

# Standardization of Brillouin data storage and processing

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## 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 Edge. 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

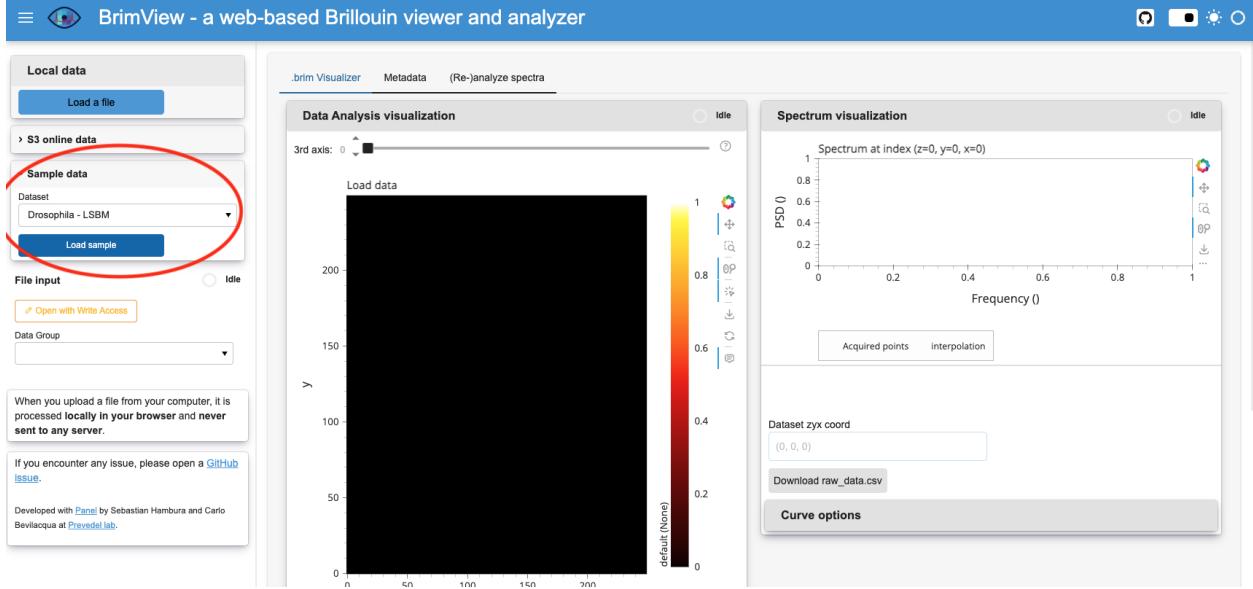


Figure 1: BrimView GUI. The widget to load sample data is encircled in red.

## 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).

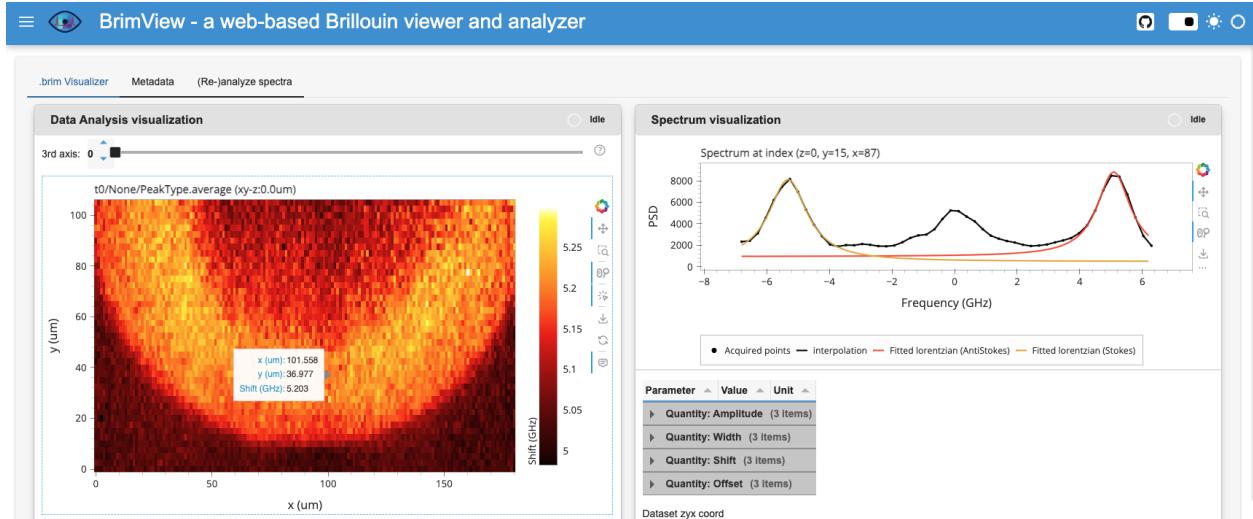


Figure 2: The spectrum and the corresponding fitted parameters can be displayed for each pixel in the image.

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).

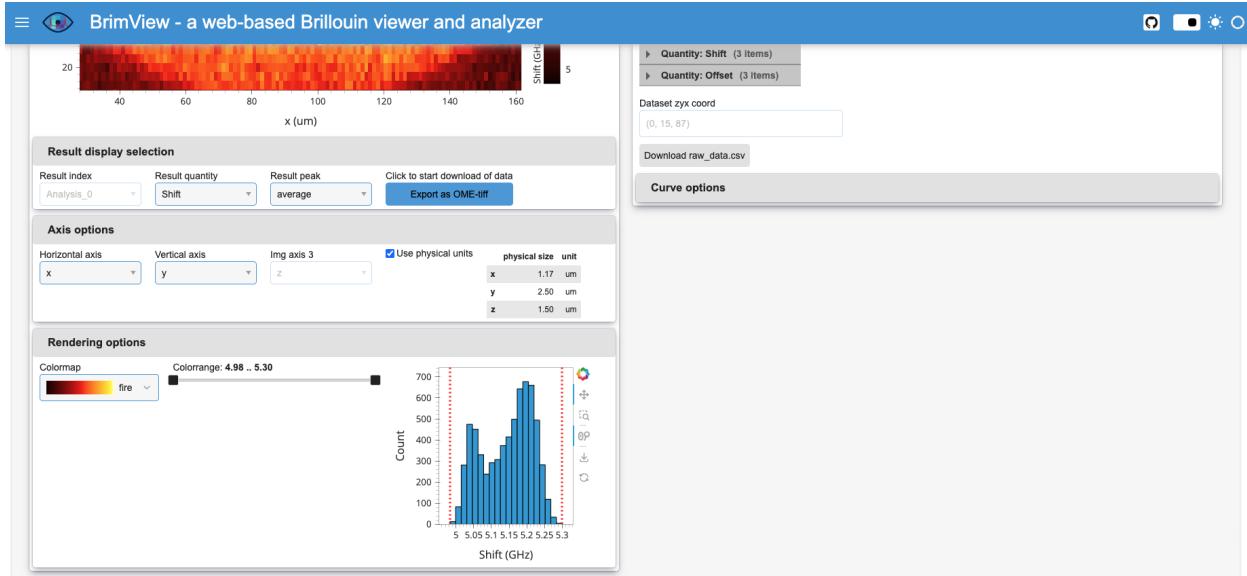


Figure 3: Different settings for displaying the image can be selected from the widgets below the images.

## 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:

```
1 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:

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

#### 2.2.2 Writing to a brimfile

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

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

```

7     dx , dy , dz = (0.4, 0.5, 2) # Stepsizes (in um)
8     n_points = Nx*Ny*Nz # total number of points
9
10    width_GHz = 0.4
11    width_GHz_arr = np.full((Nx, Ny, Nz), width_GHz)
12    shift_GHz_arr = np.empty((Nx, Ny, Nz))
13    freq_GHz = np.linspace(6, 9, 151) # 151 frequency points
14    PSD = np.empty((Nx, Ny, Nz, len(freq_GHz)))
15    for i in range(Nz):
16        for j in range(Ny):
17            for k in range(Nx):
18                index = k + Nx*j + Ny*Nx*i
19                #let's increase the shift linearly to have a readout
20                shift_GHz = freq_GHz[0] + (freq_GHz[-1]-freq_GHz[0]) * index/
21                n_points
22                spectrum = lorentzian(freq_GHz, shift_GHz, width_GHz)
23                shift_GHz_arr[i,j,k] = shift_GHz
24                PSD[i, j, k,:] = spectrum
25
26    return PSD, freq_GHz, (dz,dy,dx), shift_GHz_arr, width_GHz_arr

```

We can create a brimfile by doing:

```

1 from brimfile import File, Data, Metadata, StoreType
2 from datetime import datetime
3
4 filename = 'path/to/your/file.brim.zip'
5
6 f = File.create(filename, store_type=StoreType.AUTO)

```

We can then add the spectral data:

```

1 PSD, freq_GHz, (dz,dy,dx), shift_GHz, width_GHz = generate_data()
2
3 d0 = f.create_data_group(PSD, freq_GHz, (dz,dy,dx), name='test1')

```

and the metadata:

```

1 Attr = Metadata.Item
2 datetime_now = datetime.now().isoformat()
3 temp = Attr(22.0, 'C')
4 md = d0.get_metadata()
5
6 md.add(Metadata.Type.Experiment, {'Datetime':datetime_now, 'Temperature':temp})
7 md.add(Metadata.Type.Optics, {'Wavelength':Attr(660, 'nm')})
8 # Add some metadata to the local data group
9 temp = Attr(37.0, 'C')
10 md.add(Metadata.Type.Experiment, {'Temperature':temp}, local=True)

```

We can also add the result of the fit:

```

1 ar = d0.create_analysis_results_group({'shift':shift_GHz, 'shift_units': 'GHz',
2                                         'width': width_GHz, 'width_units':
3                                         'Hz'},
4                                         {'shift':shift_GHz, 'shift_units':
5                                         'GHz',
6                                         'width': width_GHz, 'width_units':
7                                         'Hz'},
8                                         name = 'test1_analysis')

```

We can finally close the file:

```

1 f.close()

```

### 2.2.3 Reading a brimfile

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

We first open the file:

```
1 from brimfile import File, Data, Metadata
2
3 filename = 'path/to/your/file.brim.zip'
4
5 f = File(filename)
```

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

```
1 #list all the data groups in the file
2 data_groups = f.list_data_groups(retrieve_custom_name=True)
3
4 # get the first data group in the file
5 d = f.get_data()
```

We can read the metadata:

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

We can get the results of the analysis:

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

and the corresponding image:

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

We can save the image as a TIFF:

```
1 ar_cls = Data.AnalysisResults
2 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:

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

We can finally close the file:

```
1 f.close()
```

## 3 HDF5\_BLS package

The HDF5\_BLS package is a Python package for creating BrimX files, a file format based on HDF5, designed to support all Brillouin-related data in a human-readable way, and be integrated to all existing workflows of the community. It is compatible with Python 3.10 and above.

### 3.1 Installation

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

- On Mac terminal

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

- On Windows terminal

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

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

```
1 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

Let's define a general DHO function to create the Brillouin spectra.

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

Let's now define a frequency axis to create the spectra.

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

Let's now build synthetic datasets to image different scenarios:

- 0D: Let's say we have a single spectrum, with a Brillouin shift of 5 GHz and linewidth of 1 GHz. Let's give the spectrum an amplitude of 1 and no offset.

```
1 shift_OD = 5  
2 linewidth_OD = 1  
3 PSD_OD = DHO(nu, shift_OD, linewidth_OD, 1, 0)
```

- 1D: Let's do the same for a 1D dataset now, let's think about a simple time evolution of a sample, where the shift rises quadratically from 5 to 6 GHz over time, and the linewidth from 1 to 2 GHz linearly. Here again, let's keep an amplitude of 1 with no offset.

```

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

```

- 2D: Let's consider a mapping showing a diagonal shift gradient from 5 to 6 GHz, and a diagonal linewidth gradient from 1 to 2 GHz. We keep an amplitude of 1 with no offset.

```

1 gradient_x = np.linspace(0, 1, 50)
2 gradient_y = np.linspace(0, 1, 50)
3 temp = (np.outer(gradient_y, gradient_x) + np.outer(gradient_y, gradient_x))
4 /2
5 shift_2D = temp + 5
6 linewidth_2D = temp + 1
7 PSD_2D = np.zeros((50, 50, 1024))
8 for i in range(50):
9     for j in range(50):
10        PSD_2D[i, j] = DHO(nu, shift_2D[i, j], linewidth_2D[i, j], 1, 0)

```

- 3D: Let's now think about a z-stack. In this example we'll do a z-stack of a sphere embedded in a solution. The solution will have a shift of 5GHz and linewidth 1GHz, while the sphere will have a shift of 6GHz and linewidth 2GHz. Again, we'll keep an amplitude of 1 with no offset. Again, we have an amplitude of 1 and an offset of 0 for all spectra.

```

1 x = np.linspace(-1, 1, 50)
2 y = np.linspace(-1, 1, 50)
3 z = np.linspace(-1, 1, 50)
4 shift_3D = np.zeros((50, 50, 50))
5 linewidth_3D = np.zeros((50, 50, 50))
6 PSD_3D = np.zeros((50, 50, 50, 1024))
7 for i in range(50):
8     for j in range(50):
9         for k in range(50):
10            if (x[i]**2 + y[j]**2 + z[k]**2) > 1:
11                shift_3D[i, j, k] = 5
12                linewidth_3D[i, j, k] = 1
13            else:
14                shift_3D[i, j, k] = 6
15                linewidth_3D[i, j, k] = 2
16            PSD_3D[i, j, k] = DHO(nu, shift_3D[i, j, k], linewidth_3D[i, j, k], 1, 0)

```

You can of course look at the PSD, shift and linewidth arrays with your favorite visualization tools (e.g. matplotlib).

### 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 that we'll name with example names.

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

```

1 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'll store the corresponding Power spectral density datasets, frequency array and shift and linewidth arrays. To do so, we will use the three following functions:

- "add\_frequency": to store the frequency array
- "add\_PSD": to store the Power spectral density array
- "add\_treated\_data": to store the shift and linewidth arrays

Each of these functions work the same way:

1. You indicate the dataset to add.
2. You specify where the dataset will be stored in the file (argument "parent\_group").
3. You provide a name for the dataset (argument "name").

Because you might need in the future to add other treatment modalities, we have made it so that all the datasets obtained after treatment are added in a same group. Therefore instead of "name" the "add\_treated\_data" function takes "name\_group" as argument, which is the name of the group where all the treated datasets will be stored. The names of the datasets themselves will be the type of data by default (e.g. "Shift" for the shift array, "Linewidth" for the linewidth array, etc.).

With the provided code, this gives us:

```

1 # Adding the 0D datasets
2 wrp.add_frequency(data=nu, parent_group="Brillouin/A single spectrum", name = "Frequency")
3 wrp.add_PSD(data=PSD_0D, parent_group="Brillouin/A single spectrum", name = "PSD")
4 wrp.add_treated_data(parent_group="Brillouin/A single spectrum", name_group = "Treated Data", shift = shift_0D, linewidth = linewidth_0D)
5
6 # Adding the 1D datasets
7 wrp.add_frequency(data=nu, parent_group="Brillouin/A time series", name = "Frequency")
8 wrp.add_PSD(data=PSD_1D, parent_group="Brillouin/A time series", name = "PSD")
9 wrp.add_treated_data(parent_group="Brillouin/A time series", name_group = "Treated Data", shift = shift_1D, linewidth = linewidth_1D)
10
11 # Adding the 2D datasets
12 wrp.add_frequency(data=nu, parent_group="Brillouin/A mapping", name = "Frequency")
13 wrp.add_PSD(data=PSD_2D, parent_group="Brillouin/A mapping", name = "PSD")
14 wrp.add_treated_data(parent_group="Brillouin/A mapping", name_group = "Treated Data", shift = shift_2D, linewidth = linewidth_2D)
15
16 # Adding the 3D datasets
17 wrp.add_frequency(data=nu, parent_group="Brillouin/A z-stack", name = "Frequency")
18 wrp.add_PSD(data=PSD_3D, parent_group="Brillouin/A z-stack", name = "PSD")
19 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!

Note: you can add other types of datasets to the BrimX file. The available types are:

- "Frequency" with the function "add\_frequency"
- "PSD" with the function "add\_PSD"
- "Other" with the function "add\_other", this can be anything you want to store (grayscale images, Raman spectra, fluorescence maps...)
- "Raw Data" with the function "add\_raw\_data", where you can store your data "as is" (what the spectrometer returns).
- "Abscissa" with the function "add\_abscissa" to add abscissa for your axis. Please refer to footnote <sup>1</sup>

You can also add other types of datasets after treatment, in that case you will use the "add\_treated\_data" function and just specify the datasets you want to add from this list:

- A record of shift values -> argument "shift"
- A record of linewidth values -> argument "linewidth"
- A record of the values of amplitude -> argument "amplitude"
- Values for the loss tangent -> argument "BLT"
- A record for the errors on the shift values -> argument "shift\_err"
- A record for the errors on the linewidth values -> argument "linewidth\_err"
- A record for the errors on the amplitude values -> argument "amplitude\_err"
- A record for the errors on the BLT values -> argument "BLT\_err"

### 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](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.

---

<sup>1</sup>In that case, you need to provide, aside from the dataset itself, the place where to store it and its name, the units of the abscissa (attribute "unit" given as a string, for example "mm" or "K"), the first dimension of the PSD it applies to and the last dimension of the PSD it applies to (attributes "dim\_start" and "dim\_end" respectively, given as integers and with the usual convention: starting from 0, starting index included, ending index excluded). For example:

```

1 t = np.linspace(0,10,100) # 100 values of time ranging from 0 to 10s
2 PSD = np.random.random((100,512)) # 100 PSD associated to the time array
3 wrp.add_PSD(data = PSD, parent_group = "Brillouin/A new time series", name =
   "PSD")
4 wrp.add_abscissa(data = t, parent_group = "Brillouin/A new time series",
   name = "Time", unit = "s", dim_start = 0, dim_end = 1)

```

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 names of the existing parameters so that all the community calls the same parameters the same way.

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

```
1 wrp.import_properties_data(filepath='path/to/attributes.xlsx')
```

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

```
1 wrp.import_properties_data(filepath='path/to/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](https://github.com/bio-brillouin/HDF5_BLS/blob/main/guides/Tutorial/Tutorial.pdf).

Here is a base template to get you started:

```
1 import HDF5_BLS as bls
2
3 # Create a BrimX file
4 wrp = bls.Wrapper(filepath = "path/to/file.h5")
5
6 ######
7 # Existing code to extract data from a file
8 ######
```

```

9 # Storing the data in the HDF5 file (for this example we use a random array)
10 data = np.random.random((50, 50, 512))
11 wrp.add_raw_data(data = data, parent_group = "Brillouin", name = "Raw data")
12
13 ##########
14 # Existing code to convert the data to a PSD
15 #####
16 # Storing the Power Spectral Density in the HDF5 file together with the
17 # associated frequency array (for this example we use random arrays)
17 PSD = np.random.random((50, 50, 512))
18 frequency = np.arange(512)
19 wrp.add_PSD(data = PSD, parent_group = "Brillouin", name = "Power Spectral
20 Density")
20 wrp.add_frequency(data = frequency, parent_group = "Brillouin", name =
21 Frequency)
21
22 ##########
23 # Existing code to fit the PSD to extract shift and linewidth arrays
24 #####
25 # Storing the Power Spectral Density in the HDF5 file together with the
26 # associated frequency array (for this example we use random arrays)
26 shift = np.random.random((50, 50))
27 linewidth = np.random.random((50, 50))
28 wrp.add_treated_data(parent_group = "Brillouin", name_group = "Treat_0", shift =
28     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:

```
1 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:

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

To extract the metadata that is applied to an element of the file, you can use the following code:

```
1 metadata = wrp.get_attributes("Brillouin/A single spectrum/PSD")
```

This will list all the metadata applied to the dataset located at the given path (in that case the PSD of the single spectrum).

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). Let's try with the example file we created in this tutorial.

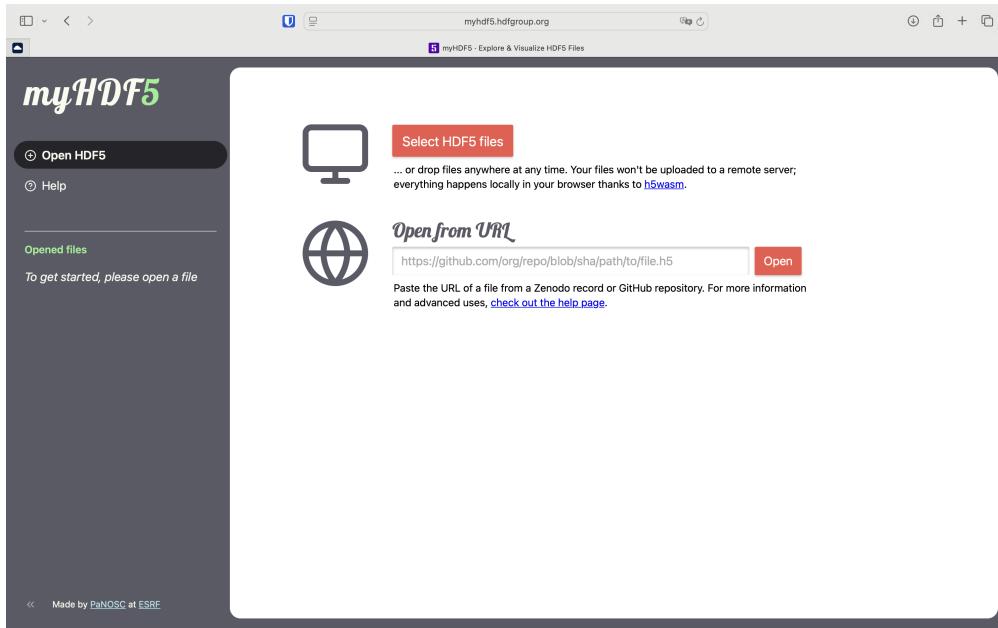


Figure 5: The welcome window of the myhdf5 application

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

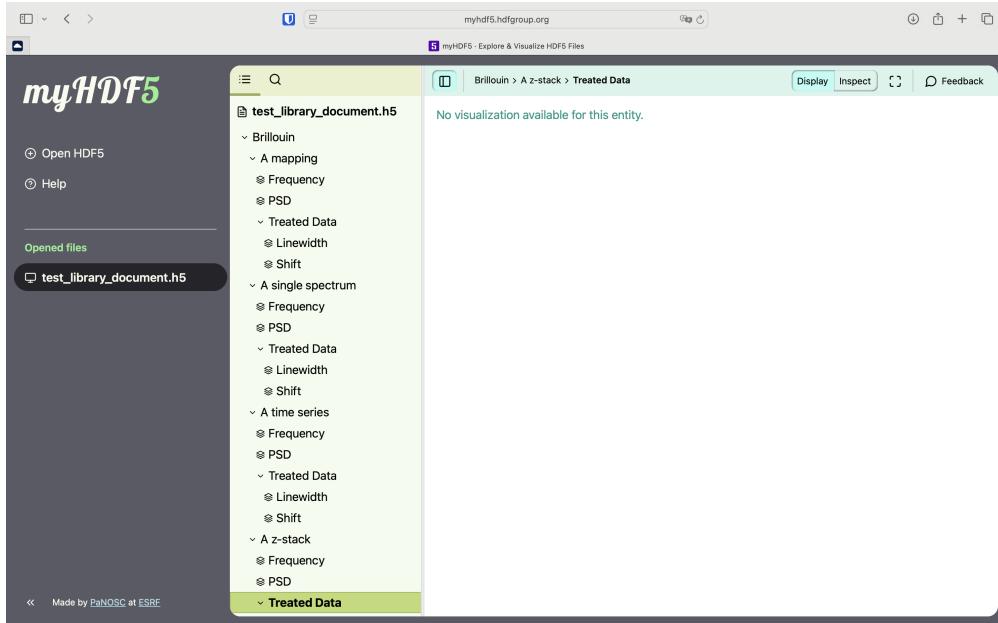


Figure 6: The developed structure view of your HDF5 file in the myhdf5 application

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

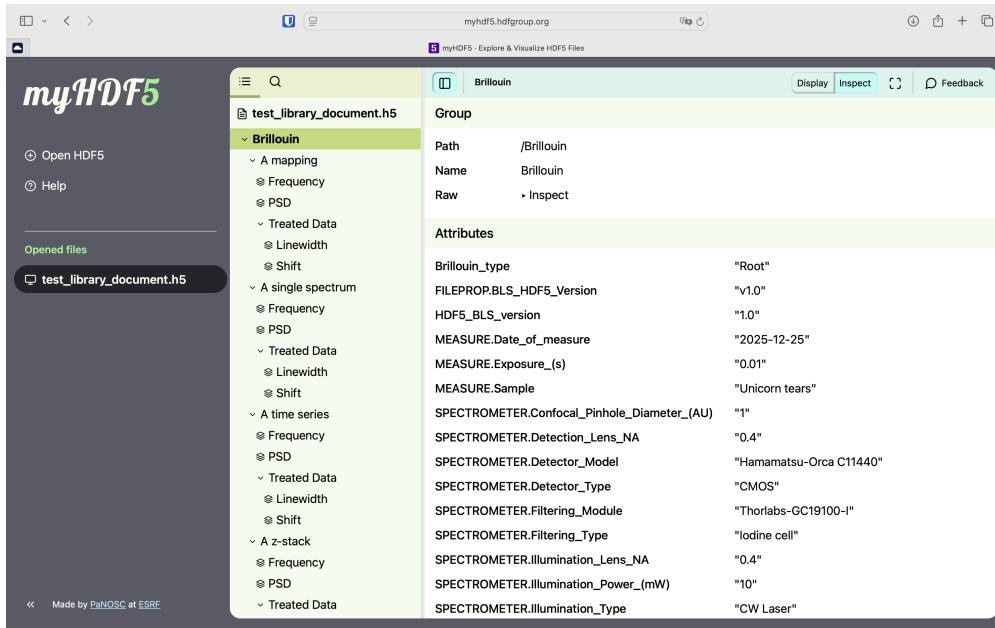


Figure 7: Visualizing the attributes stored in the "Brillouin" group



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 (thank you NASA!). 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:

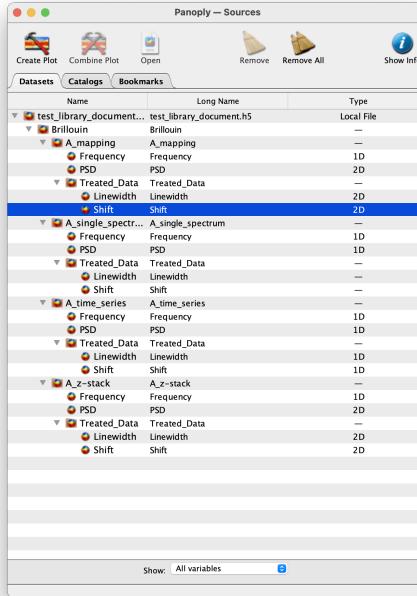


Figure 9: A simple visualization of the HDF5 file structure using the Panoply application

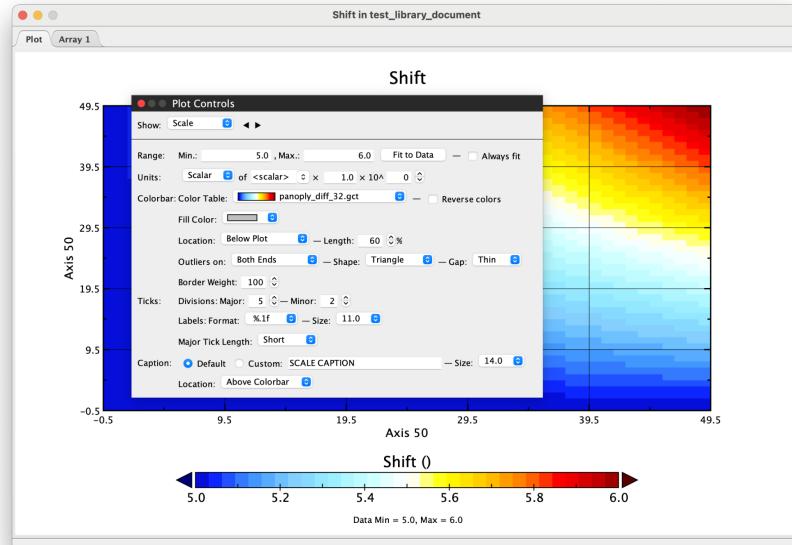


Figure 10: Visualizing datasets using the Panoply application

### 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 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).

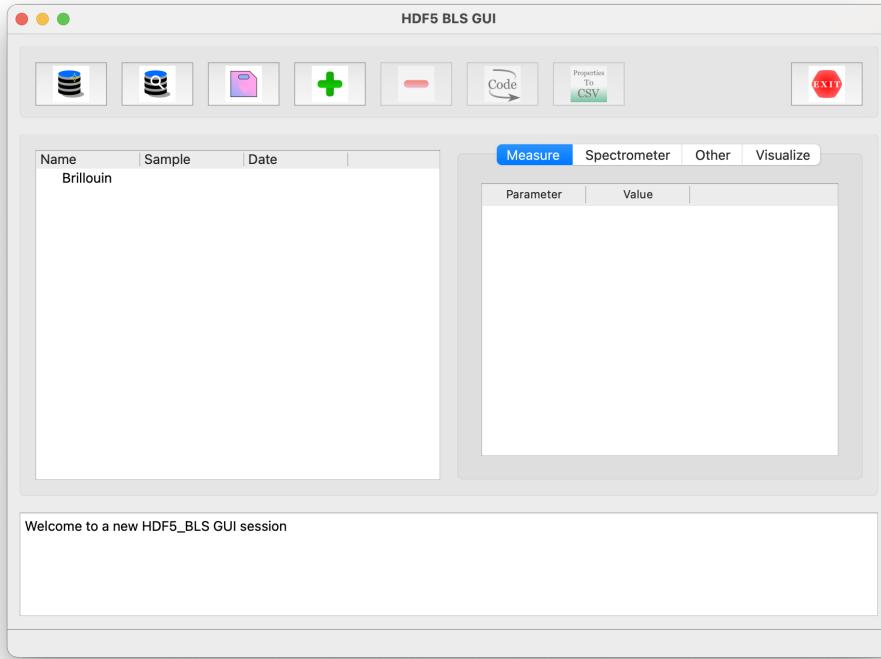


Figure 11: The welcome window of the HDF5\_BLS\_GUI

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).

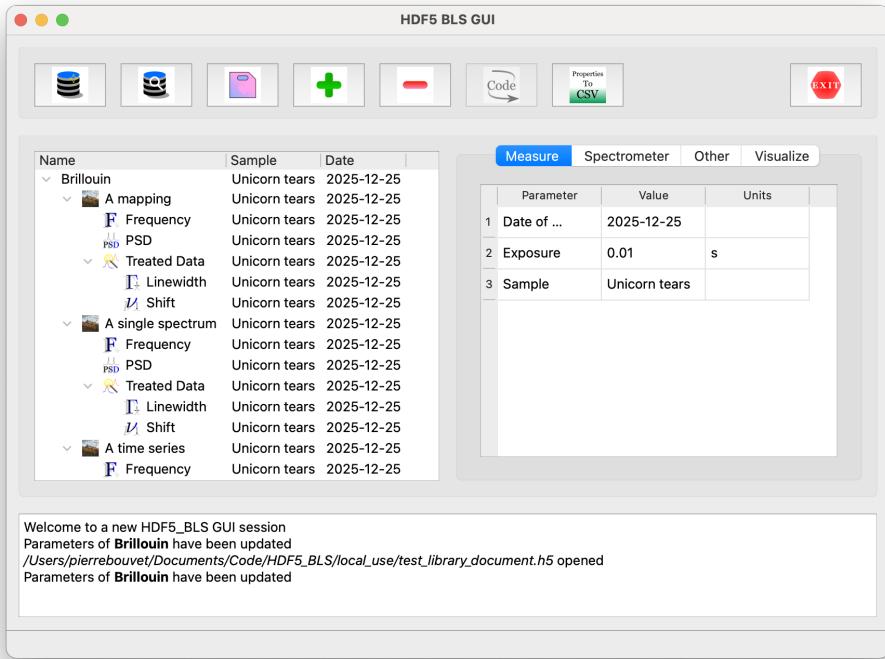


Figure 12: The structure of the example BrimX file in the HDF5\_BLS\_GUI

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](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](mailto:pierre.bouvet@meduniwien.ac.at) !

**Thank you for your help! Happy Brillouin data handling!**