KaraboData_Talk

January 11, 2019

```
In [1]: import warnings

        from IPython.display import HTML
        import matplotlib
        from matplotlib import pyplot as plt
        import numpy as np
        plt.rcParams['figure.figsize'] = (20.0, 10.0)
        matplotlib.rc('image', cmap='RdYlBu')

        warnings.filterwarnings("ignore")
        %matplotlib inline
```

1 Offline data analysis

```
<div class="intro-body">
    <div class="intro_h1"><h3>The karabo-data ecosystem</h3></div>
    <p><strong><span class="a">Martin Bergemann</span></strong><span class="b"></span><span>CAS
```

A Closer Look at Detector Data:
Data from Modular Detectors is stored across multiple files
Using standard hdf5 tools can be tricky and tedious

1.1 Solution: *karabo-data*

- Python Library that supports Analysis of EuXFEL Data.
- It is Open Source and available on the max-well cluster.

1.2 Aim:

Give you a glimpse of what is possible and provide a ground base for your own data analysis at EuXFEL

1.3 Scenario I: Take a look at some detector data

An image from a single module of the AGIP-D Detector at SPB

- How could this data be retrieved and visualized?

1.3.1 Reading single files (demo)

```
In [2]: #Live-demo
        import karabo_data as kd
        exmpl_file = '/gpfs/exfel/exp/XMPL/201750/p700000/proc/r0273/CORR-R0273-AGIPD03-S00000.h
        hdf5_file = kd.H5File(exmpl_file)
```

Data can be accessed by: * selecting trains id's * selecting train indexes * iteration over trains
Let's select data based on trains: (demo)

```
In [3]: #Live-demo (sel from train-id)
        train_id, train_data = hdf5_file.train_from_id(198425246)
        print(train_id, train_data.keys())

198425246 dict_keys(['SPB_DET_AGIPD1M-1/DET/3CH0:xtdf'])
```

```
In [4]: #Live-demo (sel from index)
        train_id, train_data = hdf5_file.train_from_index(5)
        print(train_id, train_data.keys())

198425246 dict_keys(['SPB_DET_AGIPD1M-1/DET/3CH0:xtdf'])
```

```
In [5]: #Live-demo (iteration)
        for train_id, train_data in hdf5_file.trains():
            print(train_id, train_data.keys())
            break

198425241 dict_keys(['SPB_DET_AGIPD1M-1/DET/3CH0:xtdf'])
```

Train data is of type *dictionary*. Hence the data can be accessed by giving keys:

```
In [6]: train_data['SPB_DET_AGIPD1M-1/DET/3CH0:xtdf']

Out[6]: {'detector.data': array([  0,  64, 114, ...,   0,   0,   0], dtype=uint8),
         'detector.trainId': 198425241,
         'header.dataId': 0,
         'header.linkId': 18446744069414584335,
         'header.magicNumberBegin': array([-50,  -6, -17, -66,  70,  68,  84,  88], dtype=int8),
         'header.majorTrainFormatVersion': 1,
         'header.minorTrainFormatVersion': 0,
         'header.pulseCount': 176,
         'header.reserved': array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], dtype=uint8)
         'header.trainId': 198425241,
         'image.cellId': array([  0,   1,   2,   3,   4,   5,   6,   7,   8,   9,  10,  11,  12,
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        130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142,
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        169, 170, 171, 172, 173, 174, 175], dtype=uint16),
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         [ 3.76776047e+01,  1.66408386e+01,  1.25324402e+01, ...,
           3.53553891e+00, -7.76110840e+00,  5.06602287e+00],
         [ 2.33586578e+01,  1.33027906e+01,  1.29060669e+01, ...,
          -3.58545852e+00, -8.78809452e+00, -1.76954997e+00],
         ...,
         [ 2.67929325e+01,  3.82321243e+01,  1.69615307e+01, ...,
          -5.36543350e+01,  1.77964573e+01,  2.29760933e+01],
         [ 5.43048973e+01,  2.40606403e+01,  2.68685341e+01, ...,
           1.56021561e+02,  0.00000000e+00,  1.39021225e+02],
         [ 5.41300812e+01,  3.99643478e+01,  3.18235302e+01, ...,
           4.46845245e+00, -3.83902435e+02,  1.09092340e+01]],

        [[ 2.82328766e+02,  2.13707367e+02,  3.85529510e+02, ...,
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         [ 1.72267563e+02,  2.91269714e+02,  2.23787582e+02, ...,
           1.87312103e+02,  1.91055298e+02,  1.92247986e+02],
         [ 1.74026535e+02,  2.09151901e+02,  2.23993912e+02, ...,
           1.28322266e+02,  6.25818977e+01,  1.35687103e+02],
         ...,
         [ 9.67379822e+02,  4.64296753e+02,  1.03795129e+03, ...,
           4.12897301e+01,  2.44968739e+01,  1.36369019e+02],
         [ 1.12769836e+03,  8.79650452e+02,  6.07432495e+02, ...,
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         [ 1.37194507e+03,  1.16530359e+03,  9.33655640e+02, ...,
          -1.40187941e+01, -1.80979218e+02, -1.05465247e+03]],

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           3.33557678e+02,  4.17891815e+02,  4.55165558e+02],
         [ 2.97341156e+02,  1.76079010e+02,  8.91075516e+01, ...,
           2.00919449e+02,  2.54712372e+02,  2.78320801e+02],
         ...,
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           7.16647387e+00,  2.45052700e+01,  5.89854355e+01],
         [ 1.80306104e+03,  1.42946960e+03,  9.75338379e+02, ...,
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        [ 2.03517444e+03,  1.21541614e+03,  9.28263855e+02, ...,
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       ...,

       [[ 3.09872532e+00, -5.08774281e-01,  1.51738377e+01, ...,
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        [ 1.53183994e+01,  9.43448830e+00, -9.73048973e+00, ...,
          9.80847092e+01,  9.90229797e+01,  9.15223618e+01],
        ...,
        [ 9.65496826e+01,  9.00805054e+01,  8.23390045e+01, ...,
          3.99469910e+01, -4.39730103e+02,  8.46993359e+03],
        [ 1.09837486e+02,  9.43753433e+01,  1.01021187e+02, ...,
         -7.42510234e+04, -1.19970758e+05, -7.43315469e+04],
        [ 1.11256569e+02,  9.82772827e+01,  1.06616699e+02, ...,
          7.79505127e+02, -1.85362646e+03, -1.54386367e+04]],

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         [0, 0, 0, ..., 0, 0, 0]],

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         ...,
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         [0, 0, 0, ..., 0, 0, 0],
         [0, 0, 0, ..., 0, 0, 1]],

        [[0, 0, 0, ..., 0, 0, 0],
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         [0, 0, 0, ..., 0, 0, 0],
         ...,
         [0, 0, 0, ..., 0, 0, 0],
         [0, 0, 0, ..., 0, 0, 0],
         [0, 0, 0, ..., 0, 0, 1]],

        ...,

        [[0, 0, 0, ..., 0, 0, 0],
         [0, 0, 0, ..., 0, 0, 0],
         [0, 0, 0, ..., 0, 0, 0],
         ...,
         [0, 0, 0, ..., 1, 1, 1],
         [0, 0, 0, ..., 2, 2, 2],
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        [     0,      0,      0, ...,      0,      0,      0],
        ...,
        [     0,      0,      0, ...,    515,    515,    515],
        [     0,      0,      0, ...,    515,    515,    515],
        [     0,      0,      0, ...,    515,    515,    515]],

       [[     0,      0,      0, ...,      0,      0,      0],
        [     0,      0,      0, ...,      0,      0,      0],
        [     0,      0,      0, ...,      0,      0,      0],
        ...,
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        ...,
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           572, 576, 580, 584, 588, 592, 596, 600, 604, 608, 612, 616, 620,
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                198425241, 198425241], dtype=uint64),
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          'timestamp.tid': 198425241},
         'trailer.checksum': array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], dtype=int8)
         'trailer.magicNumberEnd': array([-51, -85, -83, -34,  70,  68,  84,  88], dtype=int8),
         'trailer.status': 0,
         'trailer.trainId': 198425241}
```
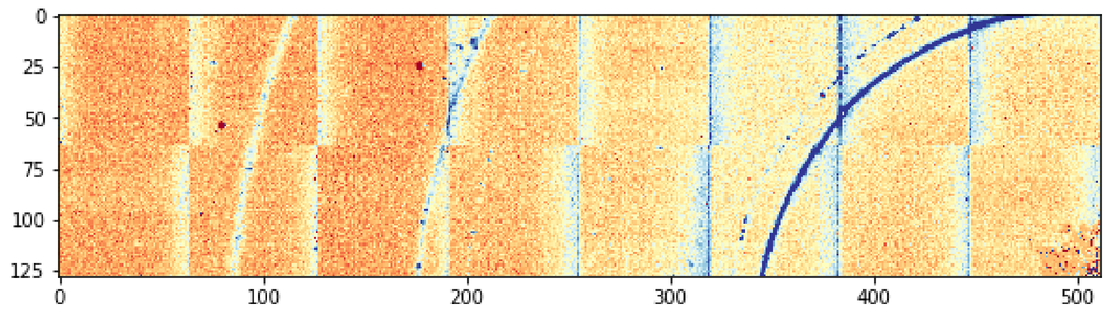

```
In [9]: train_data['SPB_DET_AGIPD1M-1/DET/3CH0:xtdf']['image.data'].shape

Out[9]: (176, 512, 128)

In [11]: #Live-demo
         type(train_data['SPB_DET_AGIPD1M-1/DET/3CH0:xtdf']['image.data'])

Out[11]: numpy.ndarray

In [12]: #Live-demo
         from matplotlib import pyplot as plt
```

```
fig = plt.figure(figsize=(10,10))
_ = plt.imshow(train_data['SPB_DET_AGIPD1M-1/DET/3CH0:xtdf']['image.data'][0].T,
               vmin=-50, vmax=100)
```



1.4 Reading whole Runs:

The main advantage of karabo-data is that not only single files at a time but whole runs can be read:

```
In [13]: #Live-demo
         run_folder = '/gpfs/exfel/exp/XMPL/201750/p700000/raw/r0273'
         run_dir = kd.RunDirectory(run_folder)
         run_dir.info()
```

```
# of trains:    156
Duration:       0:00:15.500000
First train ID: 198425241
Last train ID:  198425396

16 detector modules (SPB_DET_AGIPD1M-1)
  e.g. module SPB_DET_AGIPD1M-1 0 : 512 x 128 pixels
  176 frames per train, 27456 total frames

2 instrument sources (excluding detectors):
  - SA1_XTD2_XGM/XGM/DOOCS:output
  - SPB_XTD9_XGM/XGM/DOOCS:output

13 control sources:
  - ACC_SYS_DOOCS/CTRL/BEAMCONDITIONS
  - SA1_XTD2_XGM/XGM/DOOCS
  - SPB_IRU_AGIPD1M/PSC/HV
  - SPB_IRU_AGIPD1M/TSENS/H1_T_EXTHOUS
  - SPB_IRU_AGIPD1M/TSENS/H2_T_EXTHOUS
  - SPB_IRU_AGIPD1M/TSENS/Q1_T_BLOCK
  - SPB_IRU_AGIPD1M/TSENS/Q2_T_BLOCK
- SPB_IRU_AGIPD1M/TSENS/Q3_T_BLOCK
- SPB_IRU_AGIPD1M/TSENS/Q4_T_BLOCK
- SPB_IRU_AGIPD1M1/CTRL/MC1
- SPB_IRU_AGIPD1M1/CTRL/MC2
- SPB_IRU_VAC/GAUGE/GAUGE_FR_6
- SPB_XTD9_XGM/XGM/DOOCS
```

1.5 Data subsets

Yet another powerful tool is the ***select*** method. It selects a subset of sources and keys from the run directory:

```
In [14]: #Live-demo with glob pattern
         sel = run_dir.select('*/DET/*', 'image.*')
         sel.all_sources
```

```
Out[14]: frozenset({'SPB_DET_AGIPD1M-1/DET/0CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/10CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/11CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/12CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/13CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/14CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/15CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/1CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/2CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/3CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/4CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/5CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/6CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/7CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/8CH0:xtdf',
                    'SPB_DET_AGIPD1M-1/DET/9CH0:xtdf'})
```

Data can be access just like *previously* mentioned:

```
In [16]: #Live-demo (iterator example)
         for train_id, train_data in sel.trains():
             #print(train_id, train_data.keys())
             break
         train_id, train_data = sel.train_from_index(5)
         train_id, train_data.keys()
```

```
Out[16]: (198425246,
          dict_keys(['SPB_DET_AGIPD1M-1/DET/14CH0:xtdf', 'SPB_DET_AGIPD1M-1/DET/13CH0:xtdf', 'SP
```

1.6 What if I don't want to fire up a python console just to quickly check something?

The command `lsxfel` is a tool that provides some basic functionality using only the command line.

```
$: lsxfel /gpfs/exfel/exp/XMPL/201750/p700000/raw/r0273/
r0273 : Run directory

# of trains:    156
Duration:       0:00:15.500000
First train ID: 198425241
Last train ID:  198425396

16 detector modules (SPB_DET_AGIPD1M-1)
  e.g. module SPB_DET_AGIPD1M-1 0 : 512 x 128 pixels
  176 frames per train, 27456 total frames

2 instrument sources (excluding detectors):
  - SA1_XTD2_XGM/XGM/DOOCS:output
  - SPB_XTD9_XGM/XGM/DOOCS:output

13 control sources:
  - ACC_SYS_DOOCS/CTRL/BEAMCONDITIONS
  - SA1_XTD2_XGM/XGM/DOOCS
  - SPB_IRU_AGIPD1M/PSC/HV
  - SPB_IRU_AGIPD1M/TSENS/H1_T_EXTHOUS
  - SPB_IRU_AGIPD1M/TSENS/H2_T_EXTHOUS
  - SPB_IRU_AGIPD1M/TSENS/Q1_T_BLOCK
  - SPB_IRU_AGIPD1M/TSENS/Q2_T_BLOCK
  - SPB_IRU_AGIPD1M/TSENS/Q3_T_BLOCK
  - SPB_IRU_AGIPD1M/TSENS/Q4_T_BLOCK
  - SPB_IRU_AGIPD1M1/CTRL/MC1
  - SPB_IRU_AGIPD1M1/CTRL/MC2
  - SPB_IRU_VAC/GAUGE/GAUGE_FR_6
  - SPB_XTD9_XGM/XGM/DOOCS
```

1.7 If something goes wrong

A common source of errors is an invalid structure of the created data files. Hence a useful starting point to debug any errors is to check for valid file structures using the `karabo-data-validate` command:

```
$: karabo-data-validate /gpfs/exfel/exp/XMPL/201750/p700000/raw/r0273
Checking run directory: /gpfs/exfel/exp/XMPL/201750/p700000/raw/r0273
No problems found
```

The command checks if:

- All .h5 files in a run can be opened, and the run contains at least one usable file.

- The list of train IDs in a file has no zeros except for padding at the end.
- Each train ID in a file is greater than the one before it.
- The indexes do not point to data beyond the end of a dataset.
- The indexes point to the start of the dataset, and then to successive chunks for successive trains, without gaps or overlaps between them.

1.8 Scenario II: Extracting 1D Data

Photon flux *time-series* (by trainID)

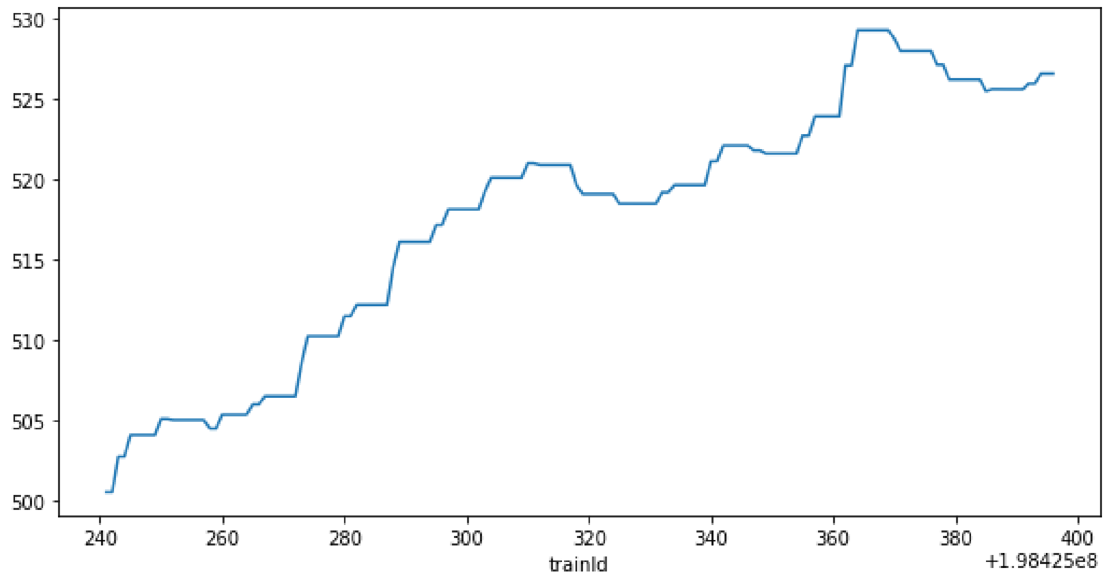
- How can 1D data be extracted and plotted?

The *get_series* method can extract a series across trainID's for a given device and property:

```
In [18]: #Live-demo
         ph_flux = run_dir.get_series('SA1_XTD2_XGM/XGM/DOOCS', 'pulseEnergy.photonFlux.value')
         ph_flux.head()
```

```
Out[18]: trainId
         198425241    500.519470
         198425242    500.519470
         198425243    502.727203
         198425244    502.727203
         198425245    504.070953
         Name: SA1_XTD2_XGM/XGM/DOOCS/pulseEnergy.photonFlux, dtype: float32
```

```
In [19]: #Live-demo
         fig = plt.figure(figsize=(10,5))
         _ = ph_flux.plot()
```



- Multiple devices and properties can be can be combined using the *get_dataframe* method:

```
In [20]: #Live-demo
         fluxes_pos = run_dir.get_dataframe(fields=[("*_XGM/*", "*.photonFlux"),
                                                    ("*_XGM/*", "*.i[xy]Pos")])
         fluxes_pos.head(10)
```

```
Out[20]:            SPB_XTD9_XGM/XGM/DOOCS/pulseEnergy.photonFlux  \
         trainId
         198425241                                     404.392822
         198425242                                     404.392822
         198425243                                     404.392822
         198425244                                     404.392822
         198425245                                     404.392822
         198425246                                     404.392822
         198425247                                     404.665680
         198425248                                     404.665680
         198425249                                     406.852539
         198425250                                     406.852539

                    SPB_XTD9_XGM/XGM/DOOCS/beamPosition.iyPos  \
         trainId
         198425241                                  -3.121433
         198425242                                  -3.121433
         198425243                                  -3.121433
         198425244                                  -3.090523
         198425245                                  -3.090523
         198425246                                  -3.090523
         198425247                                  -3.090523
         198425248                                  -3.090523
         198425249                                  -3.090523
         198425250                                  -3.090523

                    SPB_XTD9_XGM/XGM/DOOCS/beamPosition.ixPos  \
         trainId
         198425241                                   5.512009
         198425242                                   5.512009
         198425243                                   5.512009
         198425244                                   5.528512
         198425245                                   5.528512
         198425246                                   5.528512
         198425247                                   5.528512
         198425248                                   5.528512
         198425249                                   5.528512
         198425250                                   5.528512

                    SA1_XTD2_XGM/XGM/DOOCS/pulseEnergy.photonFlux  \
         trainId
```

```
198425241                                          500.519470
198425242                                          500.519470
198425243                                          502.727203
198425244                                          502.727203
198425245                                          504.070953
198425246                                          504.070953
198425247                                          504.070953
198425248                                          504.070953
198425249                                          504.070953
198425250                                          505.071930

           SA1_XTD2_XGM/XGM/DOOCS/beamPosition.iyPos  \
trainId
198425241                                        0.315761
198425242                                        0.315761
198425243                                        0.315761
198425244                                        0.341187
198425245                                        0.341187
198425246                                        0.341187
198425247                                        0.341187
198425248                                        0.341187
198425249                                        0.341187
198425250                                        0.341187

           SA1_XTD2_XGM/XGM/DOOCS/beamPosition.ixPos
trainId
198425241                                        1.293711
198425242                                        1.293711
198425243                                        1.293711
198425244                                        1.336566
198425245                                        1.336566
198425246                                        1.336566
198425247                                        1.336566
198425248                                        1.336566
198425249                                        1.336566
198425250                                        1.336566
```

1.8.1 What is *pandas*

get_dataframe and *get_series* return **pandas** objects which are extremely useful for extensive data analysis tasks. More information is available under https://pandas.pydata.org.

1.9 Scenario III: Getting data with multiple values per train

XGM intensity data is pulse resolved

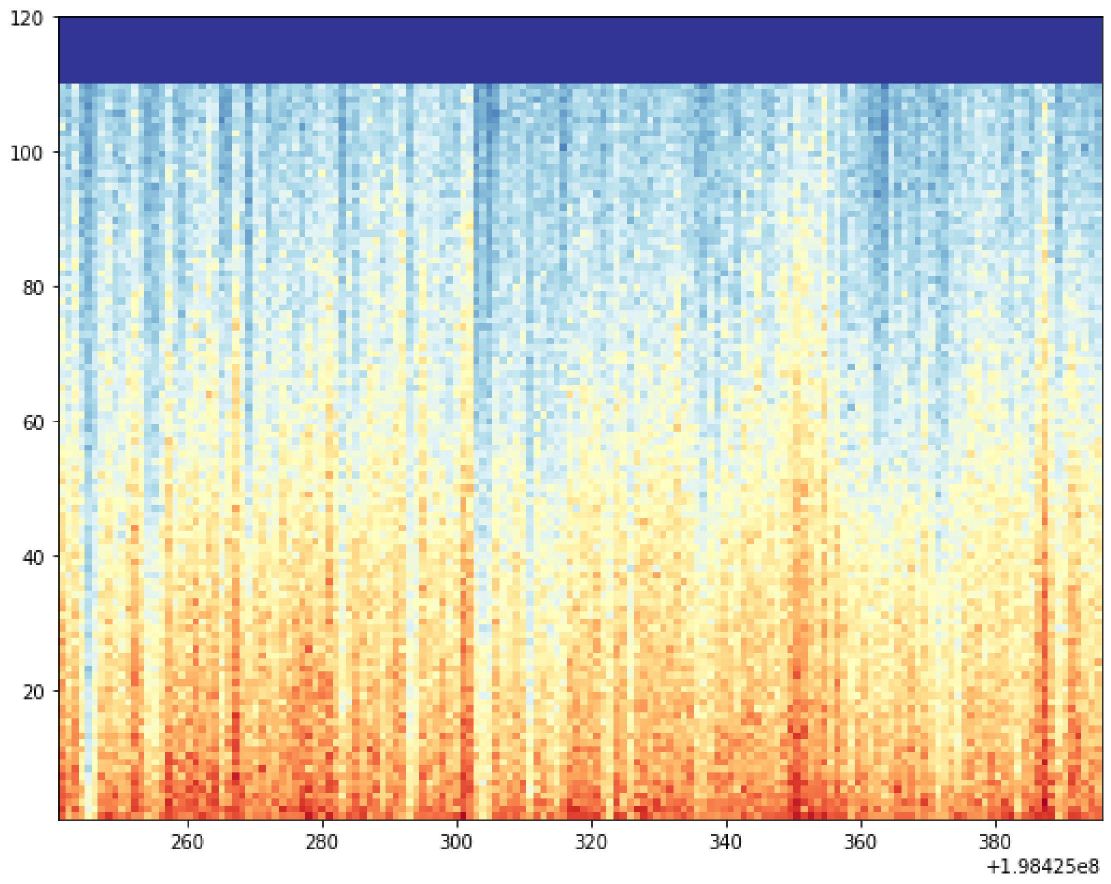
- How can this 2D data be extracted and plotted?

the *get_array* method returns a data array that contains more than one value per train. XGM intensity data is pulse resolved and serves as an example.

```
In [21]: xgm_intensity = run_dir.get_array('SA1_XTD2_XGM/XGM/DOOCS:output', 'data.intensityTD',
                                            extra_dims=['pulseId'])
         xgm_intensity
```

```
Out[21]: <xarray.DataArray (trainId: 156, pulseId: 1000)>
         array([[ 957.0532 , 1026.0005 ,  949.8755 , ...,    0.     ,    0.     ,
                    0.     ],
                [ 763.8806 ,  794.2738 ,  868.2455 , ...,    0.     ,    0.     ,
                    0.     ],
                [ 859.37   ,  995.1641 ,  838.5669 , ...,    0.     ,    0.     ,
                    0.     ],
                ...,
                [ 945.2731 ,  812.4336 ,  839.45654, ...,    0.     ,    0.     ,
                    0.     ],
                [ 903.26855,  940.15125,  953.9436 , ...,    0.     ,    0.     ,
                    0.     ],
                [ 944.08386,  949.549  ,  861.7509 , ...,    0.     ,    0.     ,
                    0.     ]], dtype=float32)
         Coordinates:
           * trainId  (trainId) uint64 198425241 198425242 ... 198425395 198425396
         Dimensions without coordinates: pulseId
```

```
In [22]: #Live-demo
         fig = plt.figure(figsize=(10,8))
         _= plt.imshow(xgm_intensity[:,:120].T,
                       extent=(xgm_intensity.trainId[0], xgm_intensity.trainId[-1], 1, 120),
                       origin='lower', cmap='RdYlBu_r')
```



a labeled array (**xarray**) is returned. More information on labeled arrays can be found on http://xarray.pydata.org

1.10 Scenario IV: Combine data and save new dataset to individual files

Suppose you want to compare data across different runs or combine various selections and then save the combined dataset to a new file.

This task could be realized with the **combine** and **write** method. This involves two different steps:

- combining
- file creation

```
In [20]: #Live-demo file combining
         xgm_intensities = run_dir.select('*/XGM/*','data.intensityTD')
         xgm_pos = run_dir.select('*/XGM/*', '*Pos')
         xgm_union = xgm_pos.union(xgm_intensities)
```

Yet another convenient way of showing the content of a selection is the **selection** method:

```
In [21]: xgm_union.selection
```

```
Out[21]: {'SA1_XTD2_XGM/XGM/DOOCS': {'beamPosition.ixPos.value',
           'beamPosition.iyPos.value'},
          'SA1_XTD2_XGM/XGM/DOOCS:output': {'data.intensityTD'},
          'SPB_XTD9_XGM/XGM/DOOCS': {'beamPosition.ixPos.value',
           'beamPosition.iyPos.value'},
          'SPB_XTD9_XGM/XGM/DOOCS:output': {'data.intensityTD'}}
```

```
In [ ]: xgm_union.write('/gpfs/exfel/data/scratch/xmpl/xmpl_xgm_subset.hdf5')
```

```
$: file /gpfs/exfel/data/scratch/xmpl/xmpl_xgm_subset.hdf5
gpfs/exfel/data/scratch/xmpl/xmpl_xgm_subset.hdf5: Hierarchical Data Format (version 5) data
```

1.11 How to install/get karabo-data?

Karabo-data is available on GitHub and there are multiple ways to install it: * it is already available on the max-well cluster nothing has to be done * it can be install using *pip* &rarr `pip install (--user) karabo_data` (preferred way) * the latest version could be downloaded from GitHub &rarr `git clone https://github.com/European-XFEL/karabo_data.git`

```
In [ ]:
```