
PyHyperScattering

Release 0+unknown

Peter Beaucage

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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 χ - 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_Pf902A", 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, Nlbxc=0,
                                                                Nlbcy=0, Nltlx=0, Nltly=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

11.1 Scope and Package Outline

PyHyperScattering is a Python package for analyzing hyperspectral scattering data - that is, x-ray and neutron scattering data that is assessed as a series rather than as a set of discrete, disconnected points.

The package is designed to provide useful tooling for end-to-end analysis using the XArray package, emphasizing the translation of bespoke, instrument-specific parameters to a common, interoperable XArray format. The package is designed to be modular and extensible, with a focus on the following key areas of data analysis:

1. Data Import and Translation “loading” (PyHyperScattering.load): Importing and translating raw data from a variety of sources into a common format. Individual loaders are provided for a variety of instruments and a variety of input formats; tooling in PyHyperScattering.load.FileLoader provides a prototype for quickly building new file-based loaders by providing only an image loading function and a metadata loading function. Intensity corrections, where possible, are applied in the loading stage.
2. Data Reduction “integration” (PyHyperScattering.integrate): Reduction of raw data to a common format of $I(q, \chi)$ or in some cases $I(q_x, q_y)$. We endeavor to use other, high-quality, community supported reduction engines such as PyFAI, PyGIX, and scikit-image warp_polar.
3. Utility Modules “util”: A collection of utility modules for such tasks as file input/output, beam centering and masking, and other common tasks.
4. Bespoke analyses “rsoxs” and others: A collection of bespoke analyses for specific measurement techniques. These analyses are intended to be a ‘cookbook’ of common recipes for users to build their own scientific data pipelines.

PyHyperScattering is unapologetically API-first, a library rather than a program. We enforce a strict separation of scientific logic code from user interfaces. This is a choice to provide the code with the best possible chance to be reused in new ways not anticipated by the original development. For instance, a data loading and reduction routine might be used in a Jupyter notebook, dispatched from a shell script, used to back a webapp using a framework like NiceGUI, used at-scale to reduce all data from a beamline via Prefect, etc. By separating UI from science, we make it possible to have the same well-tested code back all these applications.

Placeholder page.

Placeholder page.

11.2 Scope and Package Outline

We consider in-scope any aspect of loading, reduction, and analysis of hyperspectral scattering data. Details are at <scope>.

11.3 Development Philosophy

The PyHyperScattering package is designed to be modular and extensible. Our general philosophy is to accept contributions that don't break existing user experiences and don't impose too large of a documentation burden. Details at <philosophy>.

11.4 Key API Concepts / Abstract Classes

The API is built around formalized interfaces of XArrays between Loader, Integrator, and Analysis classes. Details at <api_concepts>.

11.5 Contributing

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

11.6 License

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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.

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