WP4 Data Analysis Services

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On behalf of WP4
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Vision for European Open Science Cloud

One place to

- **F**ind existence of data sets
- **A**ccess data and metadata as
- **I**nteroperable data sets
- **R**eusable data and data analysis procedures
  - ▶ reproducibility
  - ▶ ability to re-use and extend studies

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Why data analysis for FAIR data?

- To make the (raw) data usable and re-usable
  - ► significant post-processing required before knowledge can be extracted, including
  - ► calibrating the data from complex detectors
  - ► converting facility and hardware specific data into data representing the physics of the experiment
- Further data processing to extract insight from the data

- Ensure completeness of meta data
- If we have (working and meaningful) analysis routines, they contain all the required data
  - ► The source code is a complete description of the computation

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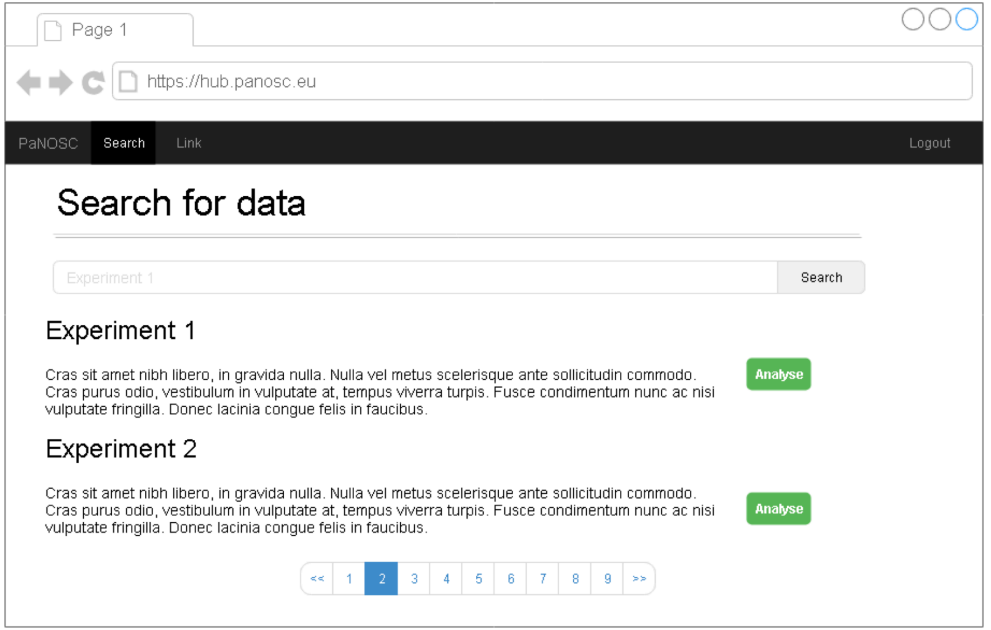
Vision for data analysis services in PaNOSC

- Search and
- Select data set from portal
- Allow data analysis on data set from this portal (or some other instance that is invoked on the fly).



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Challenges and solution elements

- Required
  - Data sets and access for analysis
    - ► Either move data or move computation to data
  - Data set → data analysis procedure
    - ► Classification of data / experiment types
  - Metadata

  - Remote interactive analysis environment
    - ► Remote Desktop (VISA), JupyterHub
  - Analysis software environment
    - ► Containers (Docker, Singularity, Virtual Machines)
    - ► Specific for each data set?

- Desirable
  - Data analysis working across facilities
    - ► Agreed API / file format (NEXUS)?
    - ► Joint use of base libraries (Silx, pyFAI, h5py, …?)

- Additional challenges
  - EOSC and the technologies we need to use are developed during this project
    - ► Difficult to plan
    - ► Opportunities for flexible adjustments

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Practical and historical aspects

- Facilities use different infrastructures
- Facilities in general support different types of experiments
- Where the experiments are of the same or similar type, the representation of the data and metadata is different
- Existing infrastructures that originate from hundreds of person years of effort are difficult to change
- To make our efforts sustainable, the PaNOSC developments must provide value to each facility (and their users)

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EOSC PaNOSC Data Analysis Portal vision

- Search for data set and select (WP3)
- For selected data set
  - Have metadata available (WP3)
  - Have choice of suggested data analysis procedures (WP3, WP4)
    - ► Could include simulation of experiment? (WP5)
    - ► Could provide link to tutorial for this type of experiment / analysis? (WP8)
  - Ability to trigger execution of these analysis procedures
    - ► Needs analysis code, software environment and data (WP4, WP6)
  - Ability to modify analysis interactively (WP4)
  - Allow download of new analysis results
- Focus on data sets connected with reproducible publications
  - Allow to view, re-execute (=reproduce) and modify (=re-use) code that created published results

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Why focus on reproducible publications as scientific use cases?

- Need to narrow down scope of project somehow
  - Publications select and describe useful parts of data from experiment
  - An analysis method used in one publication is likely to be useful for a new study
    - ► Defines (minimum set of) analysis tools/services we support
    - ► Starting point for provision of this type of analysis at the facility where the data originates
  - Publication must provide relevant meta data
  - Publications are key performance indicator
- Data sets can (often) be made public as results are published (even before 3-year embargo expires)
- Related: *every* publication *should* be reproducible
  - Journals and funding councils increasingly push for reproducible publications
  - Reproducible publications are much more easily re-usable → more effective science

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Communication in WP4

- Communication and tool infrastructure
  - WP4 specific mailing list
  - Slack channel
  - Kick-off meeting in June at EuXFEL
  - WP4 subdirectory in panosc-eu repository on Github
    - With meeting agendas and minutes
    - "resources"
      - https://github.com/panosc-eu/panosc/tree/master/Work%20Packages/WP4%20Data%20analysis%20services
    - 2-weekly video meetings of (at least) site leaders
      - Tuesdays 15:00
  - Task tracking (https://github.com/orgs/panosc-eu/projects/2)
  - https://confluence.panosc.eu/ has WP4 area
  - Invited ExPaNDS project members to join meetings

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Ongoing activities in WP4

- Active projects
  - Recruitment of staff*
  - Research “literature”
    - ► computational workflows
    - ► and design remote analysis architecture
  - Portal design*
  - Remote analysis infrastructure*
  - JupyterHub*
  - Move analysis capabilities into Jupyter notebook*
  - Hdf5 and Visualisation in notebooks*
  - Questionnaire on data analysis for participating facilities (Task 4.1)
  - Identify reproducible scientific use cases at each institute

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Recruited and contributing staff for PaNOSC WP4

- CERIC-ERIC
  - *Carlos Reis*, Marco de Simone
- ELI
  - *Jakub Grosz* (Eli Beamlines), Mariana Danielova (Eli Beamlines), Rober Racz (Eli ALPS)
- ESRF
  - *Thomas Vincent, Andy Goetz*, B. Roussel, A. Roux, A. Campbell
- ESS
  - *Kareem Galal*, Jesper Rude Selknæs, Lottie Greenwood, Alexandre Stefanov and Ashok Nulguda, Torben Nielsen, Gareth Murphy
- European XFEL
  - *Robert Rosca, Thomas Kluyver*
- ILL
  - *Jamie Hall*, *William Turner*
- EGI
  - *Giuseppe La Rocca*, Enol Fernández

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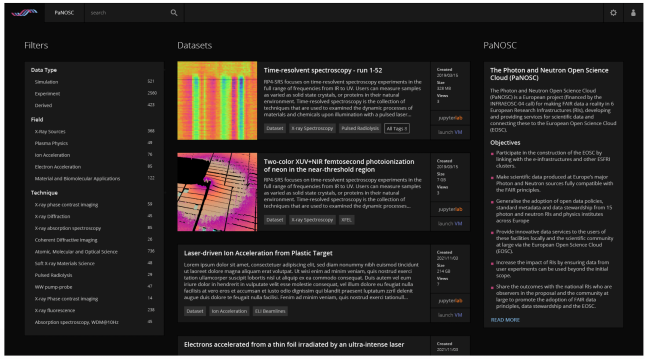
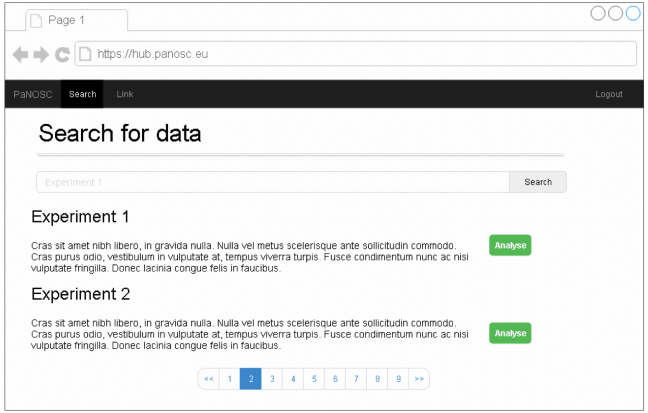
Portal

- Design of Portal, integrating requirements from WP3 and WP4
  - https://confluence.panosc.eu/display/wp4
  - Presentation Jamie Hall Wednesday 9:30 (Bassovizza)
- Aim to deploy early prototype with minimum functionality at each facility in March 2020
  - Functionality
    - ► Start remote desktop instance
    - ► Start Jupyter Notebook instance
    - ► Will need local adaption
  - Gather feedback
  - Move towards federated instance iteratively





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Remote data analysis technology 1: Remote Desktop and Virtual Machines

- Technology 1: VISA – Virtual Infrastructure for Scientific Analysis (ILL)
  - Connect Desktop GUI of Virtual Machine
  - Inside the web browser
  - Operate remotely
- Essentially creates a virtual machine for every analysis use case
  - Can support any data analysis software, any operating system.
  - Computation takes place where the data is stored
  - However:
    - ► Prescribes operating system, window manager, keyboard layout, …
    - ► Different environments for different analysis applications
- Related remote desktop technology used at other facilities (FastX).

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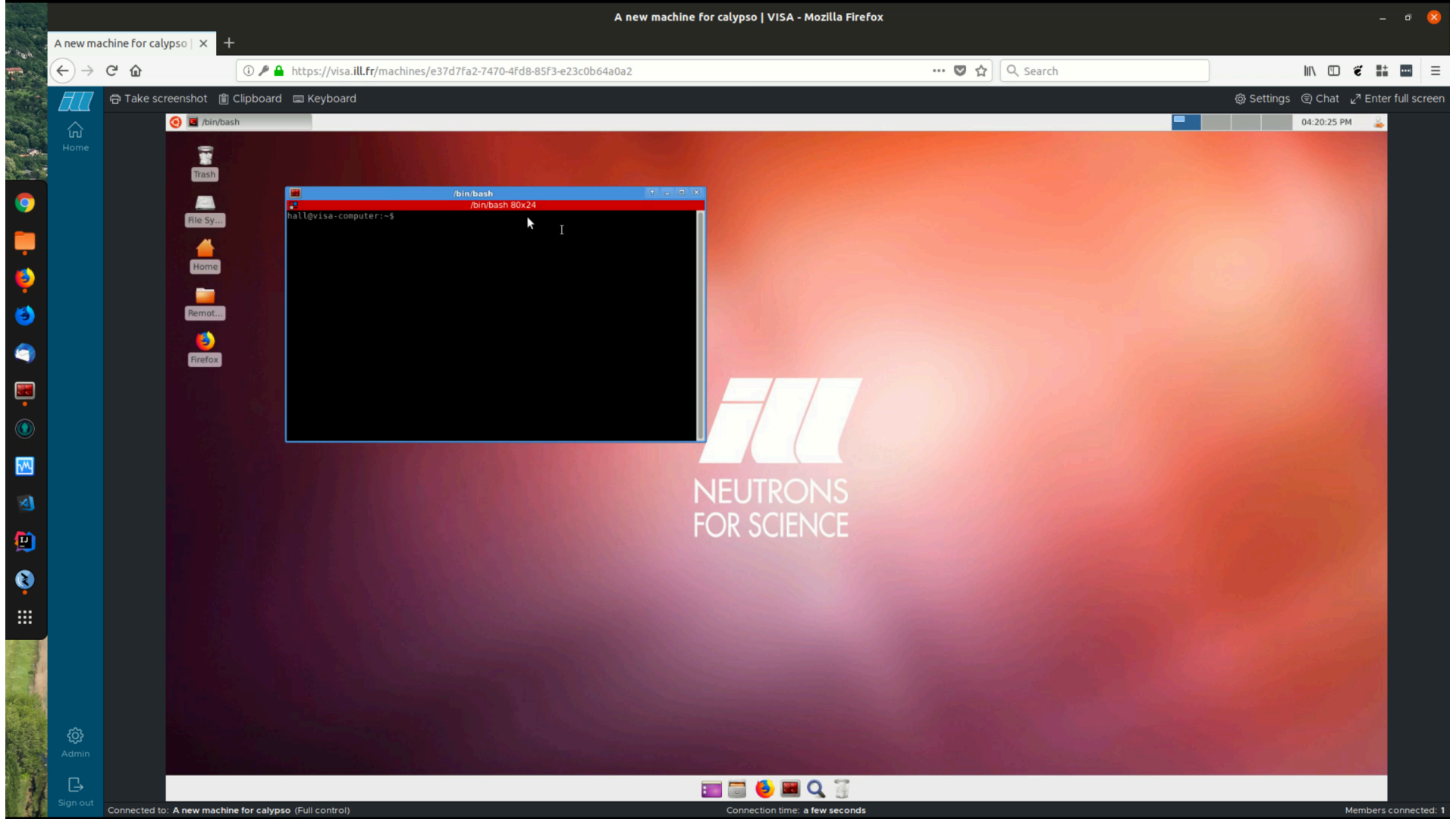
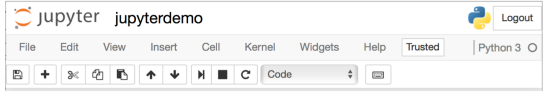

A new machine for calypso | VISA - Mozilla Firefox
A new machine for calypso
https://visa.ill.fr/machines/e37d7fa2-7470-4fd8-85f3-e23c0b64a0a2
Search
Take screenshot
Clipboard
Keyboard
Settings
Chat
Enter full screen
Home
/bin/bash
04:20:25 PM
Trash
File Sy...
Home
Remot...
Firefox
/bin/bash
/bin/bash 80x24
hall@visa-computer:~$
NEUTRONS
FOR SCIENCE
Admin
Sign out
Connected to: A new machine for calypso (Full control)
Connection time: a few seconds
Members connected: 1

Remote data analysis technology 2: Jupyter Notebook for data analysis

- Jupyter Notebook
  - Combines commands
  - Processing outputs and
  - Interpretation / annotation
- Represents the whole research to publication life cycle
  - in one virtual research environment
  - in one document
    - ► better reproducibility
- Can be shared easily (ipynb, html, pdf)
- Tools from the Jupyter ecosystem allow remote execution of notebooks

Demo: https://github.com/fangohr/jupyter-demo/



Code cells show code input and output:

```
In [1]: 1 + 2
Out[1]: 3
```

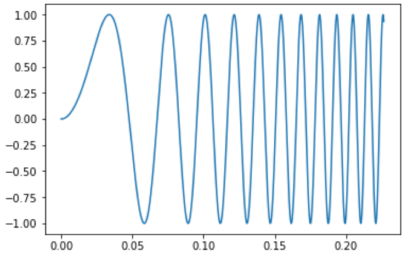
Cells can contain text and latex equations such as $f(x) = \sin(2\pi\omega t^2)$ and $\omega = 220$ Hz. We can use code to define the corresponding functions:

```
In [2]: import numpy as np
        def f(t):
            omega = 220
            return np.sin(2 * np.pi * omega * t**2)

In [3]: f(0)   # call the function
Out[3]: 0.0
```

Let's compute the data and plot the beginning of it:

```
In [4]: t = np.linspace(0, 2, 44100)
        y = f(t)
        ## Show plots inside the notebook
        %matplotlib inline
        import pylab
        pylab.plot(t[0:5000], y[0:5000])
Out[4]: [<matplotlib.lines.Line2D at 0x10a267898>]
```



Summary

It is possible to combine equations, code, data processing commands, their output, including plots, and text in one document.

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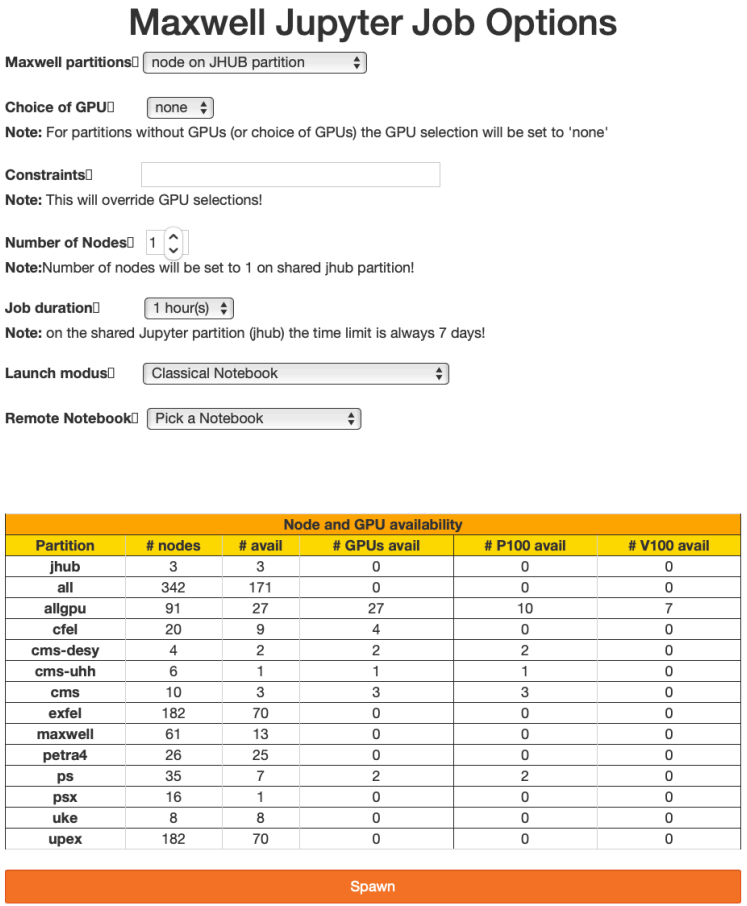
OSC

JupyterHub

- JupyterHub: service that allows
  - remote execution of notebooks
  - Offering HPC and storage resources through webportal
- All facilities working towards JupyterHub instance offered to users
  - EuXFEL, ILL: in operation
  - ESRF, CERIC-ERIC: prototype deployed
- Welcome by users
  - Example: 150 users per week at EuXFEL
  - Anecdotal evidence that Jupyter Interface can be preferred over QT Interface



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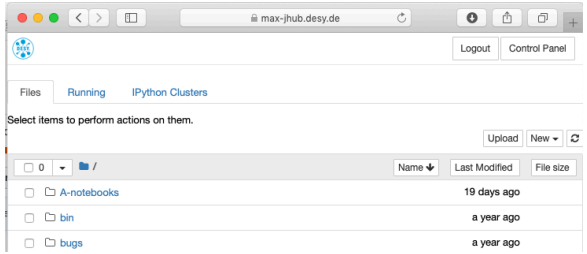
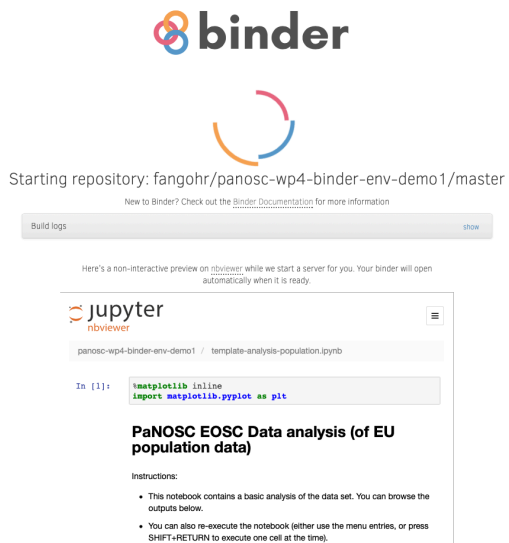
BinderHub

- JupyterHub: service that allows
  - remote execution of notebooks
  - Offering HPC and storage resources through webportal
- BinderHub (a JupyterHub with Binder-style software specification)
  - Tailored container is created based on ”binder software specifications”
    - ► `repo2docker`
      - `requirements.txt`, `environment.yml`, `Dockerfile`
  - Example: http://github.com/fangohr/panosc-wp4-binder-env-demo1
    - ► Uses global anonymous BinderHub called MyBinder. (https://mybinder.org)
  - Promising as environment that can be configured flexibly?





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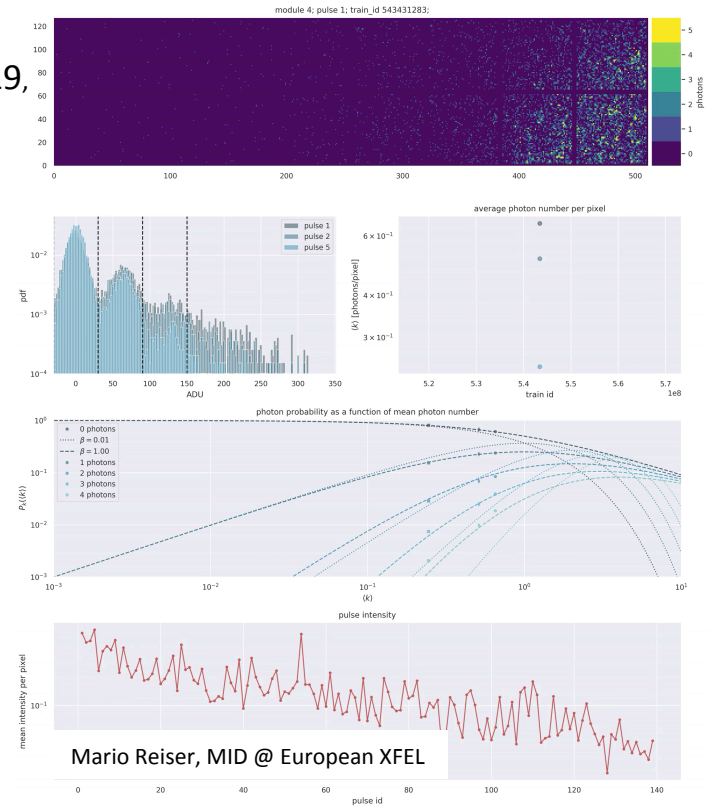
Moving data analysis into the Jupyter notebook

- Examples from ICALPECS 2019, preprint of slides at http://icalepcs2019.vrws.de/talks/tucpr02_talk.pdf
- Presentation Thomas Vincent (ESRF): *Reproducible science studies*
  Wednesday 11:30 (Bassovizza)



Mario Reiser, MID @ European XFEL

```
In [3]: import ToolBox as tb
```

X-ray Absorption Spectroscopy

Step 1: Load data and align them by train id and pulse id

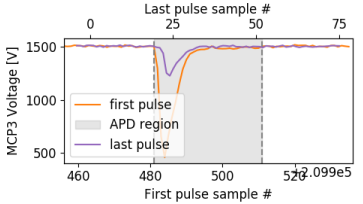
```
In [4]: proposalNB = 900074
        semesterNB = 201930
        runNB = 487
        topic = 'SCS'
        fields = ["SCS_photonFlux", "SCS_XGM", "MCP3apd", "nrj"]
        run = tb.load(fields, runNB, proposalNB, semesterNB, topic,
                      validate=True, display=False)
        nrun = tb.matchXgmTimPulseId(run)
```

```
Checking run directory: /gpfs/exfel/exp/SCS/201930/p900074/raw
/r0487/
No problems found
```

Step 2: check the pulse integration window

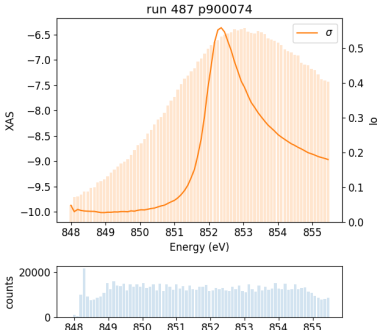
```
In [5]: tb.checkTimApdWindow(nrun, mcp=3)
```

```
no raw data for MCP3. Loading trace from MCP3
```



Step 3: bin the data and plot the XAS spectrum

```
In [6]: nrj = np.linspace(nrun.nrj.min(), nrun.nrj.max(), 80)
        xas = tb.xas(nrun, nrj, plot=True)
```



Activities on HDF5

- HDF5 used widely in facilities
- Multiple activities to improve data exploration capabilities for hdf5 files
  - Presentation Carlos Reis (CERIC ERIC), Thursday 9:40: *HDF5 Viewer – web and Jupyter Interface*
  - h5glance, silx, karabo-data-interactive, …


```
In [5]: import h5glance
        h5glance.install_ipython_h5py_display()

In [6]: f

Out[6]: example.h5
          group1
            subgroup1
              dataset1 [ ]: 200 entries, dtype: <u8
              dataset2 [ ]: 2 × 128 × 500 entries, dtype: <f4
            subgroup2

In [7]: f['group1']

Out[7]: /group1
          subgroup1
          subgroup2
```

panosc

Summary

- Many ideas and good initial progress
- Next steps
  - require more fine grained coordination
    - ► Within WP4
    - ► Within PaNOSC
  - Limit scope to be realistic
  - Deploy portal prototype (March 2020)
  - Involve all facilities
- Dedicated activities on Wednesday and Thursday for WP4
  - And joined workshops with WP3, WP6 and WP8

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