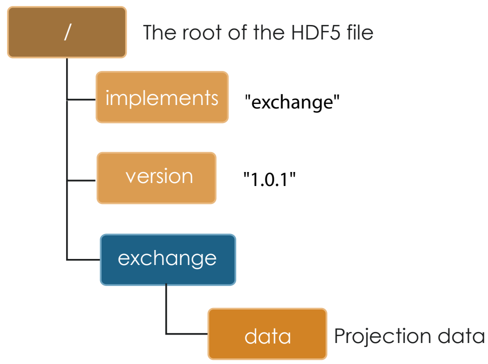

Figure 2: Diagram of a minimal Data Exchange file for a single image.

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 **??**) ”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.

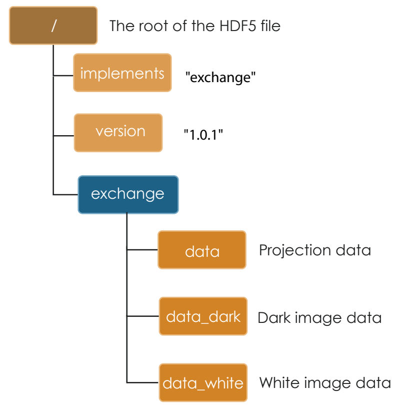

Figure 3: Diagram of a minimal Data Exchange file for a single tomographic data set including raw projections, dark and white fields. Since the positions of the rotation axis for each projection, dark and white images are not specified is assumed that the raw projections are taken at equally spaced angular 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

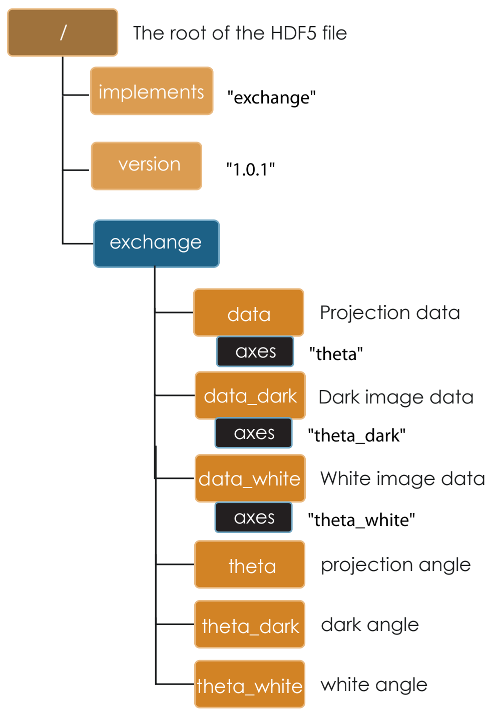

Figure 4: Diagram of a minimal Data Exchange file for a single tomographic data set including raw projections, dark and white fields. In this case the attribute `axes` indicates the presence of theta vectors containing the positions of the rotation axis for each projection, dark and white images.

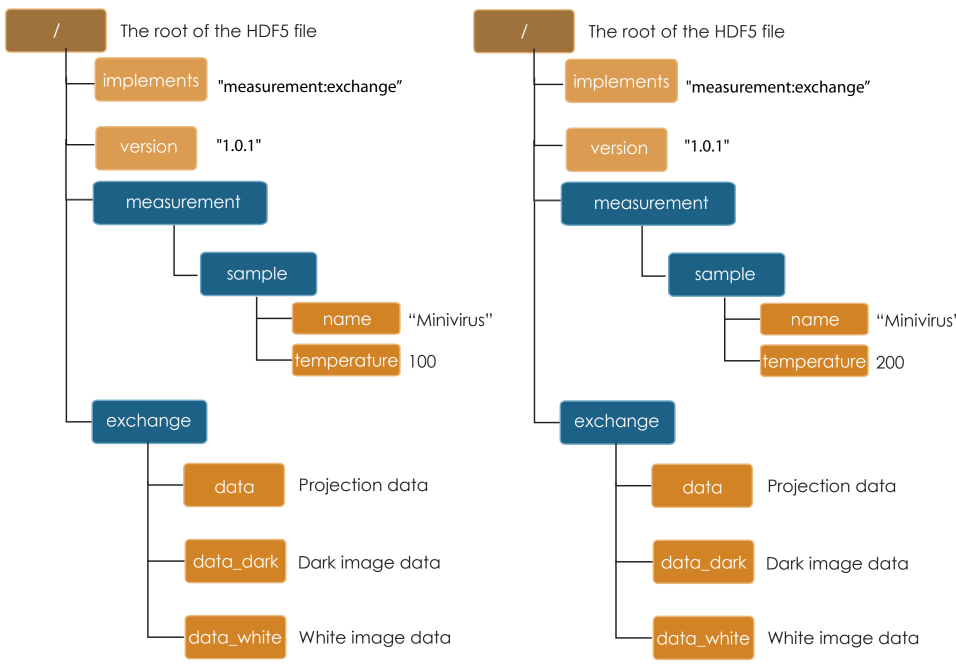

Figure 5: Diagram of two tomographic data sets taken at two different sample temperatures (100 and 200 K). To store the temperature in °C is necessary to add the attribute `units = "celsius"` to the `temperature` tag.

3.5.2 X-ray Energy Scan

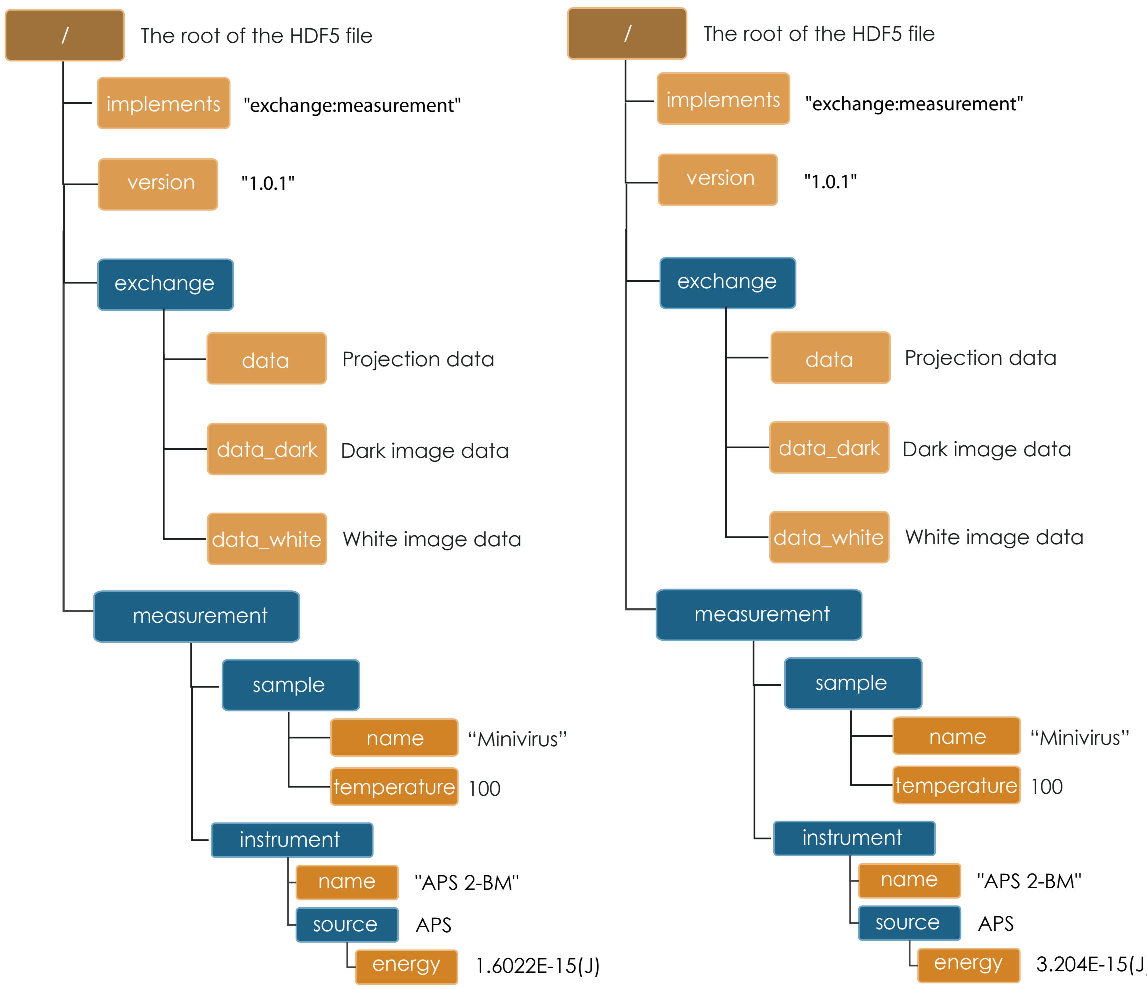

Figure 6: Diagram of two tomographic data sets taken at two different energy (10 and 20 keV). To store the temperature in keV is necessary to add the attribute `units` = `"keV"` to the `energy` tag.

3.5.3 Detector-sample Distance Scan

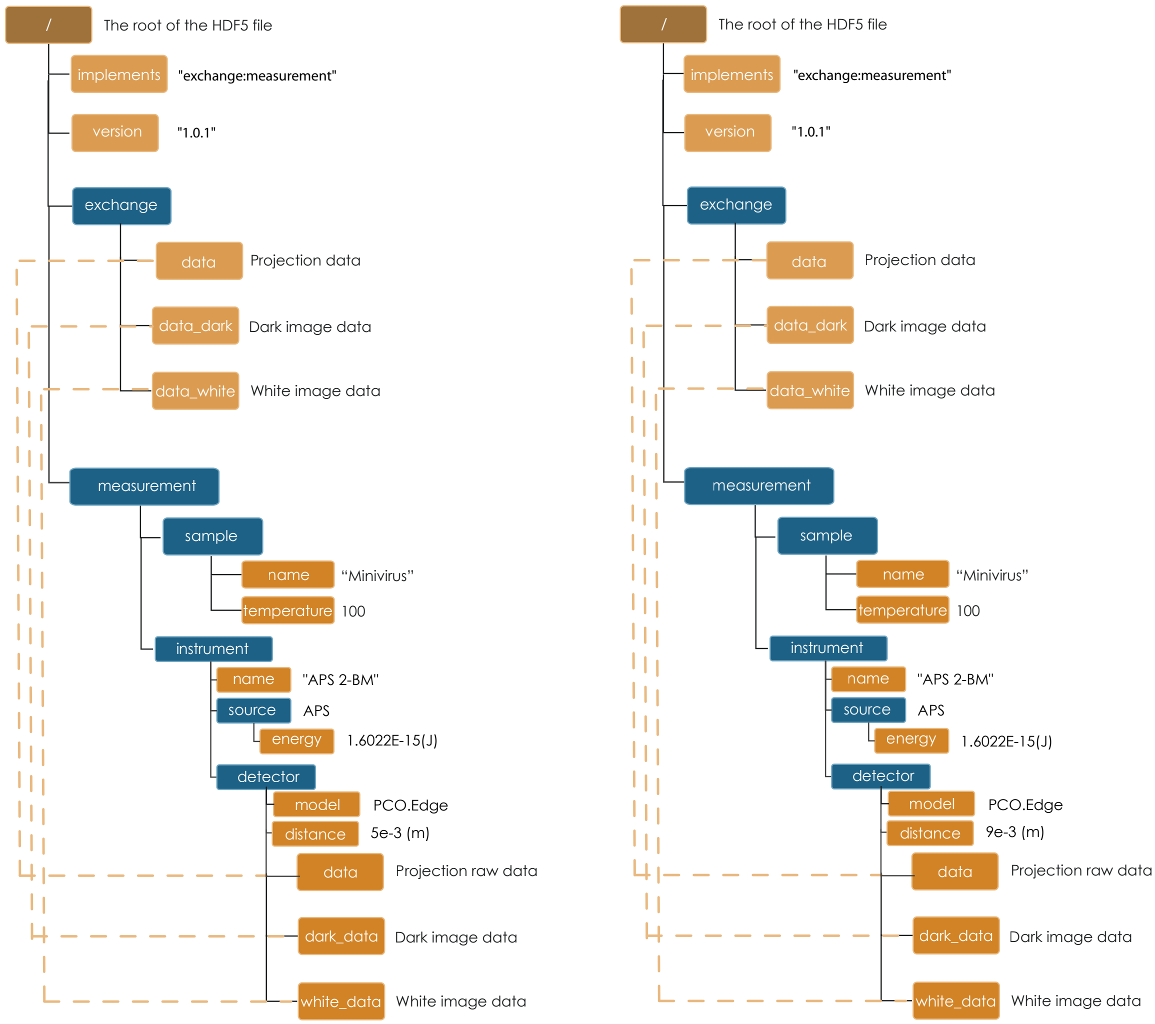

Figure 7: Diagram of two tomographic data sets collected with two different detector-sample distances (5 and 9 mm).

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.

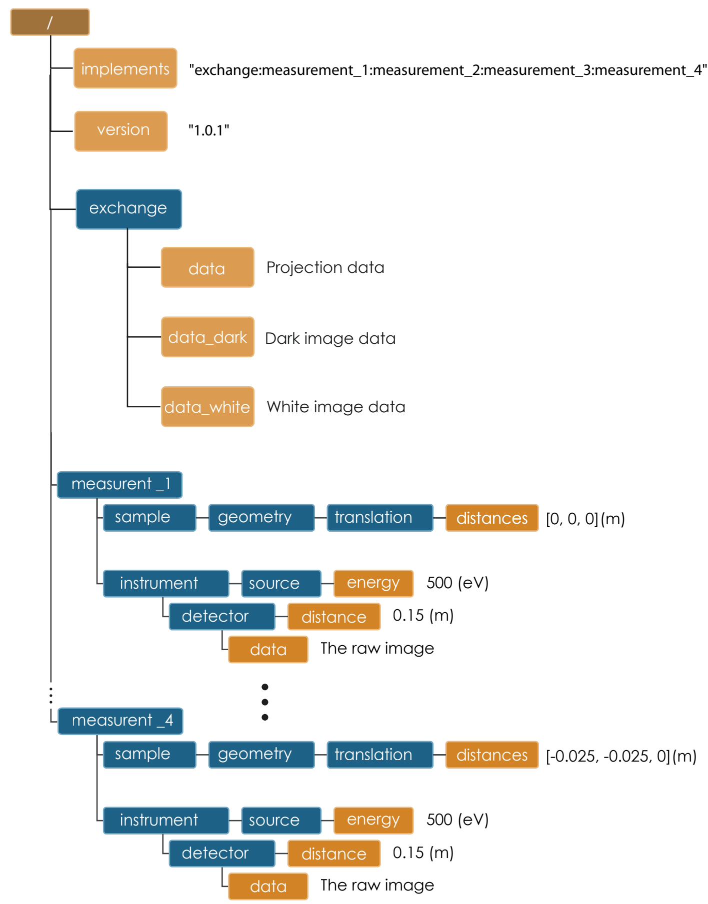

Figure 8: Diagram of a 2FXi file with 4 tomographic data sets from a nano tomography experiment.

4 Data Exchange 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: Top Level Members

Member	Type	Example
implements	string dataset	"exchange:measurement:provenance"
exchange_N	group	
`measurement_N`	group	
`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"

exchange_N

The data taken from measurements or processing.

`measurement_N`

Each measurement made on the sample.

`provenance`

The Provenance group describes all process steps that have been applied to the data.

4.2 Exchange Group

The exchange group is where scientific datasets reside. This group contains one or more array datasets containing n-dimensional data and optional descriptions of the axes (dimension scale datasets). Exactly how this group is used is dependent on the application, however the general idea is that one exchange group contains one cohesive dataset. If, for example, the dataset is processed into some other form, then another exchange group is used to store the derived data.

Multiple exchange groups are numbered consecutively as exchange_N. At a minimum, each exchange group should have a primary dataset named data. The title is optional.

Table 4: Exchange Group Members

Member	Type	Example
`title`	string dataset	"tomography projections"
data	array dataset	n-dimensional dataset

title

Descriptive title for data dataset.

data

The primary scientific dataset. Additional related datasets may have any arbitrary name. Each dataset may have description, units, and axes attributes.

Table 5: data attributes

Attribute	Type	Example
`description`	string attribute	"transmission"
`units`	string attribute	"counts"
`axes`	string attribute	"theta:y:x"

4.3 Measurement

This group holds sample and instrument information.

Table 6: Measurement Group Members

Member	Type	Example
sample	group	
instrument	group	

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 Group Members

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

experiment
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 Group Members

Member	Type	Example
translation	group	
orientation	group	

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 Group Members

Member	Type	Example
distances	3 float array dataset	(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 45)

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 Group Members

Member	Type	Example
value	6 float array dataset	

value

Dot products between the local and the global unit vectors. Unitless

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.

4.3.1.2 Experiment

This provides references to facility ids for the proposal, scheduled activity, and safety form.

Table 11: Experiment Group Members

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

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.

4.3.1.3 Experimenter Description of a single experimenter. Multiple experimenters can be represented through numbered entries such as experimenter_1, experimenter_2.

Table 12: Experimenter Group Members

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

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 a measurement.

Table 13: Instrument Group Members

Member	Type	Example
name	string dataset	"XSD/2-BM"
source	group	
shutter_N	group	
attenuator_N	group	
monochromator	group	
interferometer	group	
detector_N	group	
sample_stack	group	
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 Group Members

Member	Type	Example
name	string dataset	"APS"
datetime	string dataset (ISO 8601)	"2011-07-15T15:10Z"
beamline	string dataset	"2-BM"
distance	float dataset	-48.5
current	float dataset	0.094
energy	float dataset	4.807e-15
pulse_energy	float dataset	1.602e-15
pulse_width	float dataset	15e-11
mode	string dataset	"TOPUP"
beam_intensity_incident	float dataset	55.93
beam_intensity_transmitted	float dataset	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 shutter being used.

Table 15: Shutter Group Members

Member	Type	Example
name	string dataset	"Front End Shutter 1"
distance	float dataset	-48.5
status	string dataset	"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 the 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 Group Members

Member	Type	Example
distance	float dataset	-35.7
thickness	float dataset	1e-3
attenuator_transmission	float dataset	unit-less
type	string dataset	"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 the monochromator used in the instrument.

Table 17: Monochromator Group Members

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

type

Multilayer type.

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.

Table 18: Detector Group Members

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

manufacturer
The detector manufacturer.

model
The detector model.

serial_number
The detector serial number .

4.4 Provenance

Data provenance is the documentation of all transformations, analyses and interpretations of data. Maintaining this history allows for reproducible data. The Data Exchange format permits tracking provenance using a combination of this Provenance group plus input/output datasets in the technique specific groups. Scientific users will not generally be expected to maintain data in this group. The expectation is that analysis pipeline tools will automatically record process steps using this group. In addition, it is possible to re-run an analysis using the information provided here.

The provenance group tracks the execution order of a series of processes using numbered process groups. Each process group uses references to other groups that describe the analysis in detail. Each process group represents the status of the process and some kind of informative summary message.

Table 19: Provenance Group Members

Member	Type	Example
process_N	group	

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, scientific domain-specific information.

Table 20: Process class members

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

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 the specific process. This reference is simply the HDF5 path within this file of the technique specific process description group. The process description group should contain all parameters necessary to run the process, including the name and version of any external analysis tool used to process the data. It should also contain input and output references that point to the exchange_N groups that contain the input and output datasets of the 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: Provenance Group Example

process_1		
	status	"SUCCESS"
	reference	"/gridftp"
	message	"detector controller to cluster data transfer"
process_2		
	status	"SUCCESS"
	reference	"/sinogram"
	message	"modified axes from "theta:y:x" to "y:theta:x"
process_3		
	status	"SUCCESS"
	reference	"/ring_removal"
	message	"ring removal algorithm complete"
process_4		
	status	"SUCCESS"
	reference	"/reconstruction"
	message	"Full reconstruction complete."
process_5		
	status	"RUNNING"
	reference	"/export"
	message	"converting reconstructed data to tiff"

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.

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 45) 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.

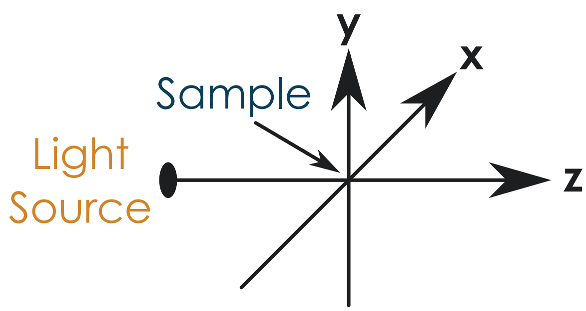

Figure 9: The coordinate system used by CXI. The intersection of the X-ray beam with the sample define the origin of the system. The z axis is parallel to the beam and points downstream.

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.