Standardization of Brillouin data storage and processing

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Contents

1 BrimView web app

You can navigate to https://biobrillouin.org/brimview/ and the webapp should load directly from the browser. We currently only support the latest version of Chrome and Egde. Firefox can be used as well by activating JSPI (a page explaining how to do should automatically show on Firefox).

1.1 Loading sample data

Once the page finishes loading (it might take a few moments), you can load sample data using the dedicated widget, as highlighted in figure 1

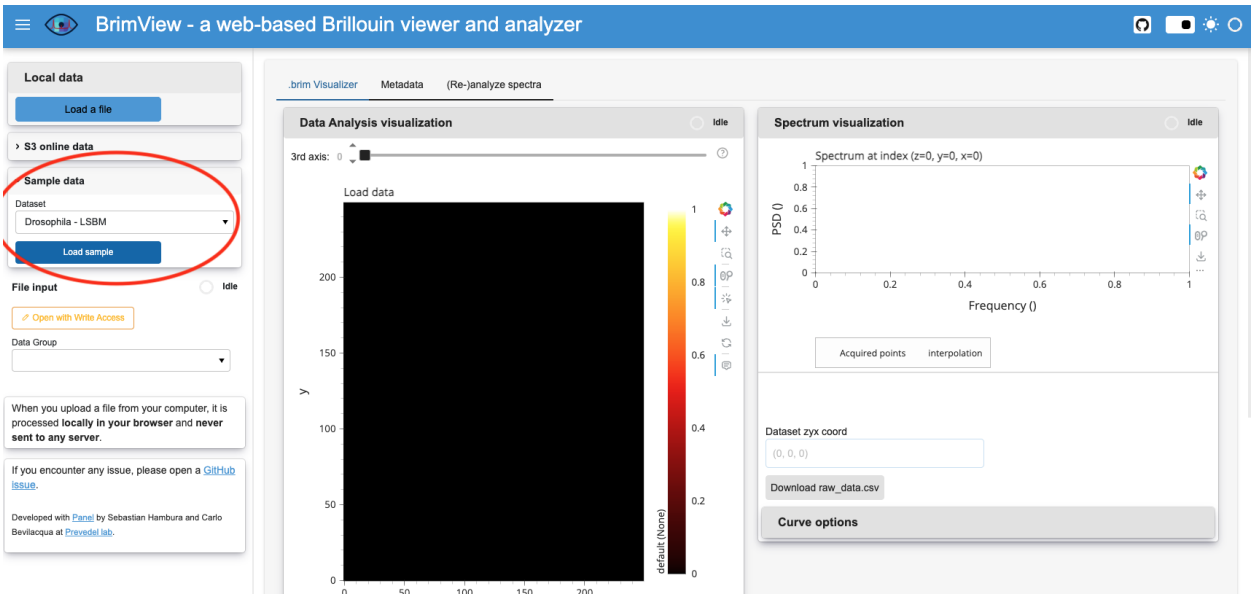


Figure 1: BrimView GUI. The widget to load sample data is encircled in red.

1.2 Exploring the data

Once the image is loaded you can click on any pixel and the corresponding spectrum will show on the right, including a table with the numerical values of the fitted parameters below (figure 2).

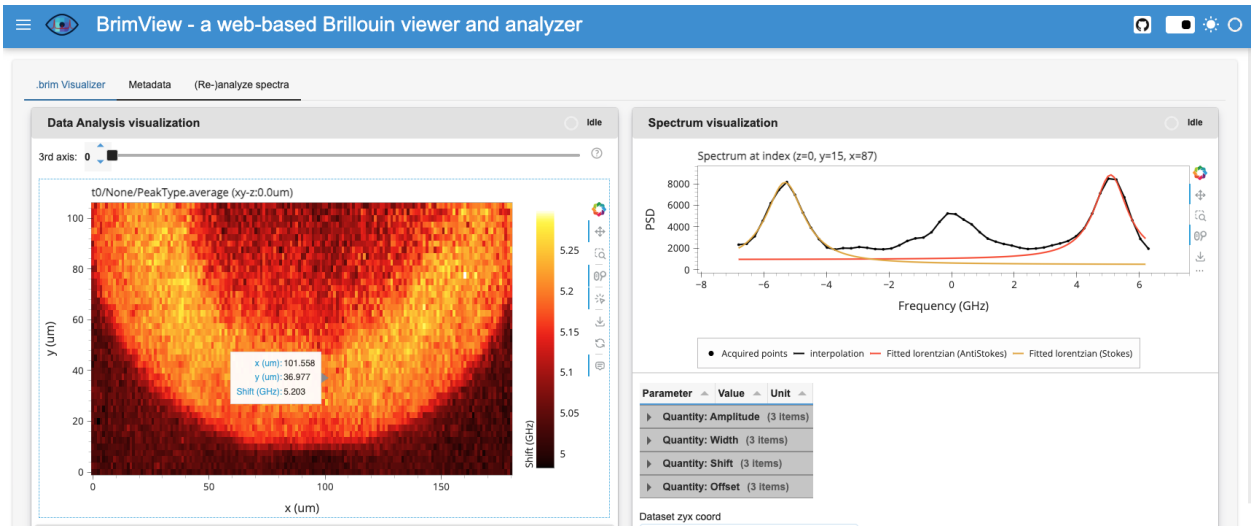


Figure 2: The spectrum and the corresponding fitted parameters can be displayed for each pixel in the image.

You can select which quantity (i.e. shift, linewidth, amplitude, ...), peak (i.e. Stokes, anti-Stokes, average), axis (x, y,z) and color range from the widgets below the image (figure 3).

Figure 3: Different settings for displaying the image can be selected from the widgets below the images.

2 Brimfile

2.1 The brim file format

We defined a new file format - brimfile (= Brillouin imaging) - with the intent of associating spatial maps to their corresponding spectral information and metadata in a well-defined yet general and flexible fashion. More information about the brimfile format can be found here.

2.2 The brimfile Python package

To easily save data to the brim file format or read from it, we developed a Python library called brimfile. The full documentation of the library can be found at https://prevedel-lab.github.io/brimfile/brimfile.html.

2.2.1 Installing brimfile

We recommend installing brimfile in a virtual environment.

After activating the new environment, simply run:

```
pip install brimfile
```

If you also need the support for exporting the analyzed data to OME-Tiff files, you can install the optional dependencies with:

```
pip install "brimfile[export-tiff]"
```

2.2.2 Writing to a brimfile

Let's first of all create a function that generate sample data:

```
import numpy as np

def generate_data():
    def lorentzian(x, x0, w):
        return 1/(1+((x-x0)/(w/2))**2)
    Nx, Ny, Nz = (7, 5, 3) # Number of points in x,y,z
```

```
    dx, dy, dz = (0.4, 0.5, 2) # Stepsizes (in um)
    n_points = Nx*Ny*Nz  # total number of points

    width_GHz = 0.4
    width_GHz_arr = np.full((Nz, Ny, Nx), width_GHz)
    shift_GHz_arr = np.empty((Nz, Ny, Nx))
    freq_GHz = np.linspace(6, 9, 151)  # 151 frequency points
    PSD = np.empty((Nz, Ny, Nx, len(freq_GHz)))
    for i in range(Nz):
        for j in range(Ny):
            for k in range(Nx):
                index = k + Nx*j + Ny*Nx*i
                #let's increase the shift linearly to have a readout
                shift_GHz = freq_GHz[0] + (freq_GHz[-1]-freq_GHz[0]) * index/
                    n_points
                spectrum = lorentzian(freq_GHz, shift_GHz, width_GHz)
                shift_GHz_arr[i,j,k] = shift_GHz
                PSD[i, j, k,:] = spectrum

    return PSD, freq_GHz, (dz,dy,dx), shift_GHz_arr, width_GHz_arr
```

We can create a brimfile by doing:

```
from brimfile import File, Data, Metadata, StoreType
from datetime import datetime

filename = 'path/to/your/file.brim.zip'

f = File.create(filename, store_type=StoreType.AUTO)
```

We can then add the spectral data:

```
PSD, freq_GHz, (dz,dy,dx), shift_GHz, width_GHz = generate_data()

d0 = f.create_data_group(PSD, freq_GHz, (dz,dy,dx), name='test1')
```

and the metadata:

```
Attr = Metadata.Item
datetime_now = datetime.now().isoformat()
temp = Attr(22.0, 'C')
md = d0.get_metadata()

md.add(Metadata.Type.Experiment, {'Datetime':datetime_now, 'Temperature':temp})
md.add(Metadata.Type.Optics, {'Wavelength':Attr(660, 'nm')})
# Add some metadata to the local data group
temp = Attr(37.0, 'C')
md.add(Metadata.Type.Experiment, {'Temperature':temp}, local=True)
```

We can also add the result of the fit:

```
ar = d0.create_analysis_results_group({'shift':shift_GHz, 'shift_units': 'GHz',
                                       'width': width_GHz, 'width_units':
                                           'Hz'},
                                      {'shift':shift_GHz, 'shift_units':
                                           'GHz',
                                       'width': width_GHz, 'width_units':
                                           'Hz'},
                                      name = 'test1_analysis')
```

We can finally close the file:

```
f.close()
```

2.2.3 Reading a brimfile

Reading from a brimfile follows a very similar logic as writing.

We first open the file:

```
from brimfile import File, Data, Metadata

filename = 'path/to/your/file.brim.zip'

f = File(filename)
```

We can list all the data group in the file and open the first one:

```
#list all the data groups in the file
data_groups = f.list_data_groups(retrieve_custom_name=True)

# get the first data group in the file
d = f.get_data()
```

We can read the metadata:

```
# get the metadata
md = d.get_metadata()
all_metadata = md.all_to_dict()
# the list of metadata is defined here https://github.com/prevedel-lab/Brillouin-standard-file/blob/main/docs/brim_file_metadata.md
time = md['Experiment.Datetime']
time.value
time.units
temp = md['Experiment.Temperature']
md_dict = md.to_dict(Metadata.Type.Experiment)
```

We can get the results of the analysis:

```
#get the list of analysis results in the data group
ar_list = d.list_AnalysisResults(retrieve_custom_name=True)
# get the first analysis results in the data group
ar = d.get_analysis_results()
```

and the corresponding image:

```
# get the image of the shift quantity for the average of the Stokes and anti-Stokes peaks
img, px_size = ar.get_image(Data.AnalysisResults.Quantity.Shift, Data.AnalysisResults.PeakType.average)
# get the units of the shift quantity
u = ar.get_units(Data.AnalysisResults.Quantity.Shift)
```

We can save the image as a TIFF:

```
ar_cls = Data.AnalysisResults
ar.save_image_to_OMETiff(ar_cls.Quantity.Shift, ar_cls.PeakType.average, filename='path/to/your/exported_tiff' )
```

We can also get the spectrum corresponding to a specific pixel:

```
coord = (1,3,4)
PSD, frequency, PSD_units, frequency_units = d.get_spectrum_in_image(coord)
```

We can finally close the file:

```
f.close()
```

3 HDF5_BLS package

3.1 Installation

The HDF5_BLS package is a Python package for creating BrimX files. It is compatible with Python 3.10 and above.

We recommend setting up a virtual environment to install the package. This can be done using the following command:

- On Mac terminal

```
python -m venv HDF5_BLS_venv
source HDF5_BLS_venv/bin/activate
```

- On Windows terminal

```
python -m venv HDF5_BLS_venv
HDF5_BLS_venv\Scripts\activate
```

On both OS, the package can be installed using pip:

```
pip install HDF5_BLS
```

3.2 An example

Here we propose to create a synthetic Brillouin dataset that we'll store in a BrimX file. We will store 3 different types of synthetic data:

- A single spectrum
- A synthetic time evolution
- A spatial mapping in 2D
- A z-stack of a sphere

3.2.1 Creating the data

We define a DHO function to create the Brillouin spectra.

```
def DHO(nu, nu0, gamma, a, b):
    return b + a * (gamma*nu0)**2/((nu**2-nu0**2)**2+(gamma*nu)**2)
```

We define a frequency axis to create the spectra.

```
nu = np.linspace(-15, 15, 1024)
```

We define the values of shift and linewidth for the different datasets to create:

- For the single spectrum, we set shift to 5 GHz and linewidth to 1 GHz, with an amplitude of 1 and no offset.

```
shift_0D = 5
linewidth_0D = 1
PSD_0D = DHO(nu, shift_0D, linewidth_0D, 1, 0)
```

- For the synthetic time evolution spectrum, we consider a shift rising quadratically from 5 to 6 GHz over time, a linewidth raising from 1 to 2 GHz linearly, and an amplitude of 1 with no offset.

```
time_1D = np.linspace(0, 10, 100)
shift_1D = 5 + time**2/100
linewidth_1D = np.linspace(1, 2, 100)
for s, l in zip(shift_1D, linewidth_1D):
    PSD_1D = DHO(nu, s, l, 1, 0)
```

- For the synthetic spatial mapping, we consider a diagonal shift gradient from 5 to 6 GHz over time, and a diagonal linewidth gradient from 1 to 2 GHz, and an amplitude of 1 with no offset.

```
gradient_x = np.linspace(0, 1, 50)
gradient_y = np.linspace(0, 1, 50)
temp = (np.outer(gradient_y, gradient_x) + np.outer(gradient_y, gradient_x)
    )/2
shift_2D = temp + 5
linewidth_2D = temp + 1
PSD_2D = np.zeros((50, 50, 1024))
for i in range(50):
    for j in range(50):
        PSD_2D[i, j] = DHO(nu, shift_2D[i, j], linewidth_2D[i, j], 1, 0)
```

- For the synthetic z-stack mapping, we consider a sphere with a shift of 6GHz and linewidth 2GHz in a solution of shift 5GHz and linewidth 1GHz, with an amplitude for all spectra of 1 and an offset of 0. The z-stack is made of 50 slices

```
x = np.linspace(-1, 1, 50)
y = np.linspace(-1, 1, 50)
z = np.linspace(-1, 1, 50)
shift_3D = np.zeros((50, 50, 50))
linewidth_3D = np.zeros((50, 50, 50))
PSD_3D = np.zeros((50, 50, 50, 1024))
for i in range(50):
    for j in range(50):
        for k in range(50):
            if (x[i]**2 + y[j]**2 + z[k]**2) > 1:
                shift_3D[i, j, k] = 5
                linewidth_3D[i, j, k] = 1
            else:
                shift_3D[i, j, k] = 6
                linewidth_3D[i, j, k] = 2
            PSD_3D[i, j, k] = DHO(nu, shift_3D[i, j, k], linewidth_3D[i, j,
                k], 1, 0)
```

We have provided in the joined Python script, options to visualize the created datasets.

3.2.2 Adding the data to a BrimX file

Here we're going to structure our file to store the four different datasets we've created. Each dataset will be stored in a separate group, and the group will be named with example names.

First we create the BrimX file at a given path, and define an object "wrp" to interact with it.

```
wrp = wrapper.Wrapper('path/to/file.h5')
```

For this example, we will structure the file as follows:

```
file.h5
|- Brillouin
|  |- A single spectrum
|  |- A time series
|  |- A mapping
|  |- A z-stack
```

In each of these groups, we will store the corresponding Power spectral density datasets, frequency array and shift and linewidth arrays. To do so, we will use the following code:

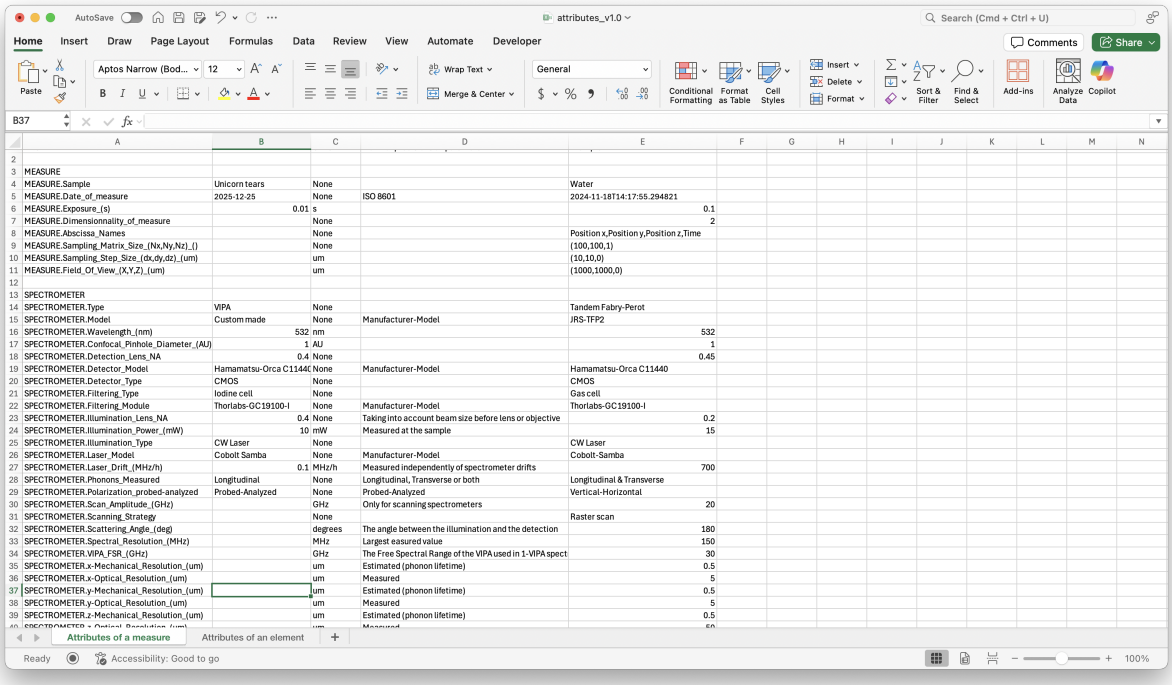
```
# Adding the 0D datasets
wrp.add_frequency(data=nu, parent_group="Brillouin/A single spectrum", name = "Frequency")
wrp.add_PSD(data=PSD_0D, parent_group="Brillouin/A single spectrum", name = "PSD")
wrp.add_treated_data(parent_group="Brillouin/A single spectrum", name_group = "Treated Data", shift = shift_0D, linewidth = linewidth_0D)

# Adding the 1D datasets
wrp.add_frequency(data=nu, parent_group="Brillouin/A time series", name = "Frequency")
wrp.add_PSD(data=PSD_1D, parent_group="Brillouin/A time series", name = "PSD")
wrp.add_treated_data(parent_group="Brillouin/A time series", name_group = "Treated Data", shift = shift_1D, linewidth = linewidth_1D)

# Adding the 2D datasets
wrp.add_frequency(data=nu, parent_group="Brillouin/A mapping", name = "Frequency")
wrp.add_PSD(data=PSD_2D, parent_group="Brillouin/A mapping", name = "PSD")
wrp.add_treated_data(parent_group="Brillouin/A mapping", name_group = "Treated Data", shift = shift_2D, linewidth = linewidth_2D)

# Adding the 3D datasets
wrp.add_frequency(data=nu, parent_group="Brillouin/A z-stack", name = "Frequency")
wrp.add_PSD(data=PSD_3D, parent_group="Brillouin/A z-stack", name = "PSD")
wrp.add_treated_data(parent_group="Brillouin/A z-stack", name_group = "Treated Data", shift = shift_3D, linewidth = linewidth_3D)
```

You are now the proud owner of a BrimX file containing synthetic Brillouin datasets!

3.2.3 Adding metadata to the BrimX file

To add metadata to the BrimX file, we will choose the easy way for this example, and just edit the standard spreadsheet given with the package and downloadable at this link: https://github.com/bio-brillouin/HDF5_BLS/blob/main/spreadsheets/attributes_v1.0.xlsx.

A list of established parameters is given, their name, units and definition is written in the different columns. For this example, we are filling the datasheet as presented on figure 4.



	A	B	C	D	E
2					
3	MEASURE				
4	MEASURE.Sample	Unicorn tears	None		Water
5	MEASURE.Date_of_measure	2025-12-25	None	ISO 8601	2024-11-18T14:17:55.294821
6	MEASURE.Exposure_(s)	0.01	s		0.1
7	MEASURE.Dimensionnality_of_measure		None		2
8	MEASURE.Abscissa_Names		None		Position x,Position y,Position z,Time
9	MEASURE.Sampling_Matrix_Size_(Nx,Ny,Nz)_()		None		(100,100,1)
10	MEASURE.Sampling_Step_Size_(dx,dy,dz)_(um)		um		(10,10,0)
11	MEASURE.Field_Of_View_(X,Y,Z)_(um)		um		(1000,1000,0)
12					
13	SPECTROMETER				
14	SPECTROMETER.Type	VIPA	None		Tandem Fabry-Perot
15	SPECTROMETER.Model	Custom made	None	Manufacturer-Model	JRS-TFP2
16	SPECTROMETER.Wavelength_(nm)	532	nm		532
17	SPECTROMETER.Confocal_Pinhole_Diameter_(AU)	1	AU		1
18	SPECTROMETER.Detection_Lens_NA	0.4	None		0.45
19	SPECTROMETER.Detector_Model	Hamamatsu-Orca C1144(	None	Manufacturer-Model	Hamamatsu-Orca C11440
20	SPECTROMETER.Detector_Type	CMOS	None		CMOS
21	SPECTROMETER.Filtering_Type	Iodine cell	None		Gas cell
22	SPECTROMETER.Filtering_Module	Thorlabs-GC19100-I	None	Manufacturer-Model	Thorlabs-GC19100-I
23	SPECTROMETER.Illumination_Lens_NA	0.4	None	Taking into account beam size before lens or objective	0.2
24	SPECTROMETER.Illumination_Power_(mW)	10	mW	Measured at the sample	15
25	SPECTROMETER.Illumination_Type	CW Laser	None		CW Laser
26	SPECTROMETER.Laser_Model	Cobolt Samba	None	Manufacturer-Model	Cobolt-Samba
27	SPECTROMETER.Laser_Drift_(MHz/h)	0.1	MHz/h	Measured independently of spectrometer drifts	700
28	SPECTROMETER.Phonons_Measured	Longitudinal	None	Longitudinal, Transverse or both	Longitudinal & Transverse
29	SPECTROMETER.Polarization_probed-analyzed	Probed-Analyzed	None	Probed-Analyzed	Vertical-Horizontal
30	SPECTROMETER.Scan_Amplitude_(GHz)		GHz	Only for scanning spectrometers	20
31	SPECTROMETER.Scanning_Strategy		None		Raster scan
32	SPECTROMETER.Scattering_Angle_(deg)		degrees	The angle between the illumination and the detection	180
33	SPECTROMETER.Spectral_Resolution_(MHz)		MHz	Largest easured value	150
34	SPECTROMETER.VIPA_FSR_(GHz)		GHz	The Free Spectral Range of the VIPA used in 1-VIPA spect	30
35	SPECTROMETER.x-Mechanical_Resolution_(um)		um	Estimated (phonon lifetime)	0.5
36	SPECTROMETER.x-Optical_Resolution_(um)		um	Measured	5
37	SPECTROMETER.y-Mechanical_Resolution_(um)		um	Estimated (phonon lifetime)	0.5
38	SPECTROMETER.y-Optical_Resolution_(um)		um	Measured	5
39	SPECTROMETER.z-Mechanical_Resolution_(um)		um	Estimated (phonon lifetime)	0.5

Figure 4: Example of the filled datasheet used to add metadata to the BrimX file

You can of course play with this file, add your own parameters, change the values for the ones given, add values for the ones not given, etc. We recommend however not changing the name of the parameters so that all the community calls the same parameters the same way.

You can then save the file at your prefered location, and apply it to the BrimX file you just created. To do so, you can use the following code:

```
wrp.import_properties_data(filepath='local_use/example_attributes.xlsx')
```

This line of code applies the metadata to the whole BrimX file. You can also apply metadata to a specific group by adding the argument "parent_group" to the function:

```
wrp.import_properties_data(filepath='local_use/example_attributes.xlsx', path =
    "Brillouin/A z-stack")
```

3.3 Template for integrating BrimX files to your workflow

You can now try integrating the use of BrimX files in your workflow. Note that the example we showed above is limited to 4 kinds of datasets (frequency, PSD, shift and linewidth). The format can handle a total of 13 different kinds of datasets that are defined in the documentation of the package: https://github.com/bio-brillouin/HDF5_BLS/blob/main/guides/Tutorial/Tutorial.pdf.

Here is a base template to get you started:

```
import HDF5_BLS as bls

# Create a BrimX file
wrp = bls.Wrapper(filepath = "path/to/file.h5")

################################################################################
# Existing code to extract data from a file
################################################################################
```

```
# Storing the data in the HDF5 file (for this example we use a random array)
data = np.random.random((50, 50, 512))
wrp.add_raw_data(data = data, parent_group = "Brillouin", name = "Raw data")

################################################################################
# Existing code to convert the data to a PSD
################################################################################
# Storing the Power Spectral Density in the HDF5 file together with the
    associated frequency array (for this example we use random arrays)
PSD = np.random.random((50, 50, 512))
frequency = np.arange(512)
wrp.add_PSD(data = PSD, parent_group = "Brillouin", name = "Power Spectral
    Density")
wrp.add_frequency(data = frequency, parent_group = "Brillouin", name = "
    Frequency")

################################################################################
# Existing code to fit the PSD to extract shift and linewidth arrays
################################################################################
# Storing the Power Spectral Density in the HDF5 file together with the
    associated frequency array (for this example we use random arrays)
shift = np.random.random((50, 50))
linewidth = np.random.random((50, 50))
wrp.add_treated_data(parent_group = "Brillouin", name_group = "Treat_0", shift =
     shift, linewidth = linewidth)
```

3.4 Extracting data from the BrimX file

You can now interact directly with the BrimX file as any other file storing data. To extract a dataset located at a known path in the file, you can use the following line of code:

```
dataset = wrp["path/to/dataset/in/the/file"][:]
```

For example, using the example BrimX file we created in this tutorial, you can extract the PSD of the first spectrum using the following code:

```
psd = wrp["Brillouin/A single spectrum/PSD"][:]
```

The paths can be obtained by visualizing the file as explained in the next section.

3.5 Visualizing the BrimX file

3.5.1 Online

You can visualize the BrimX file online using the myhdf5 web application: https://myhdf5.hdfgroup.org. This application runs locally in your web browser so you can use it safely even to observe sensitive data.

When you open the application, you can upload your BrimX file and explore its contents either by clicking the "Select HDF5 File" button or by dragging and dropping your file in the window (figure 5).

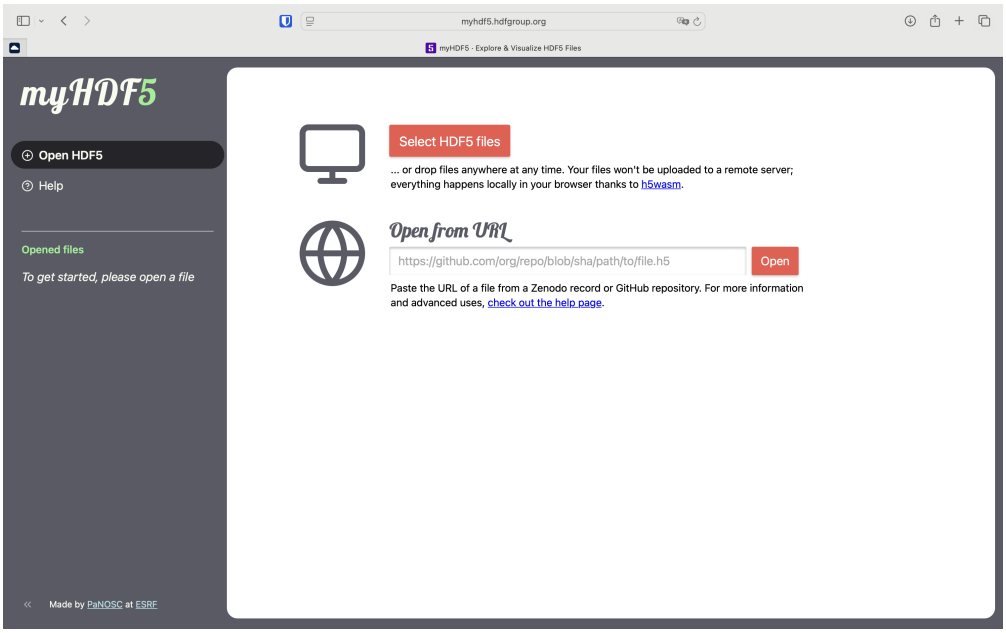


Figure 5: The welcome window of the myhdf5 application

Once your file is loaded, you can explore its contents on the left panel (figure 6).

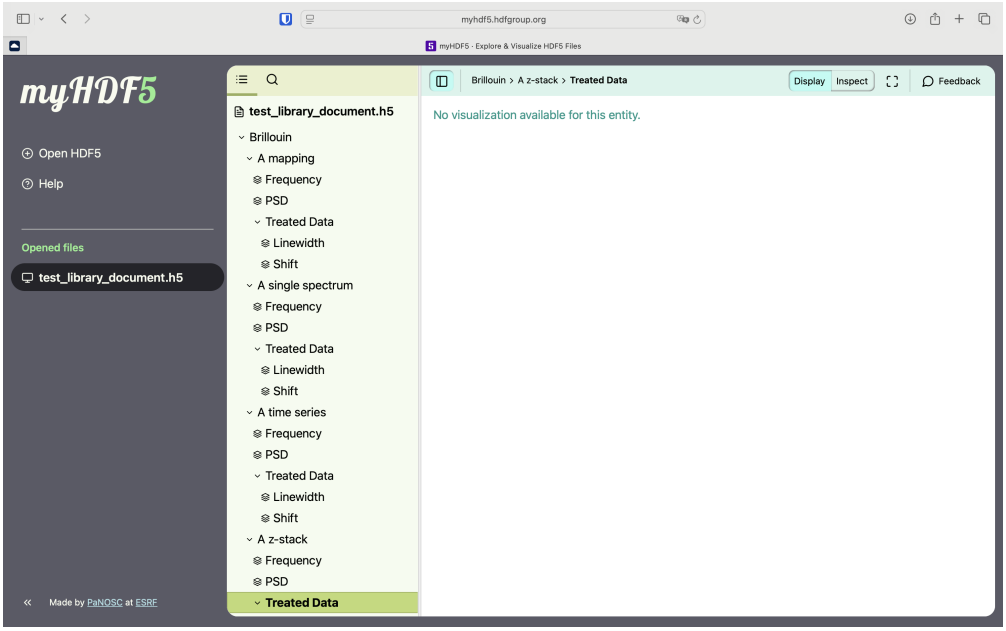


Figure 6: The developed structure view of your HDF5 file in the myhdf5 application

From there you can explore the file, visualize attributes (figure 7) and datasets of any dimension (figure 8).

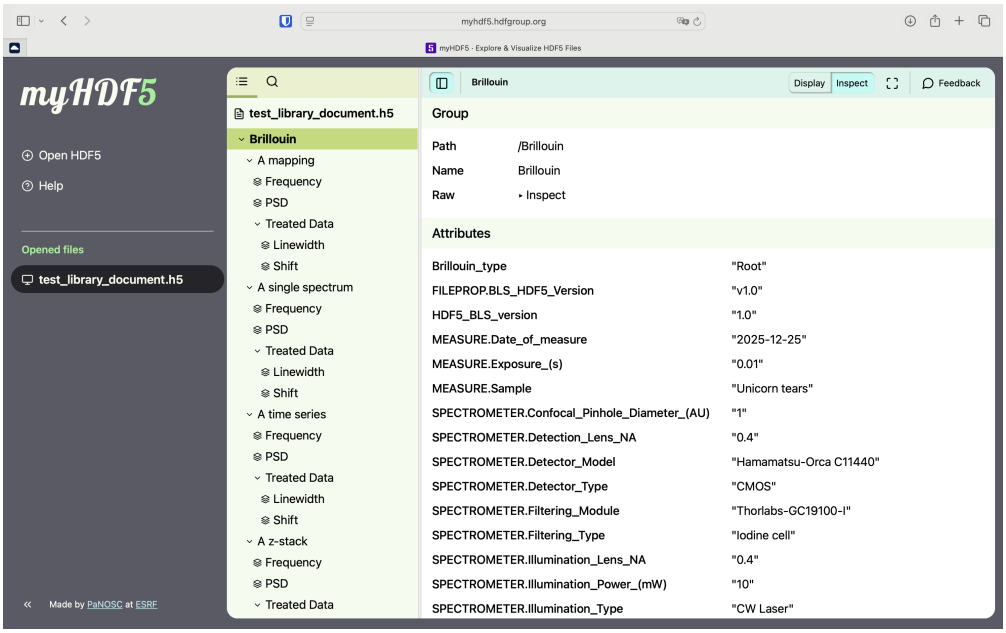


Figure 7: Visualizing the attributes stored in the "Brillouin" group

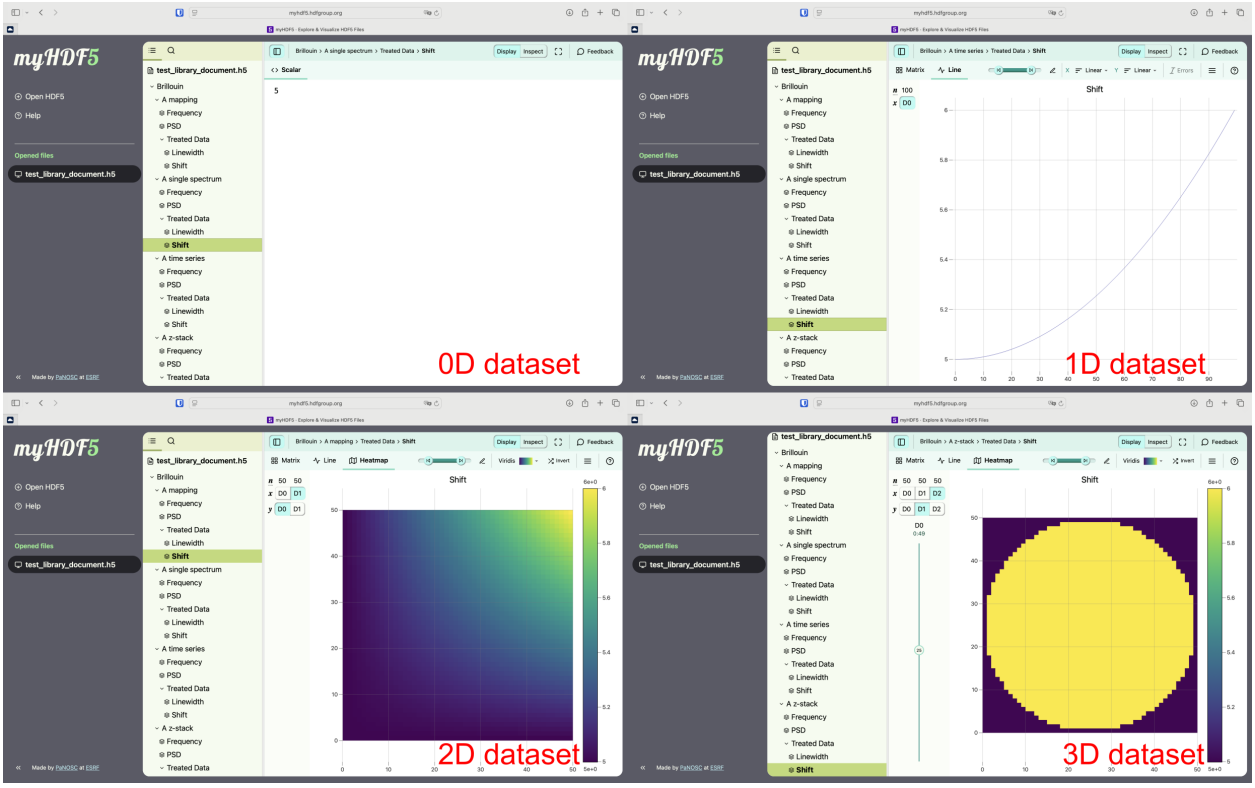


Figure 8: Visualizing the datasets using the MyHDF5 web application

3.5.2 Using Panoply

Panoply is an application developed by NASA to visualize geo-referenced data and more generally HDF5 files. It can be downloaded for free at this link: https://www.giss.nasa.gov/tools/panoply/.

Here are some screenshots of the application with the example file we created in this tutorial:

Figure 9: A simple visualization of the HDF5 file structure using the Panoply application

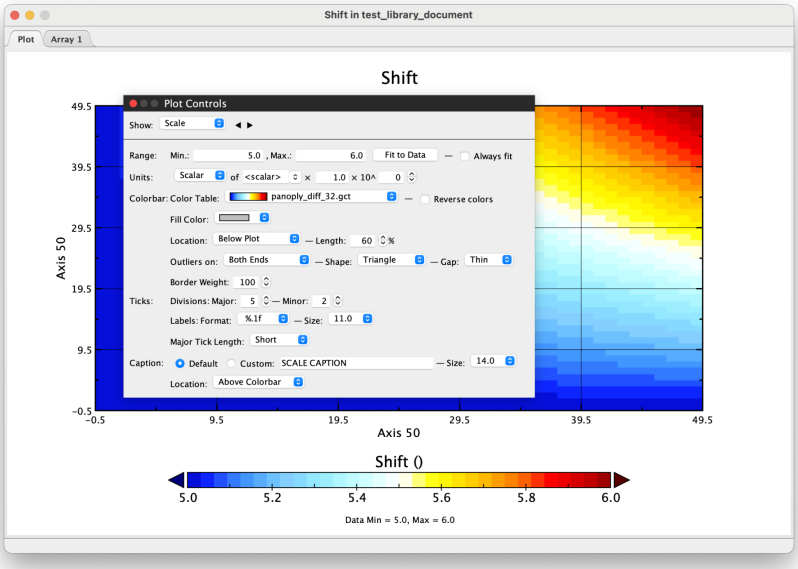


Figure 10: Visualizing datasets using the Panoply application

3.6 The HDF5_BLS_GUI

The HDF5_BLS_GUI is a graphical user interface for the HDF5_BLS package, designed to facilitate the exploration and analysis of HDF5 files. It provides a user-friendly environment for users to create and interact with their data. The GUI is meant to evolve to allow users to treat their data from it, but these developments are still in a beta phase.

To use the GUI, you need to install the package. Follow the instructions below:

- Clone the repository: `git clone https://github.com/yourusername/HDF5_BLS.git`
- Navigate to the directory: `cd HDF5_BLS`
- Install the packages for the library: `pip install -r requirements_library.txt`
- Install the packages for the GUI: `pip install -r requirements_GUI.txt`
- Run the GUI: `python HDF5_BLS_GUI/main.py`

You should see the HDF5_BLS_GUI window appear on your screen (figure 11).

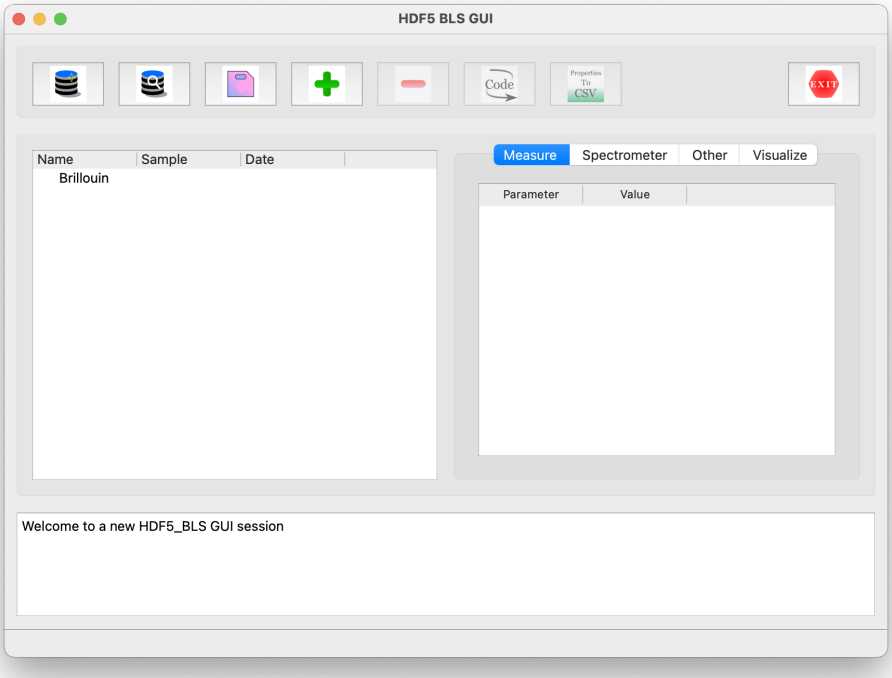


Figure 11: The welcome window of the HDF5_BLS_GUI

You can then drag and drop your data into the left panel if its addition is already supported by the GUI. If not, you'll be forced to add it from script.

You can then structure your file by creating groups, renaming them, dragging files from groups to groups, and generally use the GUI as you would a normal file explorer.

When adding a data, the GUI automatically creates a new group in the HDF5 file. You can change the name of the group by double clicking on it. You can also drag excel files with properties to the right panel to apply metadata to groups.

You can of course drag and drop the BrimX file we have created in this tutorial to the left panel to see its structure (figure 12).

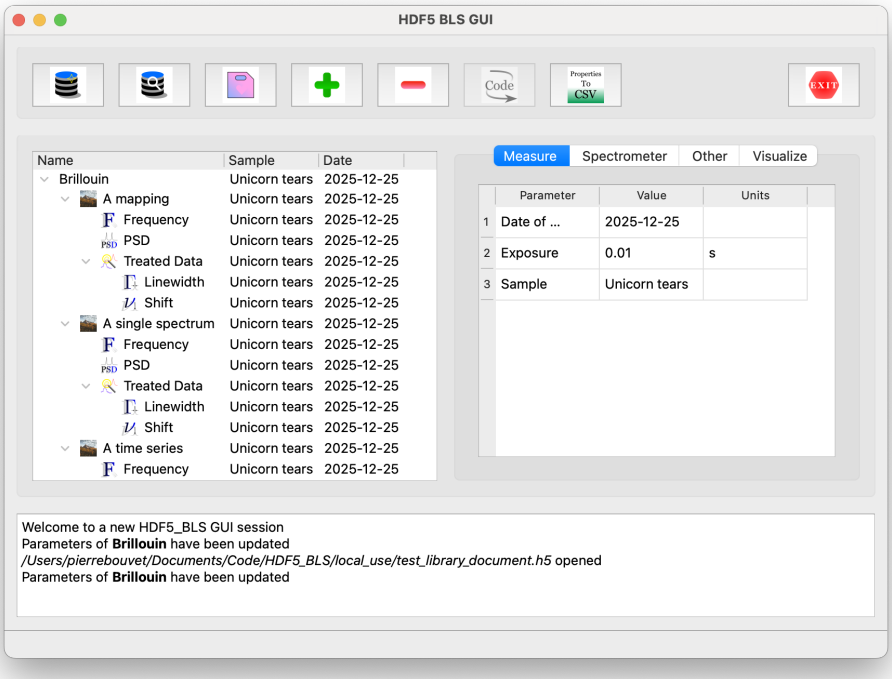


Figure 12: The structure of the example BrimX file in the HDF5_BLS_GUI

This GUI is still in development, so don't hesitate to report bugs or suggest features on the GitHub repository: https://github.com/bio-brillouin/HDF5_BLS/issues.

3.7 Ending remarks

In this tutorial, we have covered the basics of using the HDF5_BLS_GUI for exploring and managing HDF5 files. We encourage you to experiment with the GUI and provide feedback to help us improve it. You can directly contact me at pierre.bouvet@meduniwien.ac.at !

Thank you for your help! Happy Brillouin data handling!