

---

# PyHyperScattering

*Release 0+unknown*

**Peter Beaucage**

**Sep 04, 2024**



## CONTENTS

<b>1</b>	<b>Loading: getting your data into PyHyperScattering</b>	<b>1</b>
<b>2</b>	<b>Integration: raw intensity to <math>I(q)</math></b>	<b>3</b>
<b>3</b>	<b>Learning to Fly</b>	<b>5</b>
<b>4</b>	<b>Utility Modules</b>	<b>7</b>
<b>5</b>	<b>Loading Data</b>	<b>9</b>
<b>6</b>	<b>Integration</b>	<b>11</b>
<b>7</b>	<b>Custom Analysis</b>	<b>13</b>
<b>8</b>	<b>Utilities</b>	<b>15</b>
<b>9</b>	<b>User Guide</b>	<b>17</b>
<b>10</b>	<b>API Reference</b>	<b>19</b>
<b>11</b>	<b>Development and Contributing Info: TODO</b>	<b>31</b>
<b>12</b>	<b>Release Notes</b>	<b>33</b>
<b>13</b>	<b>About</b>	<b>35</b>
<b>14</b>	<b>Documentation</b>	<b>37</b>
<b>15</b>	<b>Sitemap</b>	<b>39</b>
	<b>Python Module Index</b>	<b>41</b>
	<b>Index</b>	<b>43</b>



## **LOADING: GETTING YOUR DATA INTO PYHYPERSCATTERING**



**INTEGRATION: RAW INTENSITY TO  $I(Q)$**





## LEARNING TO FLY

From this point, you're in a place where the next steps largely depend on the analysis you want to do with your data.

The tools and language are that of the xarray package, so the main goal of this section is to teach you just enough xarray to have a vocabulary for converting scientific lines of thought into commands and visualize/dissect the results.

The most important command, by far, is `select` or `.sel`



## UTILITY MODULES

Despite the power of writing your own analyses, it seems likely that many of the analyses you'll want to do won't actually be that novel.

To that end, we furnish two modules of 'canned' approaches: RSoXS and fitting. User contributions are encouraged in this area.

### 4.1 RSoXS

### 4.2 Fitting

PyHyperScattering aims to make working with hyperspectral x-ray and neutron scattering data easy, to make programs that work with such data a combination of simple, logical commands with minimal 'cruft'. In the era of modern computing, there is no reason you should have to think about for loops and how you're storing different intermediate data products - you should be able to go immediately from raw data to an analysis with clear commands, punch down to the data you need for your science quickly. The goal is for these tools to make the mechanics of hyperspectral scattering easier and in so doing, more reproducible, explainable, and robust.

It grew out of the NIST RSoXS program, but aims to be broadly applicable. If it's scattering data, you should be able to load it, reduce it, and slice it.

Run tutorials using [Binder](#):

The tools PyHyper provides are basically divided into three categories:



## **LOADING DATA**

Get your data from a source - files on disk or a network connection to a DataBroker or whatever - into a standardized structure we call a raw xarray. The metadata should be loaded and converted to a standardized set of terms, intensity corrections applied, and the frames stacked along whatever dimensions you want.



## **INTEGRATION**

Convert your data from pixel space or  $qx/qy$  space to  $\chi$ - $q$  space - perfect for slicing. generally tools here are built on pyFAI, though some variants also use `warp_polar` from numpy.





## CUSTOM ANALYSIS

Slice your data along specified dimensions and visualize the results.



## **UTILITIES**

These are pre-canned routines for common analyses, such as RSoXS anisotropic ratio or peak/background fitting. the intent here is that the barrier to building your own code is low, and contributions in module space are especially welcomed and encouraged.

Have fun!



## USER GUIDE

Work in progress cookbook for specific tasks.



## API REFERENCE

### 10.1 PyHyperScattering package

#### 10.1.1 Submodules

#### 10.1.2 PyHyperScattering.load module

##### PyHyperScattering.load.FileLoader module

**class** PyHyperScattering.load.FileLoader

Bases: object

Abstract class defining a generic scattering file loader. Input is a (or multiple) filename/s and output is a xarray I(pix\_x,pix\_y,dims,coords) where dims and coords are loaded by user request.

Difference: all coords are dims but not all dims are coords. Dims can also be auto-hinted using the following standard names: energy,exposure,pos\_x,pos\_y,pos\_z,theta.

Individual loaders can try searching metadata for other dim names but this is not guaranteed. Coords can be used to provide a list of values for a dimension when that dimension cannot be hinted, e.g. where vals come from external data.

**file\_ext** = ''

**loadFileSeries**(basepath, dims, coords={}, file\_filter=None, file\_filter\_regex=None, file\_skip=None, md\_filter={}, quiet=True, output\_qxy=False, dest\_qx=None, dest\_qy=None, output\_raw=False, image\_slice=None)

Load a series into a single xarray.

- = not implemented yet

##### Parameters

- **basepath** (*str* or *Path*) – path to the directory to load
- **dims** (*list*) – dimensions of the resulting xarray (excluding ‘pix\_x’ and ‘pix\_y’), as list of str
- **coords** (*dict*) – dictionary of any dims that are *not* present in metadata
- **file\_filter** (*str*) – string that must be in each file name
- **\*file\_filer\_regex** (*str*) – regex string that must match in each file name
- **\*file\_skip** (*str*) – string that, if present in file name, means file should be skipped.

- **md\_filter** (*dict*) – dict of *required* metadata values; points without these metadata values will be dropped
- **md\_filter\_regex** (*dict*) – dict of *required* metadata regex; points without these metadata values will be dropped
- **quiet** (*bool*) – skip printing most intermediate output if true.
- **output\_qxy** (*bool*) – output a qx/qy stack rather than a pix\_x/pix\_y stack. This is a lossy operation, the array will be remeshed. Not recommended.
- **output\_raw** (*bool*) – Do not apply pixel or q coordinates to the final stack.
- **dest\_qx** (*array-like or None*) – set of qx points that you would like the final stack to have. If None, will take the middle image and remesh to that.
- **dest\_qy** (*array-like or None*) – set of qy points that you would like the final stack to have. If None, will take the middle image and remesh to that.
- **image\_slice** (*tuple of slices*) – If provided, all images will be reduced according to these slice objects

```
loadSingleImage(filepath, coords=None, return_q=None, **kwargs)
```

```
md_loading_is_quick = False
```

```
peekAtMd(filepath)
```

## PyHyperScattering.load.ALS11012RSoXSLoader module

```
class PyHyperScattering.load.ALS11012RSoXSLoader (corr_mode=None, user_corr_func=None,
                                                    dark_pedestal=0, exposure_offset=0.002,
                                                    dark_subtract=False,
                                                    data_collected_after_mar2021=False,
                                                    constant_md={})
```

Bases: [FileLoader](#)

Loader for FITS files from the ALS 11.0.1.2 RSoXS instrument

Additional requirement: astropy, for FITS file loader

Usage is mainly via the inherited function `integrateImageStack` from `FileLoader`

```
file_ext = '(*.?).fits'
```

```
loadDarks(basepath, dark_base_name)
```

Load a series of dark images as a function of exposure time, to be subtracted from subsequently-loaded data.

### Parameters

- **basepath** (*str or Path*) – path to load images from
- **dark\_base\_name** (*str*) – str that must be in file for file to be a dark

```
loadSampleSpecificDarks(basepath, file_filter='', file_skip='donotskip', md_filter={})
```

load darks matching a specific sample metadata

Used, e.g., to load darks taken at a time of measurement in order to improve the connection between the dark and sample data.

### Parameters



- **basepath** (*str*) – path to load darks from
- **file\_filter** (*str*) – string that must be in each file name
- **file\_skip** (*str*) – string that, if in file name, means file should be skipped.
- **md\_filter** (*dict*) – dict of required metadata values. this will be appended with dark images only, no need to put that here.

**loadSingleImage**(*filepath*, *coords=None*, *return\_q=False*, *\*\*kwargs*)

THIS IS A HELPER FUNCTION, mostly - should not be called directly unless you know what you are doing

Load a single image from filepath and return a single-image, raw xarray, performing dark subtraction if so configured.

**md\_loading\_is\_quick** = True

**normalizeMetadata**(*headerdict*)

convert the local metadata terms in headerdict to standard nomenclature

**Parameters**

**headerdict** (*dict*) – the header returned by the file loader

**peekAtMd**(*file*)

load the header/metadata without opening the corresponding image

**Parameters**

**file** (*str*) – fits file from which to load metadata

## PyHyperScattering.load.SST1RSoXSLoader module

```
class PyHyperScattering.load.SST1RSoXSLoader(corr_mode=None, user_corr_func=None,
                                              dark_pedestal=100, exposure_offset=0, constant_md={},
                                              use_chunked_loading=False)
```

Bases: [FileLoader](#)

Loader for TIFF files from NSLS-II SST1 RSoXS instrument

**file\_ext** = '(.\*?)primary(.\*?)\.tiff'

**loadMd**(*filepath*)

**loadSingleImage**(*filepath*, *coords=None*, *return\_q=False*, *image\_slice=None*, *use\_cached\_md=False*, *\*\*kwargs*)

HELPER FUNCTION that loads a single image and returns an xarray with either *pix\_x* / *pix\_y* dimensions (if *return\_q == False*) or *qx* / *qy* (if *return\_q == True*)

**Parameters**

- **filepath** (*Pathlib.path*) – path of the file to load
- **coords** (*dict-like*) – coordinate values to inject into the metadata
- **return\_q** (*bool*) – return *qx* / *qy* coords. If false, returns pixel coords.

**md\_loading\_is\_quick** = True

**peekAtMd**(*filepath*)

```
pix_size_1 = 0.06
pix_size_2 = 0.06
read_baseline(baseline_csv)
read_json(jsonfile)
read_primary(primary_csv, seq_num, cwd)
read_shutter_toggle(shutter_csv)
```

## PyHyperScattering.load.SST1RSoXSDB module

```
class PyHyperScattering.load.SST1RSoXSDB(corr_mode=None, user_corr_fun=None, dark_subtract=True,
                                          dark_pedestal=0, exposure_offset=0, catalog=None,
                                          catalog_kwargs={}, use_precise_positions=False,
                                          use_chunked_loading=False, suppress_time_dimension=True)
```

Bases: object

Loader for bluesky run xarrays from NSLS-II SST1 RSoXS instrument

**background()**

**do\_list\_append(\*\*kwargs)**

**file\_ext** = ''

**loadMd(run)**

return a dict of metadata entries from the databroker run xarray

**loadMonitors(entry, integrate\_onto\_images: bool = True, useShutterThinning: bool = True, n\_thinning\_iters: int = 5)**

Load the monitor streams for entry.

Creates a dataset containing all monitor streams (e.g., Mesh Current, Shutter Timing, etc.) as data variables mapped against time. Optionally, all streams can be indexed against the primary measurement time for the images using `integrate_onto_images`. Whether or not time integration attempts to account for shutter opening/closing is controlled by `useShutterThinning`. Warning: for exposure times < 0.5 seconds at SST (as of 9 Feb 2023), `useShutterThinning=True` may excessively cull data points.

### Parameters

- **entry** (*databroker.client.BlueskyRun*) – Bluesky Document containing run information. ex: `pfs.load.SST1RSoXSDB.c[scanID]` or `databroker.client.CatalogOfBlueskyRuns[scanID]`
- **integrate\_onto\_images** (*bool, optional*) – whether or not to map timepoints to the image measurement times (as held by the ‘primary’ stream), by default True Presently bins are averaged between measurements intervals.
- **useShutterThinning** (*bool, optional*) – Whether or not to attempt to thin (filter) the raw time streams to remove data collected during shutter opening/closing, by default False As of 9 Feb 2023 at NSLS2 SST1, using `useShutterThinning= True` for exposure times of < 0.5s is not recommended because the shutter data is unreliable and too many points will be culled
- **n\_thinning\_iters** (*int, optional*) – how many iterations of thinning to perform, by default 5 If the data is becoming too sparse, try fewer iterations

**Returns**

xarray dataset containing all monitor streams as data variables mapped against the dimension “time”

**Return type**

xr.Dataset

**loadRun**(*run*, *dims=None*, *coords={}*, *return\_dataset=False*, *useMonitorShutterThinning=True*)

Loads a run entry from a catalog result into a raw xarray.

**Parameters**

- **run** (*DataBroker result*, *int of a scan id*, *list of scan ids*, *list of DataBroker runs*) – a single run from BlueSky
- **dims** (*list*) – list of dimensions you’d like in the resulting xarray. See list of allowed dimensions in documentation. If not set or None, tries to auto-hint the dims from the RSoXS plan\_name.
- **CHANGE** – List of dimensions you’d like. If not set, will set all possibilities as dimensions (x, y, theta, energy, polarization)
- **coords** (*dict*) – user-supplied dimensions, see syntax examples in documentation.
- **return\_dataset** (*bool, default False*) – return both the data and the monitors as a xr.dataset. If false (default), just returns the data.

**Returns**

raw xarray containing your scan in PyHyper-compliant format

**Return type**

raw (xarray)

**loadSeries**(*run\_list*, *meta\_dim*, *loadrun\_kwargs={}*)

Loads a series of runs into a single xarray object, stacking along meta\_dim.

Useful for a set of samples, or a set of polarizations, etc., taken in different scans.

**Parameters**

- **run\_list** (*list*) – list of scan ids to load
- **meta\_dim** (*str*) – dimension to stack along. must be a valid attribute/metadata value, such as polarization or sample\_name

**Returns**

xarray.Dataset with all scans stacked

**Return type**

raw

**loadSingleImage**(*filepath*, *coords=None*, *return\_q=False*, *\*\*kwargs*)

DO NOT USE

This function is preserved as reference for the qx/qy loading conventions.

NOT FOR ACTIVE USE. DOES NOT WORK.

**md\_loading\_is\_quick** = True

```
md_lookup = {'energy': 'en_energy_setpoint', 'exposure': 'RSoXS Shutter Opening
Time (ms)', 'polarization': 'en_polarization_setpoint', 'sam_th': 'RSoXS Sample
Rotation', 'sam_x': 'RSoXS Sample Outboard-Inboard', 'sam_y': 'RSoXS Sample
Up-Down', 'sam_z': 'RSoXS Sample Downstream-Upstream'}
```

```
md_secondary_lookup = {'energy': 'en_monoen_setpoint'}
```

```
peekAtMd(run)
```

```
pix_size_1 = 0.06
```

```
pix_size_2 = 0.06
```

```
runSearch(**kwargs)
```

Search the catalog using given commands.

**Parameters**

**\*\*kwargs** – passed through to the RawMongo search method of the catalog.

**Returns**

a catalog result object

**Return type**

result (obj)

**searchCatalog**(*outputType: str = 'default', cycle: str = None, proposal: str = None, saf: str = None, user: str = None, institution: str = None, project: str = None, sample: str = None, sampleID: str = None, plan: str = None, userOutputs: list = [], debugWarnings: bool = False, \*\*kwargs*) → DataFrame

Search the Bluesky catalog for scans matching all provided keywords and return metadata as a dataframe.

Matches are made based on the values in the top level of the ‘start’ dict within the metadata of each entry in the Bluesky Catalog (databroker.client.CatalogOfBlueskyRuns). Based on the search arguments provided, a pandas dataframe is returned where rows correspond to catalog entries (scans) and columns contain meta-data. Several presets are provided for choosing which columns are generated, along with an interface for user-provided search arguments and additional metadata. Fails gracefully on bad user input/ changes to underlying metadata scheme.

**Ex1: All of the carbon,fluorine,or oxygen scans for a single sample series in the most recent cycle:**

```
bsCatalogReduced4 = db_loader.searchCatalog(sample="BBP_", institution="NIST", cycle = "2022-2", plan="carbon|fluorine|oxygen")
```

**Ex2: Just all of the scan Ids for a particular sample:**

```
bsCatalogReduced4 = db_loader.searchCatalog(sample="BBP_PFP09A", outputType='scans')
```

**Ex3: Complex Search with custom parameters**

```
bsCatalogReduced3 = db_loader.searchCatalog(['angle', '-1.6', 'numeric'], outputType='all', sample="BBP_", cycle = "2022-2", institution="NIST", plan="carbon", userOutputs = [{"Exposure Multiplier", "exptime", r'catalog.start'}, [{"Stop Time", "time", r'catalog.stop'}]])
```

**Parameters**

- **outputType** (*str, optional*) – modulates the content of output columns in the returned dataframe ‘default’ returns scan\_id, start time, cycle, institution, project, sample\_name, sample\_id, plan name, detector, polarization, exit\_status, and num\_images ‘scans’ returns only the scan\_ids (1-column dataframe) ‘ext\_msmt’ returns default columns AND bar\_spot, sample\_rotation ‘ext\_bio’ returns default columns AND uid, saf, user\_name ‘all’ is equivalent to ‘default’ and all other additive choices
- **cycle** (*str, optional*) – NSLS2 beamtime cycle, regex search e.g., “2022” matches “2022-2”, “2022-1”
- **proposal** (*str, optional*) – NSLS2 PASS proposal ID, case-insensitive, exact match, e.g., “GU-310176”

- **saf** (*str*, *optional*) – Safety Approval Form (SAF) number, exact match, e.g., “309441”
- **user** (*str*, *optional*) – User name, case-insensitive, regex search e.g., “eliot” matches “Eliot”, “Eliot Gann”
- **institution** (*str*, *optional*) – Research Institution, case-insensitive, exact match, e.g., “NIST”
- **project** (*str*, *optional*) – Project code, case-insensitive, regex search, e.g., “liquid” matches “Liquids”, “Liquid-RSoXS”
- **sample** (*str*, *optional*) – Sample name, case-insensitive, regex search, e.g., “**BBP\_**” matches “BBP\_PF902A”
- **sampleID** (*str*, *optional*) – Sample ID, case-insensitive, regex search, e.g., “**BBP\_**” matches “BBP\_PF902A”
- **plan** (*str*, *optional*) – Measurement Plan, case-insensitive, regex search, e.g., “Full” matches “full\_carbon\_scan\_nd”, “full\_fluorine\_scan\_nd” e.g., “carbon|oxygen|fluorine” matches carbon OR oxygen OR fluorine scans
- **\*\*kwargs** – Additional search terms can be provided as keyword args and will further filter the catalog Valid input follows `metadataLabel='searchTerm'` or `metadataLabel = ['searchTerm','matchType']`. Metadata labels must match an entry in the ‘start’ dictionary of the catalog. Supported match types are combinations of ‘case-insensitive’, ‘case-sensitive’, and ‘exact’ OR ‘numeric’. Default behavior is to do a case-sensitive regex match. For metadata labels that are not valid python names, create the kwarg dict before passing into the function (see example 3). Additional search terms will appear in the output data columns. Ex1: passing in `cycle='2022'` would match `'cycle'='2022-2'` AND `'cycle'='2022-1'` Ex2: passing in `grazing=[0,'numeric']` would match `grazing==0` Ex3: create kwargs first, then pass it into the function.
 

```
kwargs = {'2weird metadata label': "Bob", 'grazing': 0, 'angle':-1.6}
db_loader.searchCatalog(sample="BBP_PFP09A", outputType='scans', **kwargs)
```
- **userOutputs** (*list of lists*, *optional*) – Additional metadata to be added to output can be specified as a list of lists. Each sub-list specifies a metadata field as a 3 element list of format: [Output column title (*str*), Metadata label (*str*), Metadata Source (raw *str*)], Valid options for the Metadata Source are any of [`r'catalog.start'`, `r'catalog.start["plan_args"]`, `r'catalog.stop'`, `r'catalog.stop["num_events"]`] e.g., `userOutputs = [[["Exposure Multiplier","exptime", r'catalog.start'], ["Stop Time","time",r'catalog.stop"]]]`
- **debugWarnings** (*bool*, *optional*) – if True, raises a warning with debugging information whenever a key can't be found.

### Returns

Pandas dataframe containing the results of the search, or an empty dataframe if the search fails

### `summarize_run(*args, **kwargs)`

Deprecated function for searching the bluesky catalog for a run. Replaced by `searchCatalog()`

To be removed in PyHyperScattering 1.0.0+.

### PyHyperScattering.load.cyrsoxsLoader module

```
class PyHyperScattering.load.cyrsoxsLoader(eager_load=False, profile_time=True,  
                                           use_chunked_loading=False)
```

Bases: object

Loader for cyrsoxs simulation files

This code is modified from Dean Delongchamp.

**file\_ext** = 'config.txt'

**loadDirectory**(*directory, method=None, \*\*kwargs*)

**loadDirectoryDask**(*directory, output\_dir='HDF5', morphology\_file=None, PhysSize=None*)

Loads a CyRSoXS simulation output directory into a Dask-backed qx/qy xarray.

**Parameters**

- **directory** (*string or Path*) – root simulation directory
- **output\_dir** (*string or Path, default /HDF5*) – directory relative to the base to look for hdf5 files in.

**loadDirectoryLegacy**(*directory, output\_dir='HDF5', morphology\_file=None, PhysSize=None*)

Loads a CyRSoXS simulation output directory into a qx/qy xarray.

**Parameters**

- **directory** (*string or Path*) – root simulation directory
- **output\_dir** (*string or Path, default /HDF5*) – directory relative to the base to look for hdf5 files in.

**md\_loading\_is\_quick** = False

**read\_config**(*fname*)

Reads config.txt from a CyRSoXS simulation and produces a dictionary of values.

**Parameters**

**fname** (*string or Path*) – path to file

**Returns**

dict representation of config file

**Return type**

config

### 10.1.3 PyHyperScattering.integrate module

#### PyHyperScattering.integrate.PFEnergySeriesIntegrator module

```
class PyHyperScattering.PFEnergySeriesIntegrator.PFEnergySeriesIntegrator(**kwargs)
```

Bases: *PFGeneralIntegrator*

**createIntegrator**(*en, recreate=False*)

**integrateImageStack**(*img\_stack, method=None, chunksize=None*)

```
integrateImageStack_dask(img_stack, chunksize=5)
```

```
integrateImageStack_legacy(img_stack)
```

```
integrateSingleImage(img)
```

```
recreateIntegrator()
```

recreate the integrator, after geometry change

```
setupDestQ(energies)
```

```
setupIntegrators(energies)
```

Sets up the integrator stack as a function of energy.

The final statement ensures that the integrator for the median of the set is created. This integrator is used to set the output q-binning.

Details: (copied from a message)

The fact that energy is changing during reduction means that if not forced to something, the output q bins of the integrator will move as well (since the pixel to q mappings are moving with energy). Because sparse data in q is a nightmare, we pick a given set of q bins corresponding to the median of the energies in the scan. That is a compromise between a few approaches. This line manually creates that integrator with default q binning settings so we can take those bins and tell all the other integrators to use that output q grid.

It would cosmically be better (for things like resolution calculation) to have the q bins actually move, but sparse arrays are computationally hard. Eventually (2-3 years of high performance Python evolution) I think that will be the right way to do it, this is an intermediate.

```
PyHyperScattering.PFEnergySeriesIntegrator.inner_generator(df_function='apply')
```

## PyHyperScattering.integrate.PFGeneralIntegrator module

```
class PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator(maskmethod='none',
                                                                maskrotate=True,
                                                                geomethod='none',
                                                                NIdistance=0, Nlbcx=0,
                                                                Nlbcy=0, Nltiltx=0, Nltilty=0,
                                                                Nlpixsizex=0, Nlpixsizey=0,
                                                                template_xr=None,
                                                                ponifile=None, energy=2000,
                                                                integration_method='csr_ocl',
                                                                correctSolidAngle=True,
                                                                maskToNan=True, npts=500,
                                                                use_log_ish_binning=False,
                                                                do_1d_integration=False,
                                                                return_sigma=False,
                                                                use_chunked_processing=False,
                                                                **kwargs)
```

Bases: object

PyFAI general integrator wrapper

```
calibrationFromNikaParams(distance, bcx, bcy, tiltx, tilty, pixsizex, pixsizey)
```

DEPRECATED as of 0.2

**Set the local calibrations using Nika parameters.**

this will probably only support rotations in the SAXS limit (i.e., where  $\sin(x) \sim x$ , i.e., a couple degrees) since it assumes the PyFAI and Nika rotations are about the same origin point (which I think isn't true).

**Args:**

distance: sample-detector distance in mm bcx: beam center x in pixels bcy: beam center y in pixels tiltx: detector x tilt in deg, see note above tilty: detector y tilt in deg, see note above pixsize: pixel size in x, microns pixsizey: pixel size in y, microns

**calibrationFromPoniFile**(*ponifile*)

Sets calibration from a pyFAI poni-file

**Parameters**

- **ponifile** (*str* or *Pathlib.path*) – a pyFAI poni file containing the geometry
- **raw\_xr** (*raw format xarray*) – optional, raw xr with correct pixel dimensions for creating an empty mask if necessary

**calibrationFromTemplateXRParams**(*raw\_xr*)

Sets calibration from a pyFAI values in a template xarray

**Parameters**

**raw\_xr** (*raw format xarray*) – a raw\_xr bearing the metadata in members

**property energy****integrateImageStack**(*img\_stack*, *method=None*, *chunksize=None*)**integrateImageStack\_dask**(*data*, *chunksize=5*)**integrateImageStack\_legacy**(*data*)**integrateSingleImage**(*img*)**loadEdfMask**(*\*\*kwargs*)

Loads an edf-format mask (probably from pyFAI.calib2?).

**Parameters**

**filetoload** (*pathlib.Path* or *string*) – path to edf format mask

**loadImageMask**(*\*\*kwargs*)

loads a mask from a generic image

**Parameters**

- **maskpath** ((*pathlib.Path* or *String*)) – path to load
- **maskrotate** (*bool*) – rotate mask using `np.flipud(np.rot90(mask))`

**loadNikaMask**(*rotate\_image=True*, *\*\*kwargs*)

Loads a Nika-generated HDF5 or tiff mask and converts it to an array that matches the local conventions.

**Parameters**

- **filetoload** (*pathlib.Path* or *string*) – path to hdf5/tiff format mask from Nika.
- **rotate\_image** (*bool*, *default True*) – rotate image as should work



**loadPolyMask**(*maskpoints*=[], *\*\*kwargs*)

loads a polygon mask from a list of polygon points

Args: (list) *maskpoints*: a list of lists of points, e.g.

```
[
    [ #begin polygon 1
      [0,0],[0,10],[10,10],[10,0]
    ], [ #later polygons]
]
```

(tuple) **maskshape**: (x,y) dimensions of mask to create

if not passed, will assume that the maximum point is included in the mask

**loadPyHyperMask**(*\*\*kwargs*)

Loads a mask json file saved by PyHyper's drawMask routines.

**Parameters**

**maskpath**((*pathlib.Path* or *string*)) – path to load json file from

property **ni\_beamcenter\_x**

property **ni\_beamcenter\_y**

property **ni\_distance**

property **ni\_pixel\_x**

property **ni\_pixel\_y**

property **ni\_tilt\_x**

property **ni\_tilt\_y**

**recreateIntegrator**()

recreate the integrator, after geometry change

property **wavelength**

`PyHyperScattering.PFGeneralIntegrator.inner_generator(df_function='apply')`

## PyHyperScattering.integrate.WPIntegrator module

Integrator for qx/qy format xarrays using `skimage.transform.warp_polar` or a custom cuda-accelerated version, `warp_polar_gpu`

#### 10.1.4 PyHyperScattering.util module

PyHyperScattering.util.Fitting module

PyHyperScattering.util.HDR module

PyHyperScattering.util.IntegrationUtils module

PyHyperScattering.util.FileIO module

PyHyperScattering.util.RSoXS module

#### 10.1.5 Module contents

## DEVELOPMENT AND CONTRIBUTING INFO: TODO

PyHyperScattering is an open-source collaboration maintained by the [National Institute of Standards and Technology \(NIST\)](#). This package is under active development, and the team welcome DMs with questions on the NIST RSoXS slack, Nikea, and NSLS2 slack channels, or by email to [Dr. Peter Beaucage](#). For more information about contributing, development philosophy, and licensing, see [the Development page](#).

### 11.1 Scope and Package Outline

TODO

### 11.2 Contributing

Contributions are welcome! Please view our [Contributor Guidelines](#) on github.

### 11.3 License

This software was developed by employees of the National Institute of Standards and Technology (NIST), an agency of the Federal Government and is being made available as a public service. Pursuant to title 17 United States Code Section 105, works of NIST employees are not subject to copyright protection in the United States. This software may be subject to foreign copyright. Permission in the United States and in foreign countries, to the extent that NIST may hold copyright, to use, copy, modify, create derivative works, and distribute this software and its documentation without fee is hereby granted on a non-exclusive basis, provided that this notice and disclaimer of warranty appears in all copies. THE SOFTWARE IS PROVIDED ‘AS IS’ WITHOUT ANY WARRANTY OF ANY KIND, EITHER EXPRESSED, IMPLIED, OR STATUTORY, INCLUDING, BUT NOT LIMITED TO, ANY WARRANTY THAT THE SOFTWARE WILL CONFORM TO SPECIFICATIONS, ANY IMPLIED WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE, AND FREEDOM FROM INFRINGEMENT, AND ANY WARRANTY THAT THE DOCUMENTATION WILL CONFORM TO THE SOFTWARE, OR ANY WARRANTY THAT THE SOFTWARE WILL BE ERROR FREE. IN NO EVENT SHALL NIST BE LIABLE FOR ANY DAMAGES, INCLUDING, BUT NOT LIMITED TO, DIRECT, INDIRECT, SPECIAL OR CONSEQUENTIAL DAMAGES, ARISING OUT OF, RESULTING FROM, OR IN ANY WAY CONNECTED WITH THIS SOFTWARE, WHETHER OR NOT BASED UPON WARRANTY, CONTRACT, TORT, OR OTHERWISE, WHETHER OR NOT INJURY WAS SUSTAINED BY PERSONS OR PROPERTY OR OTHERWISE, AND WHETHER OR NOT LOSS WAS SUSTAINED FROM, OR AROSE OUT OF THE RESULTS OF, OR USE OF, THE SOFTWARE OR SERVICES PROVIDED HEREUNDER. With respect to the example data package, the following terms apply: The data/work is provided by NIST as a public service and is expressly provided “AS IS.” NIST MAKES NO WARRANTY OF ANY KIND, EXPRESS, IMPLIED OR STATUTORY, INCLUDING, WITHOUT LIMITATION, THE IMPLIED WARRANTY OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE, NON-INFRINGEMENT AND DATA ACCURACY. NIST does

not warrant or make any representations regarding the use of the data or the results thereof, including but not limited to the correctness, accuracy, reliability or usefulness of the data. NIST SHALL NOT BE LIABLE AND YOU HEREBY RELEASE NIST FROM LIABILITY FOR ANY INDIRECT, CONSEQUENTIAL, SPECIAL, OR INCIDENTAL DAMAGES (INCLUDING DAMAGES FOR LOSS OF BUSINESS PROFITS, BUSINESS INTERRUPTION, LOSS OF BUSINESS INFORMATION, AND THE LIKE), WHETHER ARISING IN TORT, CONTRACT, OR OTHERWISE, ARISING FROM OR RELATING TO THE DATA (OR THE USE OF OR INABILITY TO USE THIS DATA), EVEN IF NIST HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES. To the extent that NIST may hold copyright in countries other than the United States, you are hereby granted the non-exclusive irrevocable and unconditional right to print, publish, prepare derivative works and distribute the NIST data, in any medium, or authorize others to do so on your behalf, on a royalty-free basis throughout the world. You may improve, modify, and create derivative works of the data or any portion of the data, and you may copy and distribute such modifications or works. Modified works should carry a notice stating that you changed the data and should note the date and nature of any such change. Please explicitly acknowledge the National Institute of Standards and Technology as the source of the data: Data citation recommendations are provided at <https://www.nist.gov/open/license>. Permission to use this data is contingent upon your acceptance of the terms of this agreement and upon your providing appropriate acknowledgments of NIST's creation of the data/work.

## RELEASE NOTES

Release notes for each release are on the *GitHub releases page* <<https://github.com/usnistgov/PyHyperScattering/releases>>

Major changes are discussed here:

Preparing for v1.0 release, which includes breaking changes that make xarray Datasets the underlying data structure.



## ABOUT

PyHyperScattering aims to make working with hyperspectral x-ray and neutron scattering data easy” to make programs that work with such data a combination of simple, logical commands with minimal ‘cruft’. In the era of modern computing, there is no reason you should have to think about for loops and how you’re storing different intermediate data products - you should be able to go immediately from raw data to an analysis with clear commands, punch down to the data you need for your science quickly. The goal is for these tools to make the mechanics of hyperspectral scattering easier and in so doing, more reproducible, explainable, and robust.

PyHyperScattering is an open-source collaboration maintained by the [National Institute of Standards and Technology \(NIST\)](#). This package is under active development, and the team welcome DMs with questions on the NIST RSoXS slack, Nikea, and NSLS2 slack channels, or by email to [Dr. Peter Beaucage](#). For more information about contributing, development philosophy, and licensing, see [the Development page](#).





## DOCUMENTATION

<i>Getting Started</i> Tutorials to help you get your analysis up and running. Beginners should start here.	<i>User Guide</i> A collection of How-To guides (recipes) for specific data reduction, analysis, and visualization tasks.
<i>API Reference</i> Detailed technical reference; presents documentation at the function, class, and module level.	<i>Development</i> Information and resources regarding the scope and development philosophy of this project, along with information on contributing and licensing.



## SITEMAP

- [genindex](#)
- [modindex](#)
- [search](#)



## PYTHON MODULE INDEX

### p

- PyHyperScattering, [30](#)
- PyHyperScattering.integrate, [26](#)
- PyHyperScattering.integrate.WPIntegrator, [29](#)
- PyHyperScattering.load, [19](#)
- PyHyperScattering.PFEnergySeriesIntegrator,  
[26](#)
- PyHyperScattering.PFGeneralIntegrator, [27](#)
- PyHyperScattering.util, [30](#)
- PyHyperScattering.util.FileIO, [30](#)
- PyHyperScattering.util.Fitting, [30](#)
- PyHyperScattering.util.HDR, [30](#)
- PyHyperScattering.util.IntegrationUtils, [30](#)
- PyHyperScattering.util.RSoXS, [30](#)



## A

ALS11012RSoXSLoader (class in *PyHyperScattering.load*), 20

## B

background() (*PyHyperScattering.load.SSTIRSoXSDB* method), 22

## C

calibrationFromNikaParams() (*PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator* method), 27

calibrationFromPoniFile() (*PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator* method), 28

calibrationFromTemplateXRParams() (*PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator* method), 28

createIntegrator() (*PyHyperScattering.PFEnergySeriesIntegrator.PFEnergySeriesIntegrator* method), 26

cyrsoxsLoader (class in *PyHyperScattering.load*), 26

## D

do\_list\_append() (*PyHyperScattering.load.SSTIRSoXSDB* method), 22

## E

energy (*PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator* property), 28

## F

file\_ext (*PyHyperScattering.load.ALS11012RSoXSLoader* attribute), 20

file\_ext (*PyHyperScattering.load.cyrsoxsLoader* attribute), 26

file\_ext (*PyHyperScattering.load.FileLoader* attribute), 19

file\_ext (*PyHyperScattering.load.SSTIRSoXSDB* attribute), 22

file\_ext (*PyHyperScattering.load.SSTIRSoXSLoader* attribute), 21

FileLoader (class in *PyHyperScattering.load*), 19

## I

inner\_generator() (in module *PyHyperScattering.PFEnergySeriesIntegrator*), 27

inner\_generator() (in module *PyHyperScattering.PFGeneralIntegrator*), 29

integrateImageStack() (*PyHyperScattering.PFEnergySeriesIntegrator.PFEnergySeriesIntegrator* method), 26

integrateImageStack() (*PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator* method), 28

integrateImageStack\_dask() (*PyHyperScattering.PFEnergySeriesIntegrator.PFEnergySeriesIntegrator* method), 26

integrateImageStack\_dask() (*PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator* method), 28

integrateImageStack\_legacy() (*PyHyperScattering.PFEnergySeriesIntegrator.PFEnergySeriesIntegrator* method), 27

integrateImageStack\_legacy() (*PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator* method), 28

integrateSingleImage() (*PyHyperScattering.PFEnergySeriesIntegrator.PFEnergySeriesIntegrator* method), 27

integrateSingleImage() (*PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator* method), 28

## L

loadDarks() (*PyHyperScattering.load.ALS11012RSoXSLoader* method), 20

loadDirectory() (*PyHyperScattering.load.cyrsoxsLoader* method), 26

- loadDirectoryDask() (PyHyperScattering.load.cyrsoxsLoader method), 26
- loadDirectoryLegacy() (PyHyperScattering.load.cyrsoxsLoader method), 26
- loadEdfMask() (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator method), 28
- loadFileSeries() (PyHyperScattering.load.FileLoader method), 19
- loadImageMask() (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator method), 28
- loadMd() (PyHyperScattering.load.SSTIRSoXSDB method), 22
- loadMd() (PyHyperScattering.load.SSTIRSoXSLoader method), 21
- loadMonitors() (PyHyperScattering.load.SSTIRSoXSDB method), 22
- loadNikaMask() (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator method), 28
- loadPolyMask() (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator method), 28
- loadPyHyperMask() (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator method), 29
- loadRun() (PyHyperScattering.load.SSTIRSoXSDB method), 23
- loadSampleSpecificDarks() (PyHyperScattering.load.ALS11012RSoXSLoader method), 20
- loadSeries() (PyHyperScattering.load.SSTIRSoXSDB method), 23
- loadSingleImage() (PyHyperScattering.load.ALS11012RSoXSLoader method), 21
- loadSingleImage() (PyHyperScattering.load.FileLoader method), 20
- loadSingleImage() (PyHyperScattering.load.SSTIRSoXSDB method), 23
- loadSingleImage() (PyHyperScattering.load.SSTIRSoXSLoader method), 21
- ## M
- md\_loading\_is\_quick (PyHyperScattering.load.ALS11012RSoXSLoader attribute), 21
- md\_loading\_is\_quick (PyHyperScattering.load.cyrsoxsLoader attribute), 26
- md\_loading\_is\_quick (PyHyperScattering.load.FileLoader attribute), 20
- md\_loading\_is\_quick (PyHyperScattering.load.SSTIRSoXSDB attribute), 23
- md\_loading\_is\_quick (PyHyperScattering.load.SSTIRSoXSLoader attribute), 21
- md\_lookup (PyHyperScattering.load.SSTIRSoXSDB attribute), 23
- md\_secondary\_lookup (PyHyperScattering.load.SSTIRSoXSDB attribute), 24
- module
- PyHyperScattering, 30
  - PyHyperScattering.integrate, 26
  - PyHyperScattering.integrate.WPIntegrator, 29
  - PyHyperScattering.load, 19
  - PyHyperScattering.PFEnergySeriesIntegrator, 26
  - PyHyperScattering.PFGeneralIntegrator, 27
  - PyHyperScattering.util, 30
  - PyHyperScattering.util.FileIO, 30
  - PyHyperScattering.util.Fitting, 30
  - PyHyperScattering.util.HDR, 30
  - PyHyperScattering.util.IntegrationUtils, 30
  - PyHyperScattering.util.RSoXS, 30
- ## N
- ni\_beamcenter\_x (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator property), 29
- ni\_beamcenter\_y (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator property), 29
- ni\_distance (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator property), 29
- ni\_pixel\_x (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator property), 29
- ni\_pixel\_y (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator property), 29
- ni\_tilt\_x (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator property), 29
- ni\_tilt\_y (PyHyperScattering.PFGeneralIntegrator.PFGeneralIntegrator property), 29
- normalizeMetadata() (PyHyperScattering.load.ALS11012RSoXSLoader method), 21
- ## P
- peekAtMd() (PyHyperScattering.load.ALS11012RSoXSLoader method), 21



`peekAtMd()` (*PyHyperScattering.load.FileLoader* method), 20  
`peekAtMd()` (*PyHyperScattering.load.SSTIRSoXSDB* method), 24  
`peekAtMd()` (*PyHyperScattering.load.SSTIRSoXSLoader* method), 21  
`PFEnergySeriesIntegrator` (class in *PyHyperScattering.PFEnergySeriesIntegrator*), 26  
`PFGGeneralIntegrator` (class in *PyHyperScattering.PFGGeneralIntegrator*), 27  
`pix_size_1` (*PyHyperScattering.load.SSTIRSoXSDB* attribute), 24  
`pix_size_1` (*PyHyperScattering.load.SSTIRSoXSLoader* attribute), 21  
`pix_size_2` (*PyHyperScattering.load.SSTIRSoXSDB* attribute), 24  
`pix_size_2` (*PyHyperScattering.load.SSTIRSoXSLoader* attribute), 22  
`PyHyperScattering` module, 30  
`PyHyperScattering.integrate` module, 26  
`PyHyperScattering.integrate.WPIntegrator` module, 29  
`PyHyperScattering.load` module, 19  
`PyHyperScattering.PFEnergySeriesIntegrator` module, 26  
`PyHyperScattering.PFGGeneralIntegrator` module, 27  
`PyHyperScattering.util` module, 30  
`PyHyperScattering.util.FileIO` module, 30  
`PyHyperScattering.util.Fitting` module, 30  
`PyHyperScattering.util.HDR` module, 30  
`PyHyperScattering.util.IntegrationUtils` module, 30  
`PyHyperScattering.util.RSoXS` module, 30

## R

`read_baseline()` (*PyHyperScattering.load.SSTIRSoXSLoader* method), 22  
`read_config()` (*PyHyperScattering.load.cyrsoxsLoader* method), 26  
`read_json()` (*PyHyperScattering.load.SSTIRSoXSLoader* method), 22  
`read_primary()` (*PyHyperScattering.load.SSTIRSoXSLoader* method), 22  
`read_shutter_toggle()` (*PyHyperScattering.load.SSTIRSoXSLoader* method), 22

`recreateIntegrator()` (*PyHyperScattering.PFEnergySeriesIntegrator.PFEnergySeriesIntegrator* method), 27  
`recreateIntegrator()` (*PyHyperScattering.PFGGeneralIntegrator.PFGGeneralIntegrator* method), 29  
`runSearch()` (*PyHyperScattering.load.SSTIRSoXSDB* method), 24

## S

`searchCatalog()` (*PyHyperScattering.load.SSTIRSoXSDB* method), 24  
`setupDestQ()` (*PyHyperScattering.PFEnergySeriesIntegrator.PFEnergySeriesIntegrator* method), 27  
`setupIntegrators()` (*PyHyperScattering.PFEnergySeriesIntegrator.PFEnergySeriesIntegrator* method), 27  
`SSTIRSoXSDB` (class in *PyHyperScattering.load*), 22  
`SSTIRSoXSLoader` (class in *PyHyperScattering.load*), 21  
`summarize_run()` (*PyHyperScattering.load.SSTIRSoXSDB* method), 25

## W

`wavelength` (*PyHyperScattering.PFGGeneralIntegrator.PFGGeneralIntegrator* property), 29