

REIXS Soft
X-ray
Spectroscopy
Workshop

Patrick
Braun

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REIXS Soft X-ray Spectroscopy Workshop

On-the-fly data processing and visualization: An introduction to the
python *reixs* package

Outline

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- 1 What is the *reixs* python package and why use it
- 2 Programming Fundamentals
- 3 Starting and Setting Up
- 4 Examples
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- 6 Summary & Questions

What is the *reixs* python package

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- Tool for data processing and visualization - based on the needs of the user community at the REIXS beamline
- Disclaimer: dominant focus on the RIXS endstation
- Ships as python package and is distributed on *PyPi*
- Runs as stand-alone python code but works best when integrated in a Jupyter notebook environment for interactive computing

Why develop the *reixs* python package

- Native integration for beamline data with commercial plotting software lacking
 - Pre-Processing required before data can be visualized - multi-step process (e.g. strip the scan of interest out of data file, ...)
 - Data reduction complex: combine information such as independent axis, detector scale, and matrix from multiple files (i.e. header file, auxiliary files)
 - Mutual energy calibration of the monochromator and spectrometer difficult for new users
- ⇒ Users collect data but do not utilize it to the fullest extend
- ⇒ Focus on the data interpretation rather than the processing

Why use the *reixs* python package

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- On-the-fly data processing is important for decision making while measuring - especially when controlling the beamline remotely and scripting scans
- Analysis package provides real-time interaction with acquired spectra
- Directly compatible with the beamline data format
- Allows to quickly reduce higher-dimensional data to 1D
- Supports the export to commercial plotting software
- It is easy to use - no programming skills required and you will receive hands-on training today!

Objectives for today

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After this session, users will be able to

- run the *reixs* data analysis package;
- extract and export scans of interest;
- use reduction methods to exploit multi-channel analyzer data;
- apply mathematical operations to the collected data;
- plot and interact with visualized data.

Nomenclature

Variable

A *variable* is a name for a value. Variables are created on demand whenever a value is assigned to them and stored in memory.
e.g. `variable = "Hello"`

Function

A block of code that performs a specific task.

Class

A "blueprint" (constructor) for creating objects.

Types of Data

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- Strings
 - collection of characters
 - may include letters and numbers
 - string literals are written by enclosing them in single ('Hello') or double quotes ("Hello")
- Integer numbers
- Objects
 - A collection of data/properties (variables) and methods (functions)
 - Methods are functions that belong to the object
 - An object is a specific instance of a class

Function calls

```
# Setup a variable "my_variable"  
# Store values of function "my_function"  
# Pass on arguments "arg1" and "arg2"  
# Pass on key-word arguments "kwarg1" and "kwarg2"
```

```
my_variable =  $\square$   
   $\rightarrow$  my_function(arg1, arg2, kwarg1=True, kwarg2=False)
```

```
# Note the parentheses after "my_function"  
# Need to specify arguments;  
# Key-word arguments not required (default to pre-set  $\square$   
   $\rightarrow$  values)
```

Calling a class method

```
# Similarly to functions: execute class method  
↪ associated with object
```

```
# Create object "my_object" of the "SomeObject" class  
# Existing method "my_method"
```

```
my_object = SomeObject()  
my_object.my_method(arg1, arg2, kwarg1=True, kwarg2=False)
```

Quickstart: starting the jupyter environment

```
Anaconda Powershell Prompt (Anaconda3)
(base) PS C:\> jupyter notebook
[I 2023-04-24 11:48:21.032 LabApp] JupyterLab extension loaded from C:\Users\braunp\Anaconda3\lib\site-packages\jupyterlab
[I 2023-04-24 11:48:21.032 LabApp] JupyterLab application directory is C:\Users\braunp\Anaconda3\share\jupyter\lab
[I 11:48:21.038 NotebookApp] Serving notebooks from local directory: C:\
[I 11:48:21.038 NotebookApp] Jupyter Notebook 6.4.12 is running at:
[I 11:48:21.038 NotebookApp] http://localhost:8888/?token=3d1eaa9114d187c5bda4ad08c57a07c70dcb88be65c03086
[I 11:48:21.038 NotebookApp] or http://127.0.0.1:8888/?token=3d1eaa9114d187c5bda4ad08c57a07c70dcb88be65c03086
[I 11:48:21.038 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 11:48:21.063 NotebookApp]

To access the notebook, open this file in a browser:
file:///C:/Users/braunp/AppData/Roaming/jupyter/runtime/nbserver-16852-open.html
Or copy and paste one of these URLs:
http://localhost:8888/?token=3d1eaa9114d187c5bda4ad08c57a07c70dcb88be65c03086
or http://127.0.0.1:8888/?token=3d1eaa9114d187c5bda4ad08c57a07c70dcb88be65c03086
```

Figure: Starting Jupyter Notebook

Quickstart: jupyter browser

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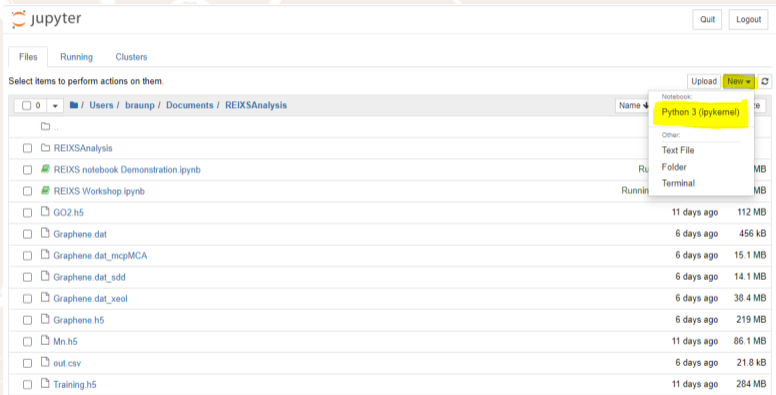
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The screenshot displays the JupyterLab web interface. At the top, there are 'Quit' and 'Logout' buttons. Below them are tabs for 'Files', 'Running', and 'Clusters'. A message says 'Select items to perform actions on them.' Below this is a breadcrumb path: '/ Users / braunp / Documents / REIXSAnalysis'. A file browser table lists various files and folders. A 'New' dropdown menu is open, showing options: 'Notebook', 'Python 3 (ipykernel)', 'Other:', 'Text File', 'Folder', and 'Terminal'. The 'Python 3 (ipykernel)' option is highlighted in yellow.

Name	Size	Modified
..		
REIXSAnalysis		
REIXS notebook Demonstration.ipynb		
REIXS Workshop.ipynb		
GO2.h5	112 MB	11 days ago
Graphene.dat	456 kB	6 days ago
Graphene.dat_mcpMCA	15.1 MB	6 days ago
Graphene.dat_sdd	14.1 MB	6 days ago
Graphene.dat_xeol	38.4 MB	6 days ago
Graphene.h5	219 MB	6 days ago
Mn.h5	86.1 MB	11 days ago
out.csv	21.8 kB	6 days ago
Training.h5	284 MB	11 days ago

Figure: Integrated file browser allows to choose directory

Quickstart: jupyter notebook

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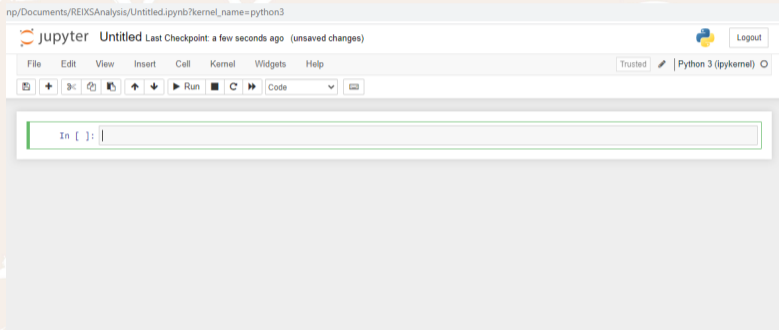


Figure: Empty Jupyter Notebook with python3 kernel

Quickstart: using the example import

```
# Import module to load REIXS scans from package  
from reixs.LoadData import *  
  
# Import bokeh plotting module  
from bokeh.io import output_notebook  
  
# Enable bokeh plotting within the notebook environment  
output_notebook(hide_banner=True)  
  
# Select the base directory  
# Can use absolute or relative path  
basedir = '.' # We choose the current folder
```

Quickstart: pattern to load data

```
# Scan analysis always follows the same pattern  
# (1) Create an object to load scans  
# (2) Load scans as desired  
# (3) Plot all loaded scans  
# (4) Export the scans to ASCII
```

```
scans = Load1d()  
scans.load(basedir, 'Training.h5', 'Mono Energy', 'TEY', 6)  
scans.load(basedir, 'Training.h5', 'Mono_  
↪Energy', 'PFY[0]', 6)  
scans.plot()  
scans.exporter()
```

Quickstart: output from the previous code

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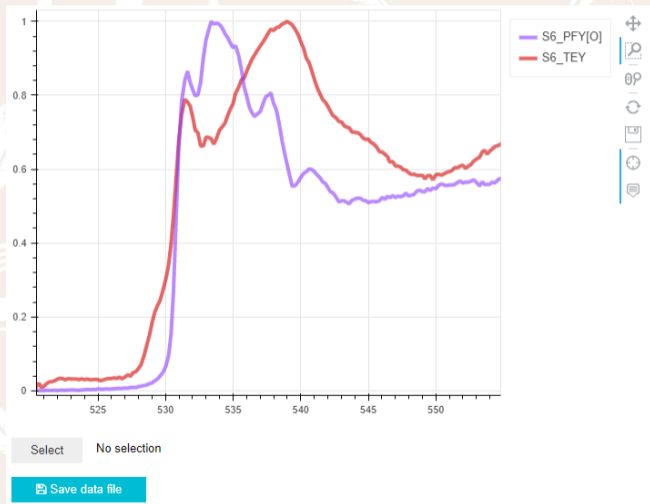
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Docstrings: Interactive Helptools are available by pressing Shift + Tab

```
In [7]: # Scan analysis always follows the same pattern
        # (1) Create an object to load scans
        # (2) Load scans as desired
        # (3) Plot all loaded scans
        # (4) Export the scans to ASCII

        scans = Load1d()
        scans.load(basedir, 'Training.h5', 'Mono Energy', 'TEY', 6)
        scans.plot()
```

Signature: scans.load(basedir, file, x_stream, y_stream, *args, **kwargs)

Docstring:

Load one or multiple specific scan(s) for selected streams.

Parameters

basedir : string

Specify the absolute or relative path to experimental data.

file : string

Specify the file name (either ASCII or HDF5).

x_stream : string

Specify the data for the horizontal axis.

Use: "Mono Energy", "MCP Energy", "SDD Energy", "XEOL Energy", "Points", or any SCA scalar array.

y_stream : string

Specify the data for the vertical axis.

Use: "TEY", "TFY", "PFY", "iPFY", "XES", "rXES", "specPFY",
"XRF", "rXRF", "XEOL", "rXEOL", "POV", "TOY", "EY", "Sample", "Mesh", "ET", or any SCA scalar array.

***args** : int

Separate scan numbers with comma.

****kwargs**: multiple, optional

Options:

norm : boolean

Norm the spectra to [0,1].

default: True

xoffset : list of tuples

Offset the x-axis by applying a polynomial fit.

Errors and Tracebacks: Intimidating but provide useful information

```
scans = Load1d()  
scans.load(basedir, 'Training.h5', 'Mono Energy', 'TEEY', 6)
```

```
KeyError: 'TEEY'
```

```
UserWarning: Stream not defined. Only mnemonics  
↳ supported! Special Stream not defined.
```

```
7 scans = Load1d()  
----> 8 scans.load(basedir, 'Training.h5', 'Mono  
↳ Energy', 'TEEY', 6)
```

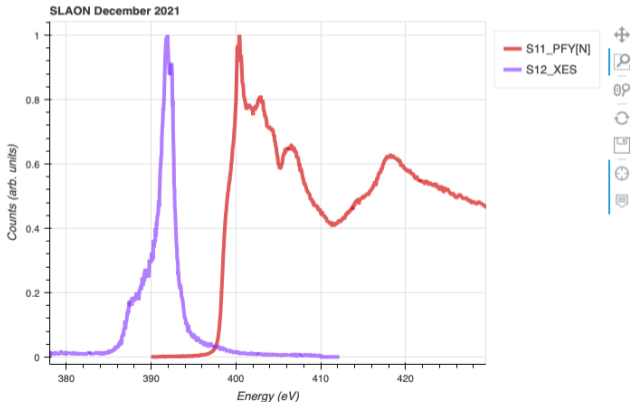
Plot x-ray emission and absorption spectra on common energy scale

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```
xas = Load1d()  
xas.load(basedir, 'Plate5_Ruhul.dat', 'Mono Energy', 'PFY[N]', 11, norm=True)  
xas.load(basedir, 'Plate5_Ruhul.dat', 'MCP Energy', 'XES', 12, norm=True, xoffset=[(377.9, 380), (382.8, 385)],  
xas.plot(xlabel='Energy (eV)', title='SLAON December 2021', ylabel='Counts (arb. units)')
```



Silicon Drift Detector Data at your fingertips

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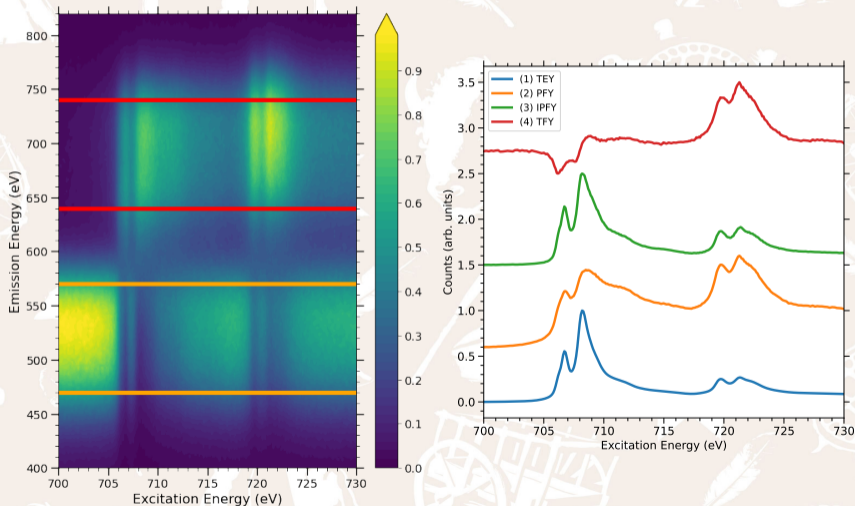
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- Descriptive information about a resource but does not include the actual experimental data
- Captures a snapshot of the beamline
- Useful to monitor beamline components and check beamline setup, i.e. time evolution of a specific PV
- Allows to log pertinent information for each scan and generate an automated experimental log, i.e. spreadsheet
- All information encapsulated in the HDF5 file

HDF5 Data Structure

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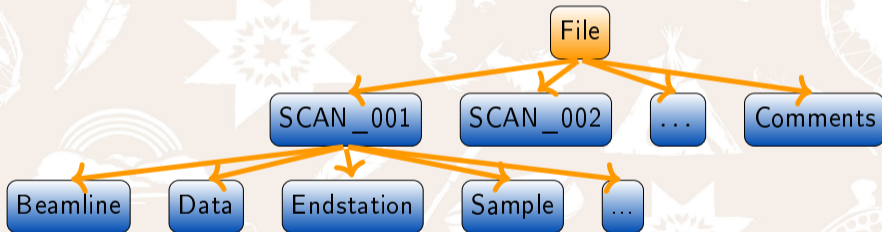
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Plot meta data as a function of scan number

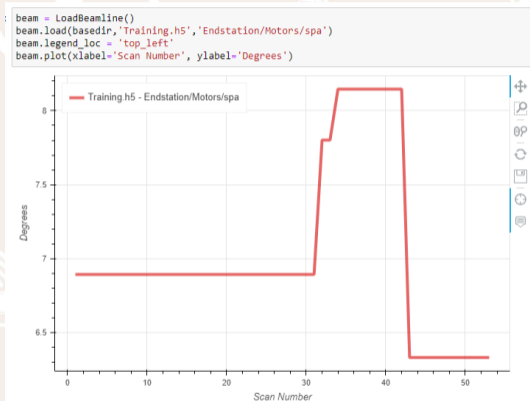


Figure: Variation of the spectrometer angle for the different scans in the data file.

Under Development: Generate measurement log from HDF5 entries

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	Command	Sample Stage (ssh)	SS (ssv)	SS (ssd)	Spectrom (XES dist)	SpectromFlux (XES angl)	4-Jaw (mm)	Mono G	Mono M	Polarizati	Status
3	ascan engy 559.998 559.998 19 30	0.45	-3.9	0	844.1715	6.893	8 Ni LEG	NICKEL	LINEAR H	Scan successfully com	
4	ascan engy 559.991 559.991 19 30	0.45	-3.9	0	844.1715	6.893	7.999 Ni LEG	NICKEL	LINEAR H	Scan successfully com	
5	rscan engy 530 560 150 1	0.45	-3.9	0	844.1715	6.893	8 Ni LEG	NICKEL	LINEAR H	Scan successfully com	
6	rscan engy 520 555 175 1	0.45	-3.9	0	844.1715	6.893	8 Ni LEG	NICKEL	LINEAR H	Scan successfully com	
7	rscan engy 520 528 40 530 20	0.45	-3.9	0	844.1715	6.893	7.999 Ni LEG	NICKEL	LINEAR H	Scan successfully com	

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- Focus on the science rather than the technicalities of data plotting
 - Make decisions on-the-fly
 - Use all information contained in multi-channel analyzers
- ⇒ Learn how to use the program now!

Questions & Resources

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Contact Information

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<https://github.com/pmb399/REIXSAnalysis>