FERMI Data Analysis

Simon Schreck

January 2018

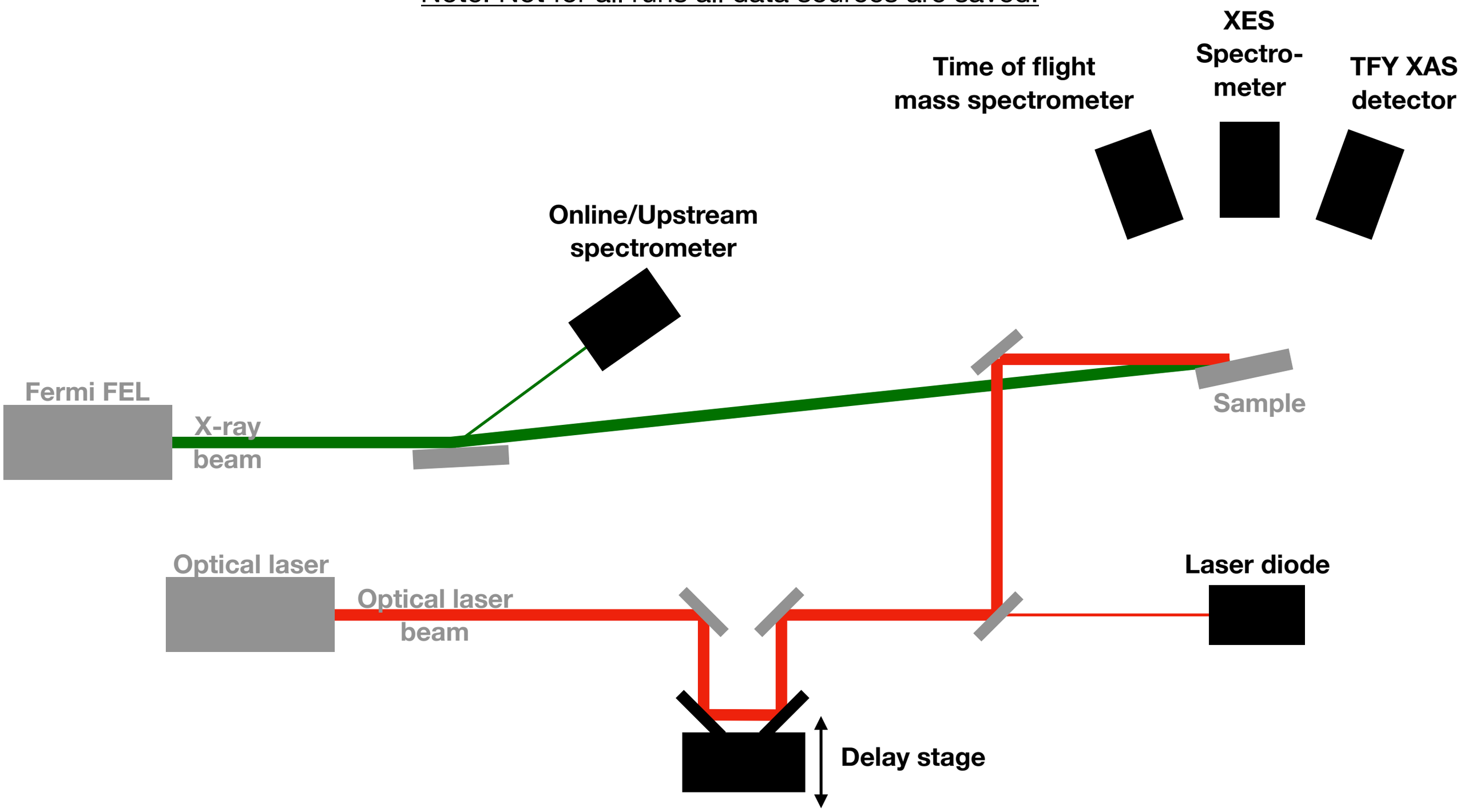
Stockholm University
Department of Physics, Chemical Physics Division

Content

- Experiment Overview
- Data acquisition and data structure
- Data sources
- Data reduction
  - Data collection
- To come… Data Binning

Experiment Overview

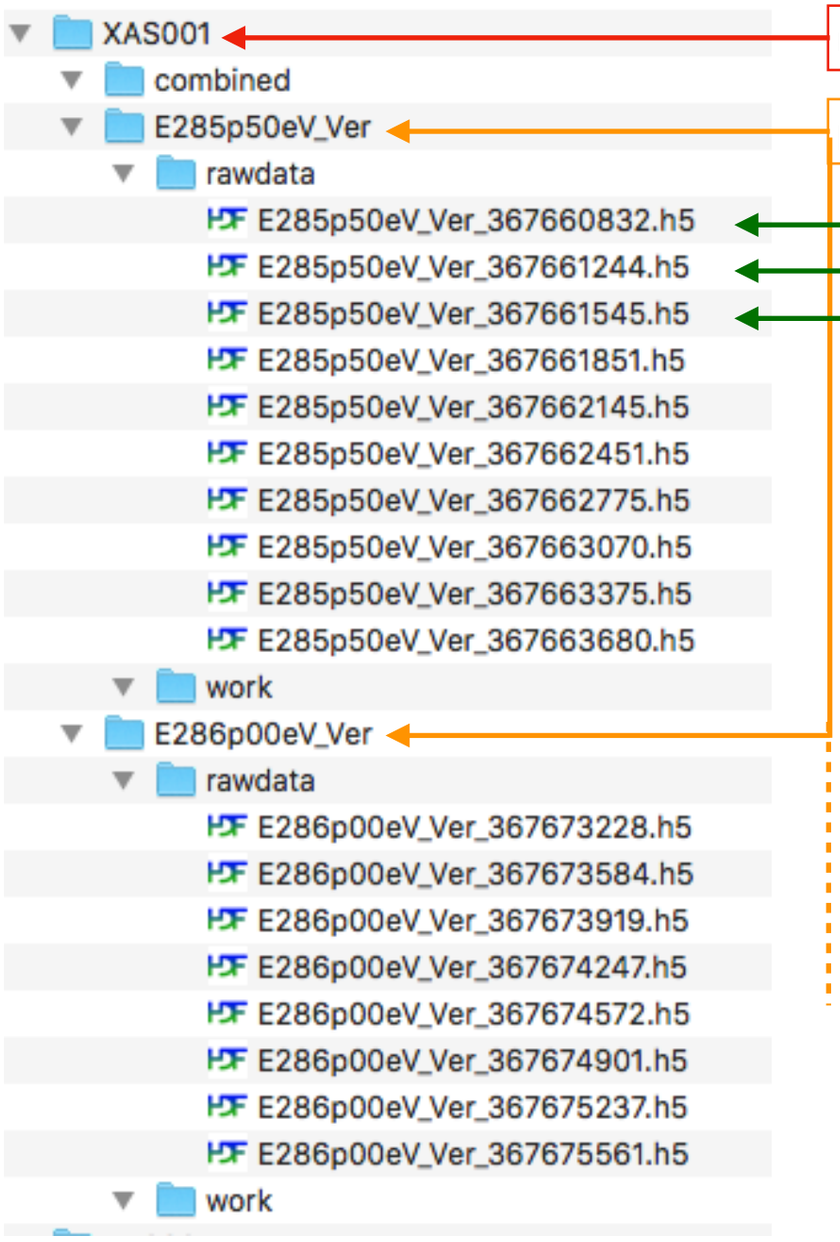
Each black box in the diagram represents a data source that is described in more detail on the following pages.
All data sources are read out shot-to-shot.
Note: Not for all runs all data sources are saved!



Data Acquisition and Folder Structure

For XAS Runs

For one XAS run (e.g. ’XAS001’) we recorded several FEL photon energies and for each FEL photon energy several delays. For each delay we recorded a number of shots - typically a few 100.
This resulted in the following folder structure for the raw data:



run folder

photon energy folders One folder for each energy measured

delay files One file for each delay measured

Each delay file contains the data for all shots recorded at this delay.
See details on the next slide.

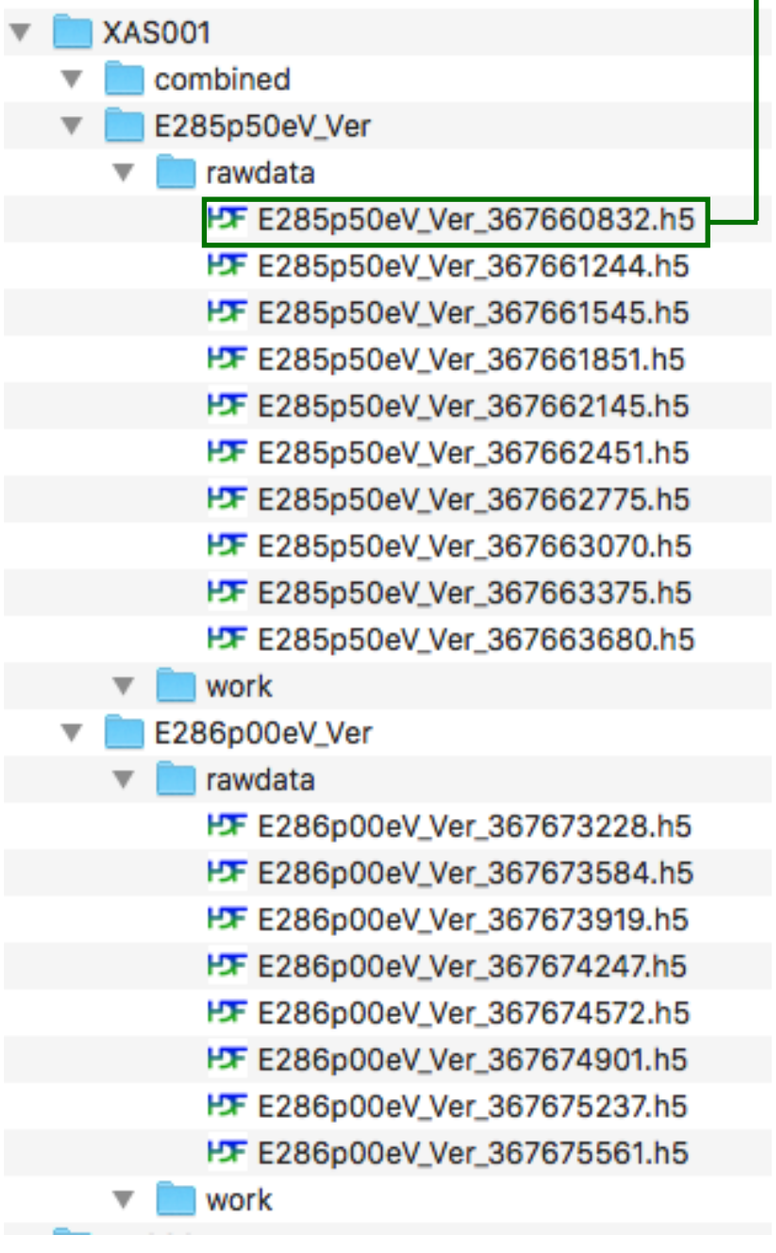
Notes:

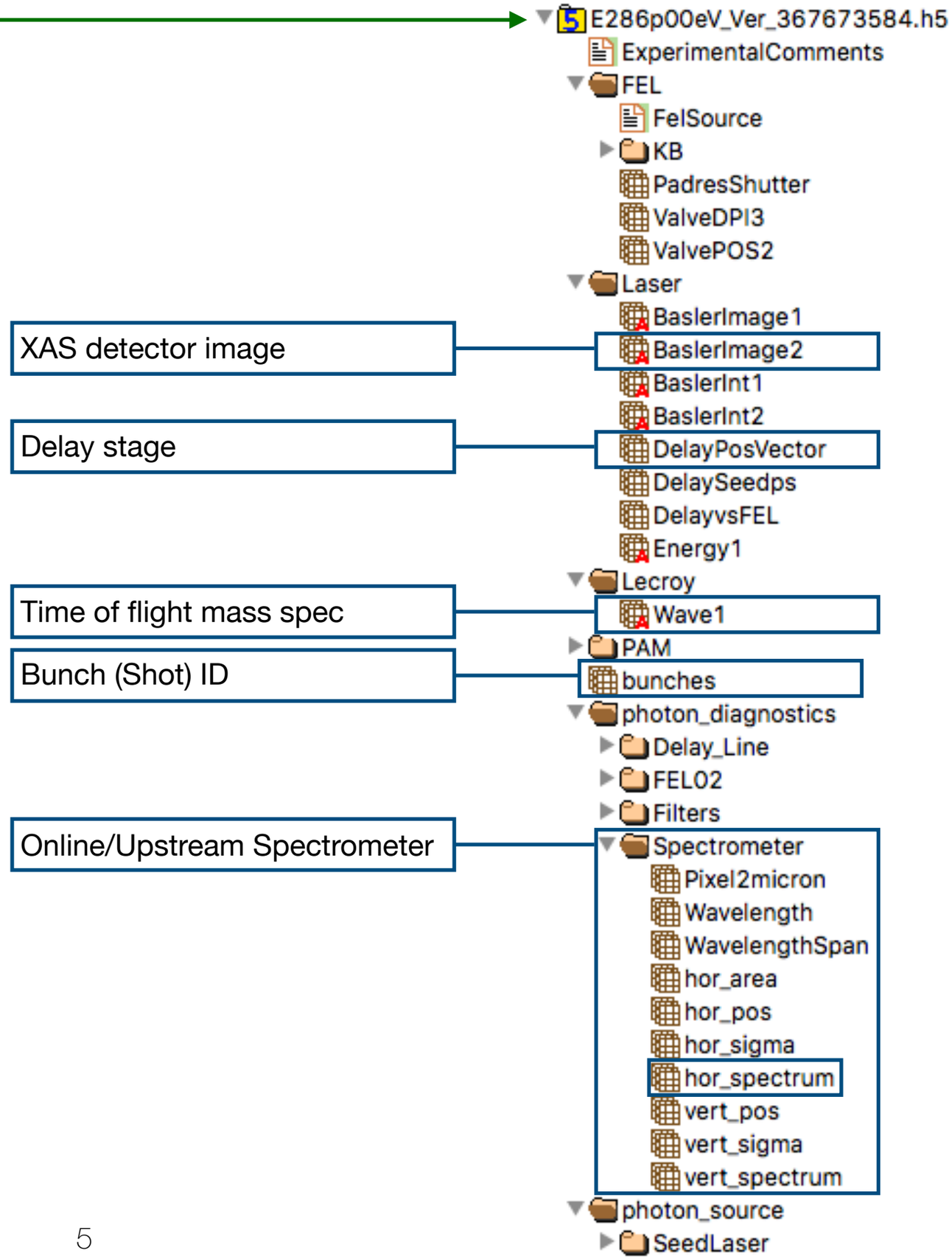
- For NoPump runs (runs without the optical laser, e.g. ’XAS005_NoPump) there is only one delay file per photon energy folder.
- The folders ’combined’ and ’work’ are empty.
- The folder ’combined’ is later used to save the reduced (combined) data.
- The folder ’work’ will be unused.

Delay File Structure (HDF5)

Raw data file

The delay files are in HDF5 format. Each delay file contains many variables of different format. Only a few of them are of interested for us. A few examples on the right.





Online/Upstream Spectrometer

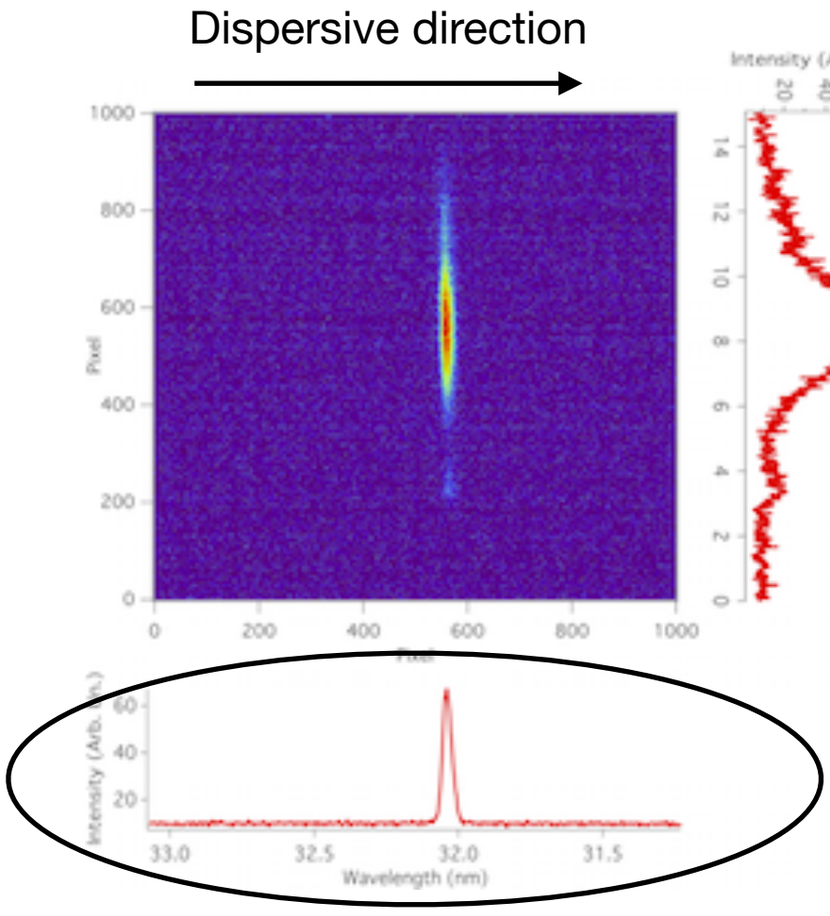
The **online/upstream spectrometer** is a CCD camera that sees a small fraction of the incident x-ray beam, which is diffracted (energy dispersed) onto the camera.

We use only the projection onto the dispersive direction, which is called ‚hor_spectrum‘ and saved under:

/photon_diagnostics/Spectrometer/hor_spectrum

From ‚hor_spectrum‘ we extract:

- Incident intensity (I0) = area under peak
- Incident photon energy = peak position
- Bandwidth of incident photon energy = peak width



hor_spectrum

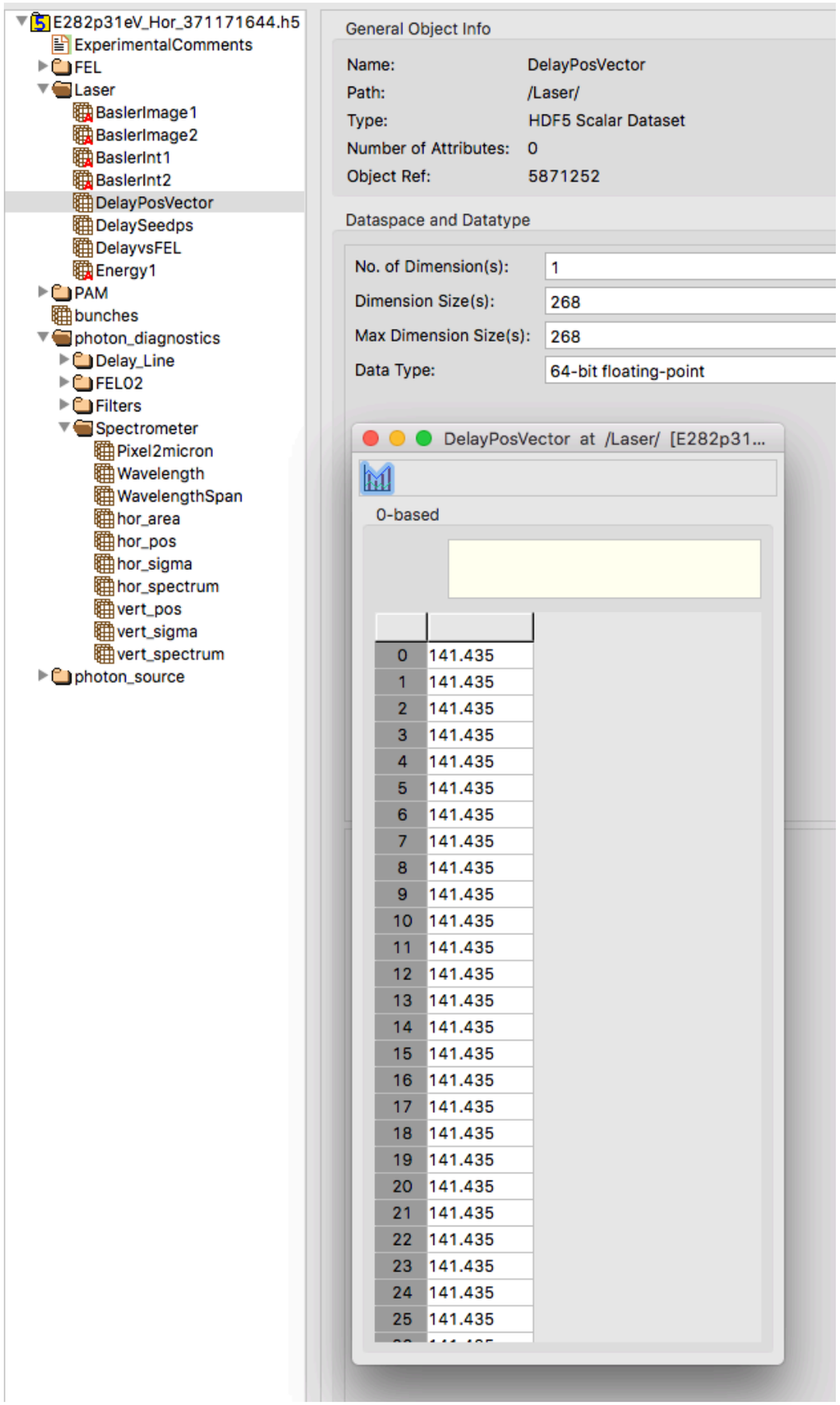
Delay stage

The **delay stage** is a linear drive that moves two mirrors which ultimately changes the path length of the optical laser and with this the delay between X-ray and optical laser pulse.

The delay stage position in mm is saved under:

/Laser/DelayPosVector

With the delay stage position and the time-zero position the delay can be calculated for each shot in femtoseconds.



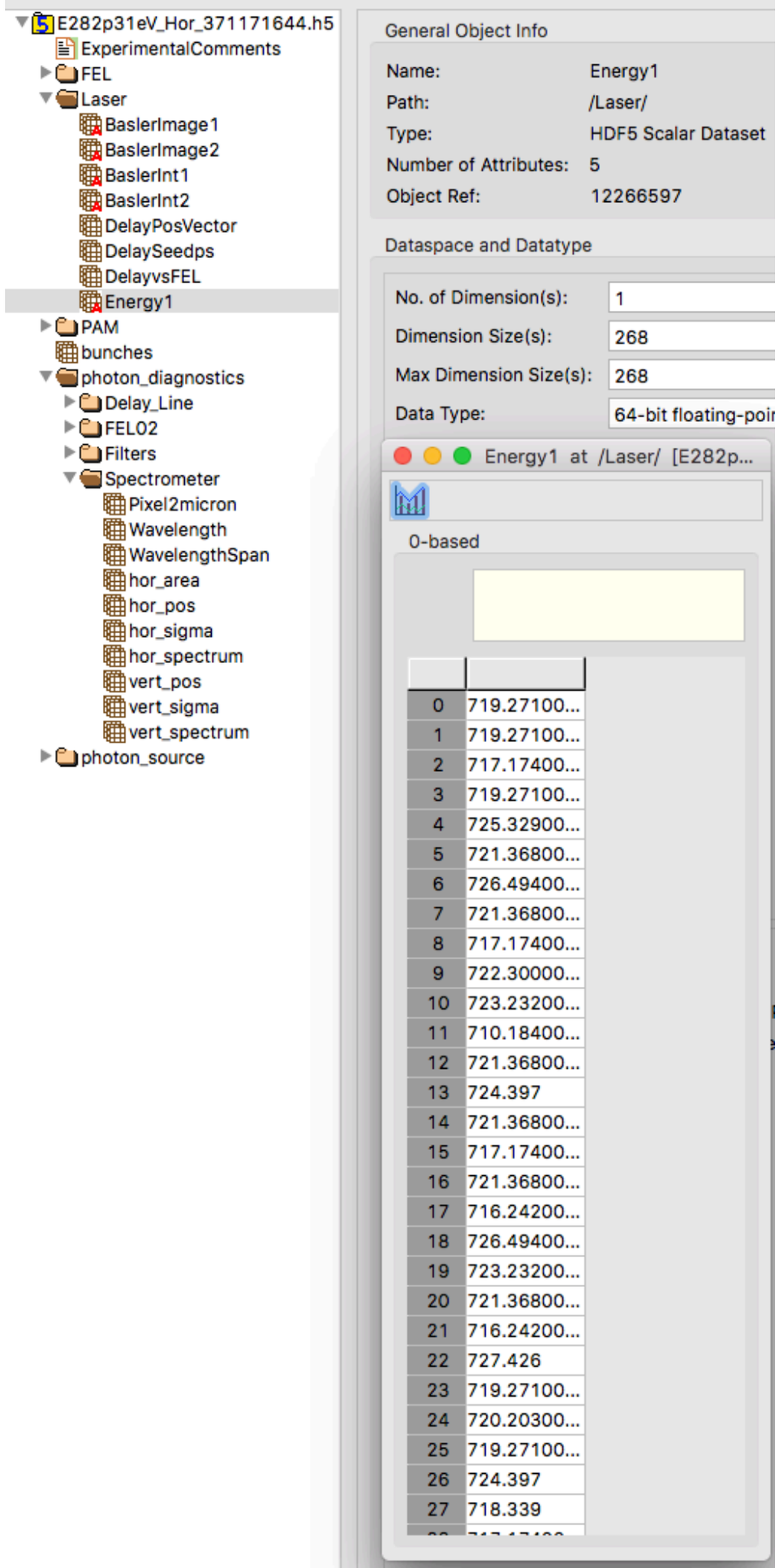
Laser diode

The **laser diode** is a photodiode that sees a fraction of the incident optical laser beam and with this supplies an intensity that is proportional to the laser intensity on the sample.

The laser diode reading in µJ is saved under:

/Laser/Energy1

For now we don’t use the laser diode in the analysis, but it is saved in the processes data in case we need it later.



TFY XAS detector

The **TFY** (total fluorescence yield) **XAS detector** is a CCD camera that looks at the phosphor screen behind our MCP x-ray detector. Each bright spot, which we called a blob, on the detector corresponds to one photon.

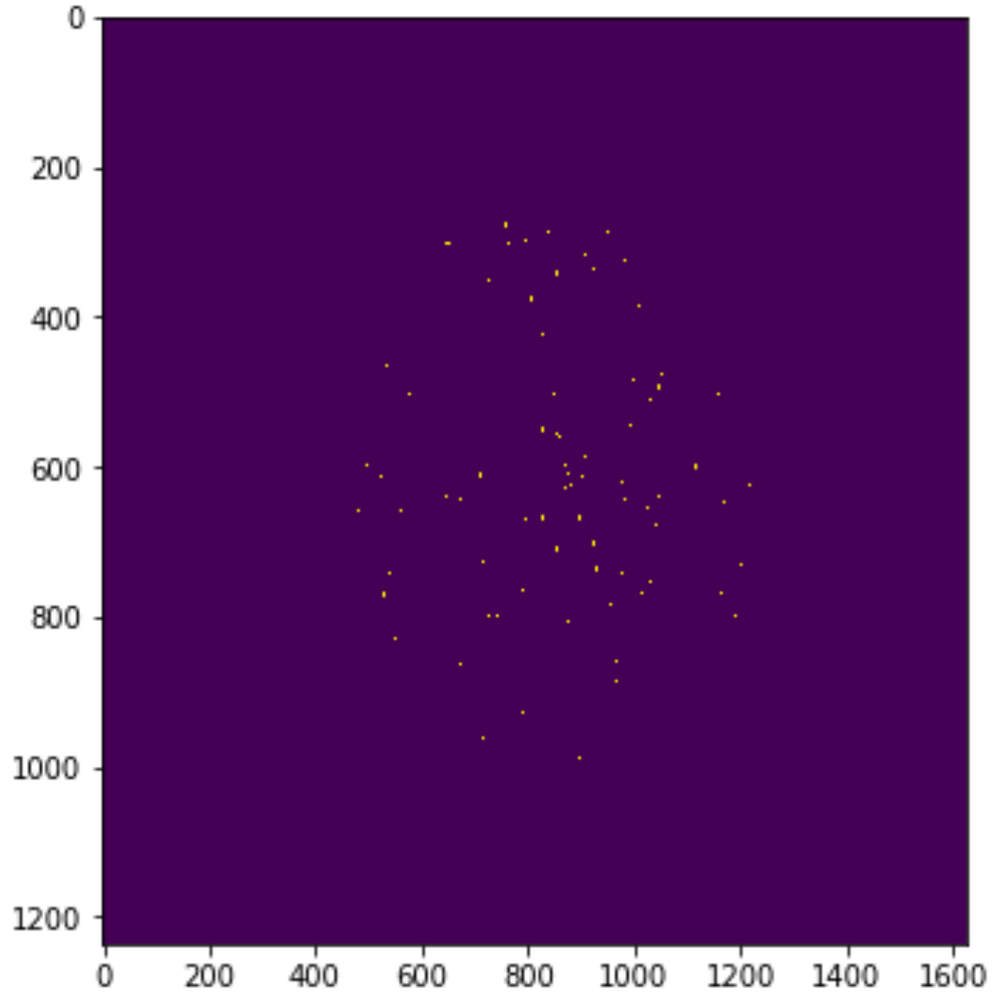
The integrated intensity on the camera (after proper background treatment) is promotional to the total fluoresce coming from the sample and with this prontoional to the absorption.

The camera image is saved under:

/Laser/BaslerImage2

For some runs also the integrated intensity is saved directly under:

/Laser/BaslerInt2



XES Spectrometer

The **XES Spectrometer** is a CCD camera in the same way as for the TFY XAS detector. However, since the x-rays are dispersed by a grating before hitting the XES CCD camera, one dimension of the camera is the dispersive direction.

Projection onto the dispersive direction under consideration of the curvature yields the x-ray emission spectrum.

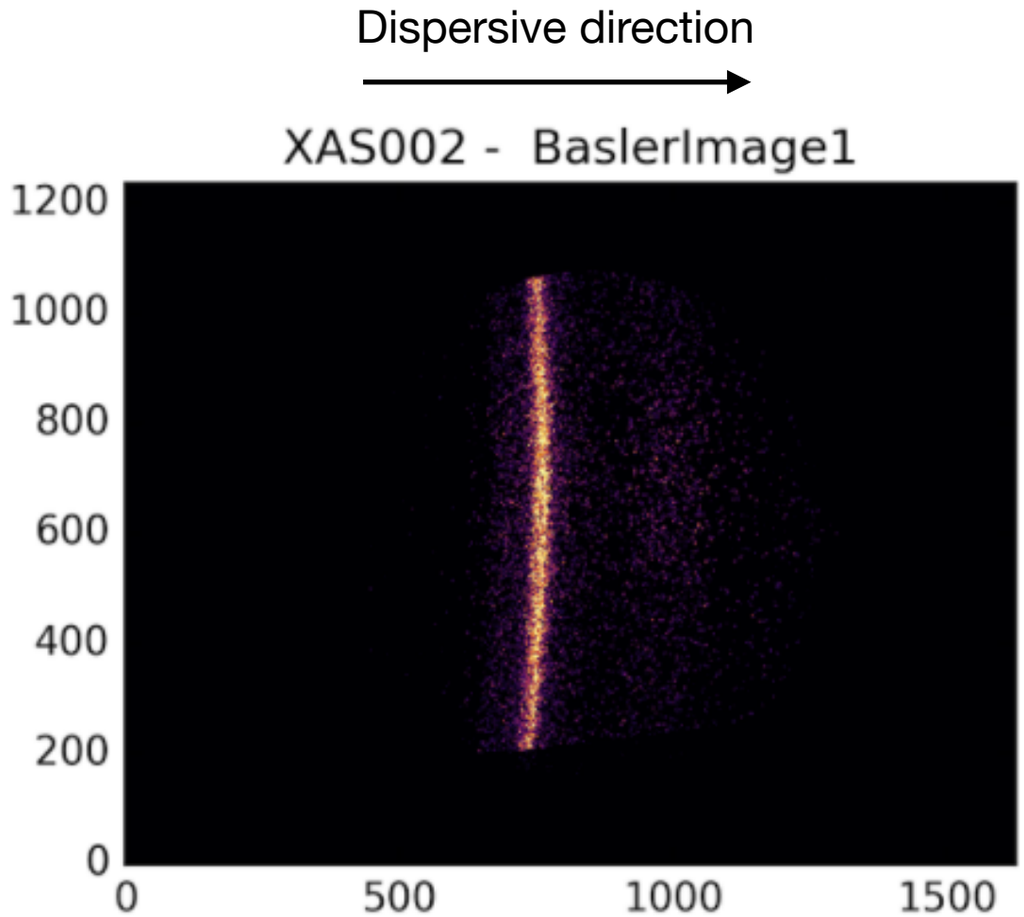
The camera image is saved under:

/Laser/BaslerImage1

For some runs also the integrated intensity is saved directly under:

/Laser/BaslerInt1

XES analysis is not yet included in the scripts! (As of Jan 2018)



The above image is the sum of many 100 shots. On a single shot there will be only a 1 to a few blobs!

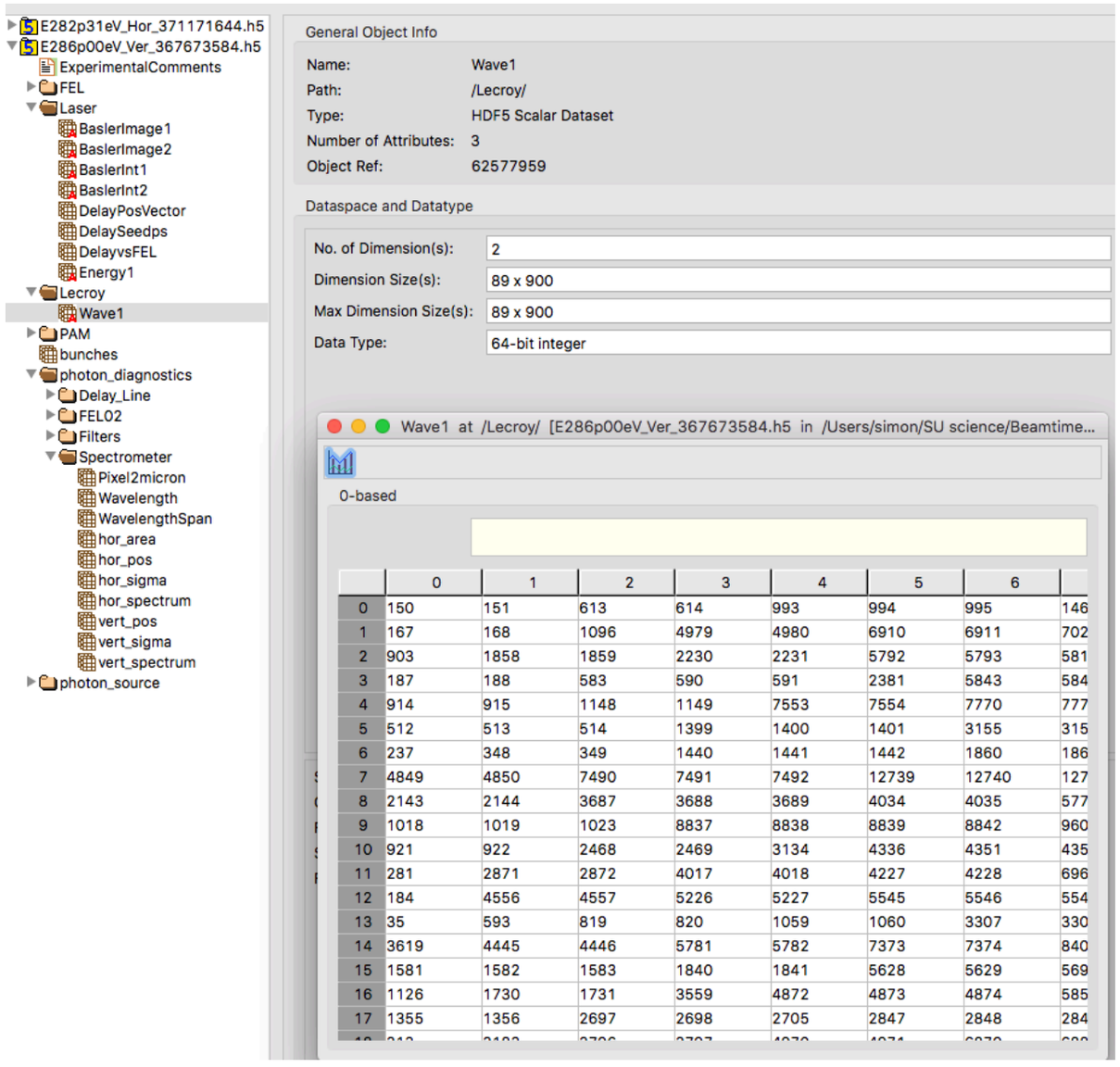
Time of Flight Mass Spectrometer

The **time of flight mass spectrometer** records molecules of a specific mass that desorbed from the surface as a function of time after the optical laser hit the sample.

In the data source the arrival time of each count is saved in units of 5e-9 sec.

The arrival times for each shot are saved under:

/Lecroy/Wave1



	0	1	2	3	4	5	6	
0	150	151	613	614	993	994	995	146
1	167	168	1096	4979	4980	6910	6911	702
2	903	1858	1859	2230	2231	5792	5793	581
3	187	188	583	590	591	2381	5843	584
4	914	915	1148	1149	7553	7554	7770	777
5	512	513	514	1399	1400	1401	3155	315
6	237	348	349	1440	1441	1442	1860	186
7	4849	4850	7490	7491	7492	12739	12740	127
8	2143	2144	3687	3688	3689	4034	4035	577
9	1018	1019	1023	8837	8838	8839	8842	960
10	921	922	2468	2469	3134	4336	4351	435
11	281	2871	2872	4017	4018	4227	4228	696
12	184	4556	4557	5226	5227	5545	5546	554
13	35	593	819	820	1059	1060	3307	330
14	3619	4445	4446	5781	5782	7373	7374	840
15	1581	1582	1583	1840	1841	5628	5629	569
16	1126	1730	1731	3559	4872	4873	4874	585
17	1355	1356	2697	2698	2705	2847	2848	284

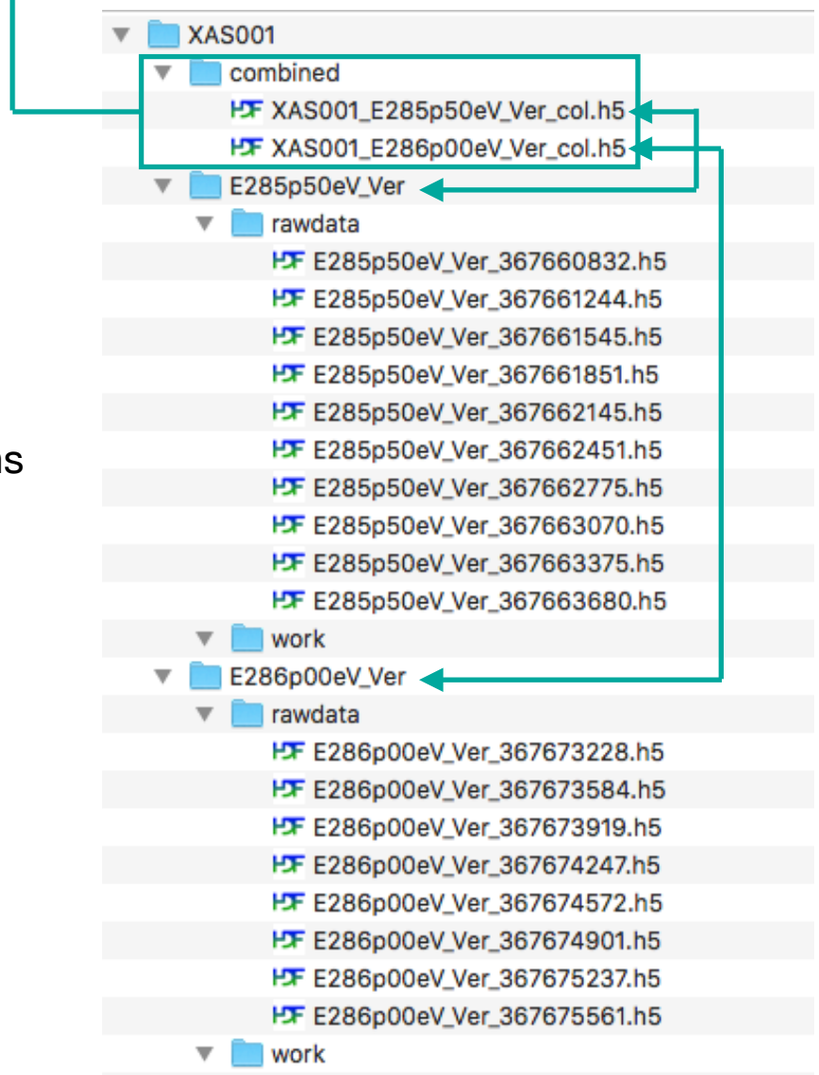
Data Reduction Structure

The reduction of the raw data is done in two steps:

Step 1: Data Collection (script: *16_data_collection.ipynb)*

- In this step all relevant data from the raw HDF5 files (delay files) are collected and saved in a new HDF5 file.
- For the more complex data sources (e.g. XAS detector or online/upstream spectrometer) the data are reduced to more compact formats. E.g. for the XAS detector the image is reduced to a single number representing the integrated intensity in the image.
- The data from all delay files within one photon energy folder are combined in a single HDF5 file with the name *run_photonenergy_polarization*_col.h5 e.g.: *XAS001_E285p50eV_Ver_col.h5*
  This combined file is saved in the ‚combined' folder of the run folder.

- In the combined files the data from each data source is saved for each shot.



Step 2: Data Binning

- In this step all combined files for a number of selected runs (or a single run) are loaded.
- Filters are applied on a shot-to-shot basis on all shots in the selected runs.
  E.g. Filtering out all shots with an incident intensity below a certain value.
- All *good shots* (the ones not filtered out) are then binned into a 2d-raster with dimensions photon energy X delay.
- *… more infos to come ….*

Data Collection

(script: *16_data_collection.ipynb)*

The data collection script consists of three cells:

1. **Initialization**

   Initialize python by loading packages and defining some settings.
   This cell needs to be run only once after starting the juyter notebook.

2. **Define Parameters**

   Define which data to collect and parameters for e.g. the XAS detector camera.
   This cell needs to run whenever you have changed a parameter defined here.

3. **Do the Data Collection**

   This cell performs the main data collection.
   In the top part of the cell you can define which run(s) (run, run type, beamtime) to collect the data from.
   Also you have to set correct main data path.

3. Do the Data Collection

(Cell 3 in script: *16_data_collection.ipynb)*

The main data collection consists of a three nested loops with the following structure:

1. **Loop over selected runs**

   - Collect data which are global for the entire run (harmonic, polarization)

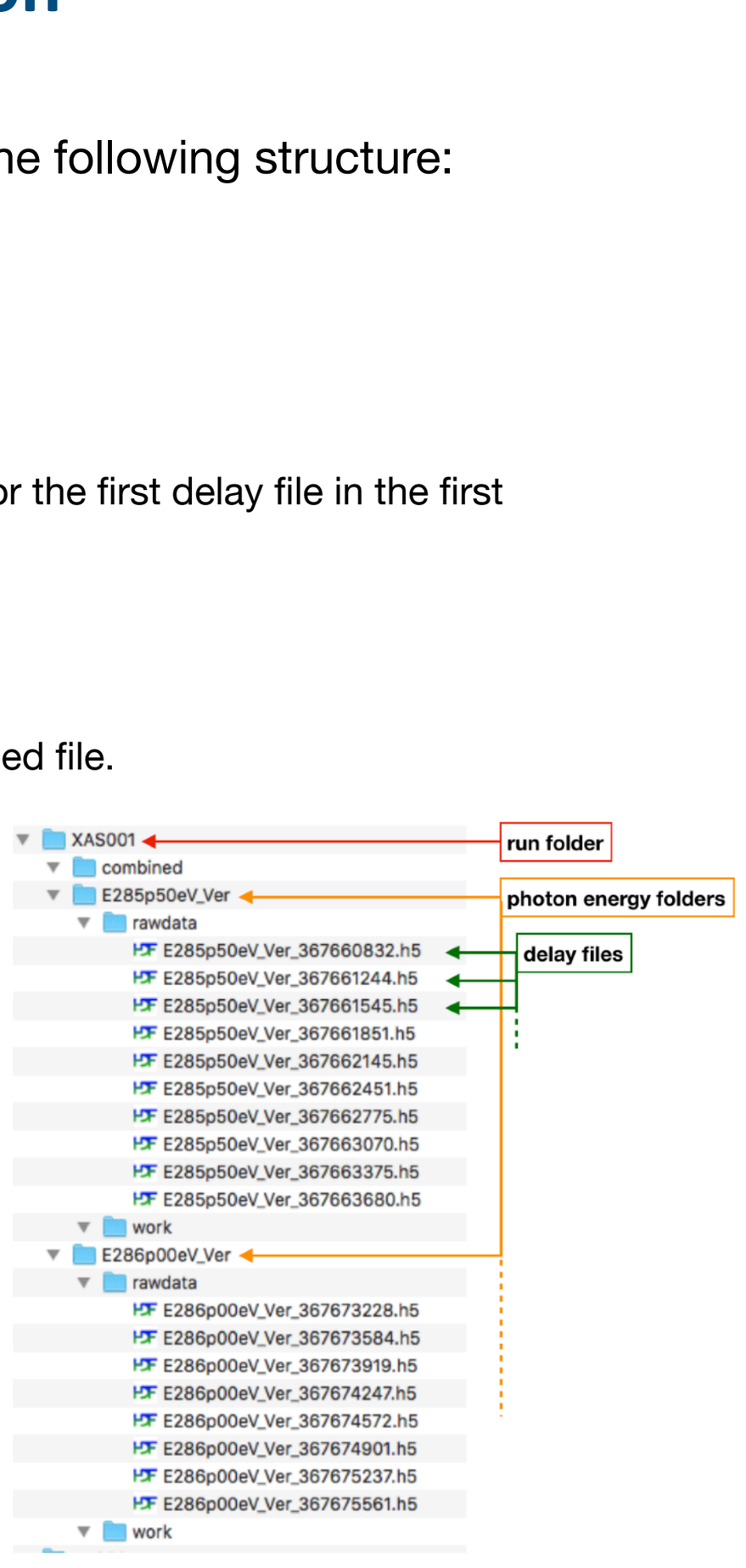
      1.1. **Loop over photon energy folders for this run**

         - Check that all data that should be collected do exist (checks this for the first delay file in the first photon energy folder)

            1.1.1. **Loop over delay files for this photon energy folder**

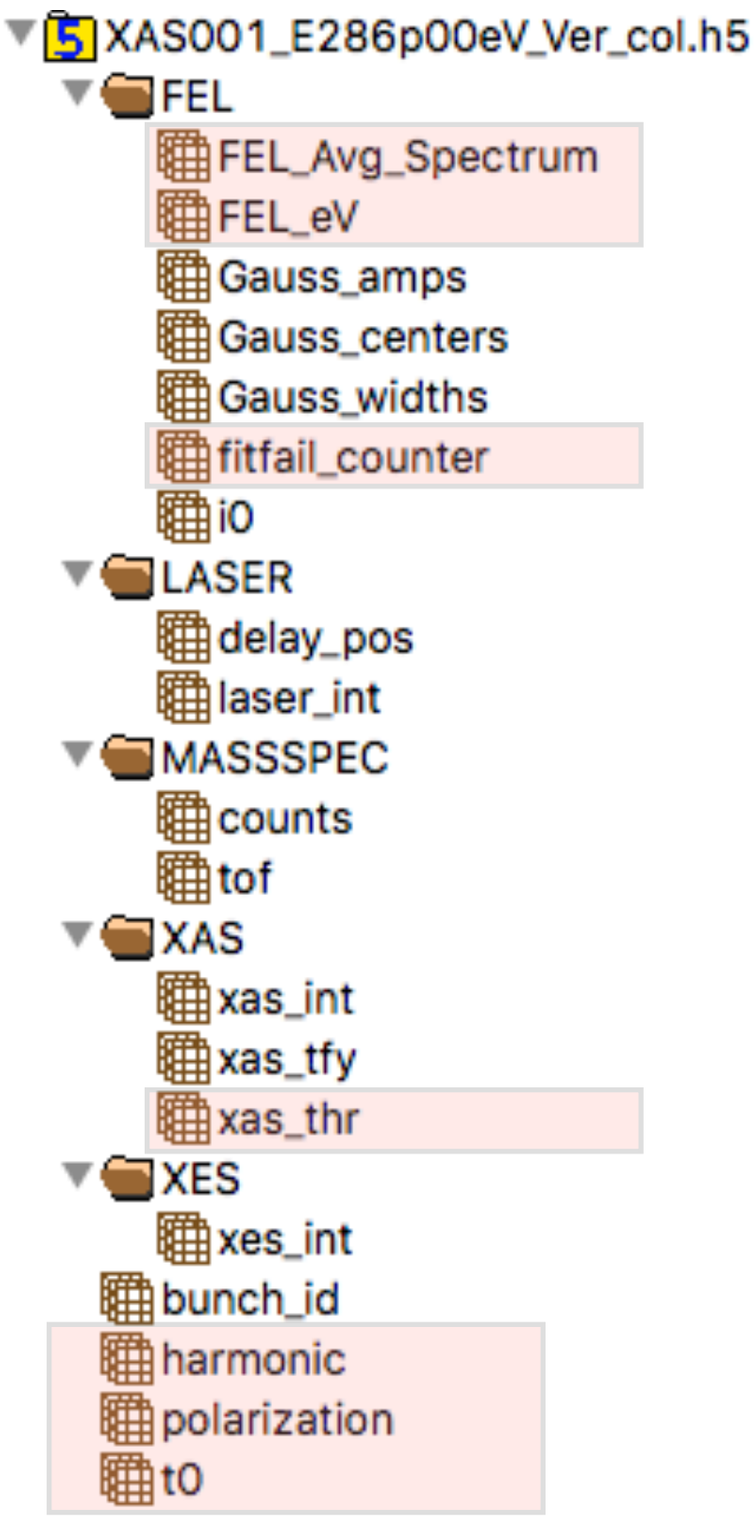
               - Collect the data for all delay files

               - Save the collected data for this photon energy folder in the combined file.



Collected Date in the Combined File

After running the Data Collection



Global data (not shot-to-shot)

- FEL_Avg_Spectrum and FEL_eV

  each 1d array with length 1000

  Average spectrum of all shots form the online/upstream spectrometer (FEL_Avg_Spectrum is the intensity and FEL_eV is the photon energy)
- fitfail_counter

  integer number

  Number of shots for which the gaussian fit of the FEL spectrum failed. Typically 0…10
- xas_thr

  floating point number

  Intensity threshold for the XAS meteor images. This number is set in the data collection parameters.
- harmonic

  integer number

  FEL harmonic
- Polarisation

  integer number

  FEL polarization: 1 = linear vertical, 0 = linear horizontal
- t0

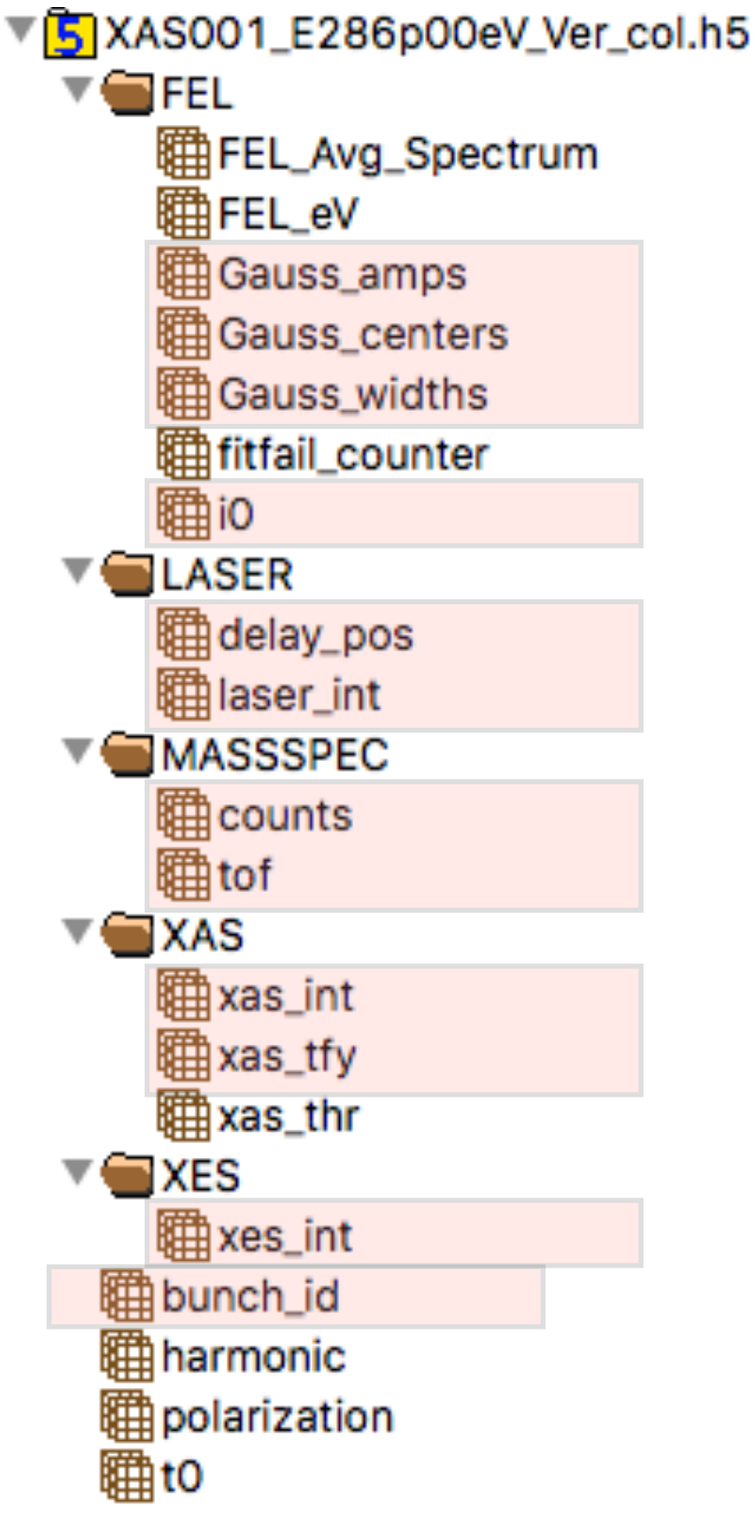
  floating point number

  Zime zero position on the delay stage in mm as it was set during data acquisition.

  NOTE: THIS IS NOT THE FINAL CALIBRATED TIME ZERO!

Collected Date in the Combined File

After running the Data Collection



Shot-to-shot data

- Gauss_amps, Gauss_centers and Gauss_width

  each 1d array with length of number of shots

  Amplitude, central photon energy and photon energy width of the incident x-ray pulse retrieved from a gauss fit to the online spectrometer.
- i0

  1d array with length of number of shots

  Incident x-ray intensity calculated as the intensity in the online spectrometer over a region of interest.
- delay_position and laser_int

  each 1d array with length of number of shots

  Delay stage position in mm and laser diode reading in µJ
- MASSSPEC

  Unused for now…
- xas_int and xas_tfy

  each 1d array with length of number of shots

  Both give the integrated intensity on the XAS detector (difference is the thresholding).

  USE xas_tfy FOR NOW!
- xes_int

  Unused for now…
- bunch_id

  each 1d array with length of number of shots

  Unique number identifying each shot. Monotonically increasing from shot to shot.