Data analysis with Jupyter Notebook for Open Science

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Photon and Neutron Open Science Cloud

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Photon and Neutron Open Science Cloud – team effort

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- ESRF: European Synchrotron Radiation Facility
- ILL: Institut Laue-Langevin
- EuXFEL: European X-ray Free Electron Laser Facility
- ESS: The European Spallation Source
- CERIC-ERIC: The Central European Research Infrastructure Consortium
- ELI: Extreme Light Infrastructure

Outline

- Open Science, Data Analysis, Jupyter
- PaNOSC requirements and vision
- Challenges
- Summary

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823852.

Data Analysis for Open Science

- (FAIR) data is central for Open Science
- *Data* provides potential for new understanding
- *Data analysis* extracts the meaning from the data
- Publications based on data
  - Data sources should be known
  - Central findings (figures, tables, numbers) should be reproducible

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Jupyter Notebook

- Cells contain
  - (formatted) text
  - Code
  - Output from code execution
  - (multimedia)
- Can execute cells interactively
- Can save, close, load and re-execute
- Can export to other file formats
- Remote execution via https possible

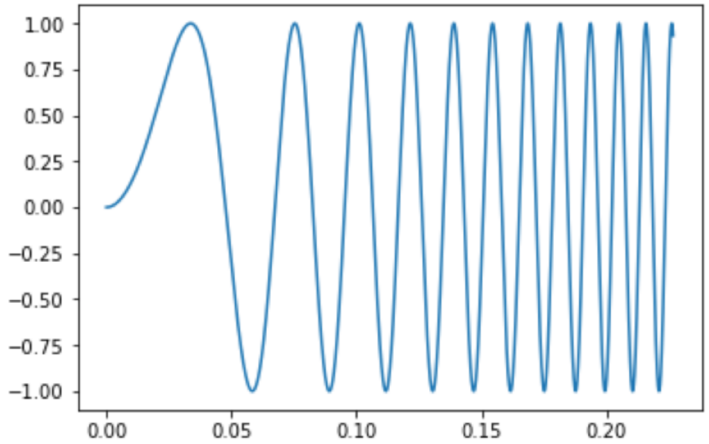
Cells can contain text and latex equations such as $f(x) = \sin(2\pi\omega t^2)$ and $\omega = 220$ Hz.
We can use code to define the corresponding functions:

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

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

In [3]:
```
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[3]:
```
[<matplotlib.lines.Line2D at 0x1047ada58>]
```



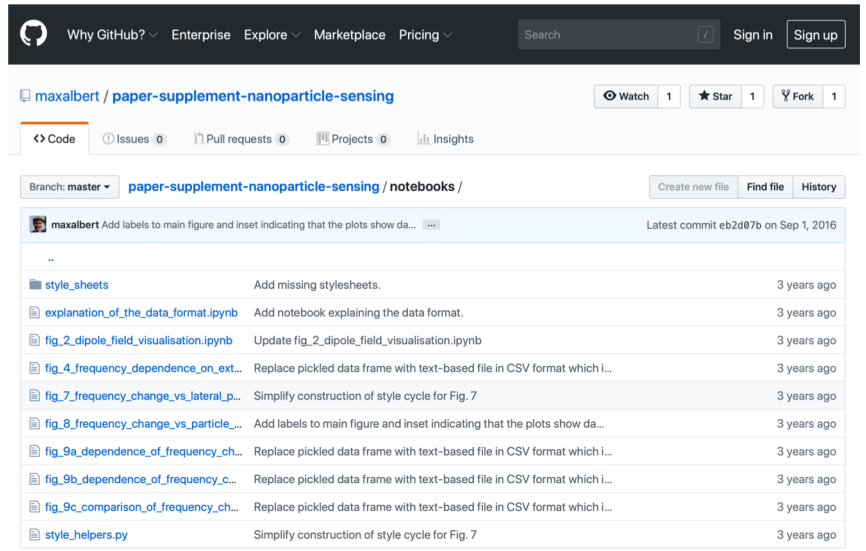
We can integrate media: images, videos, interactive elements and sound:

In [4]:
```
from IPython.display import Audio
Audio(y, rate=44100)    # plays the data in y as audible signal
```

Out[4]:

Jupyter Notebook for Open Science

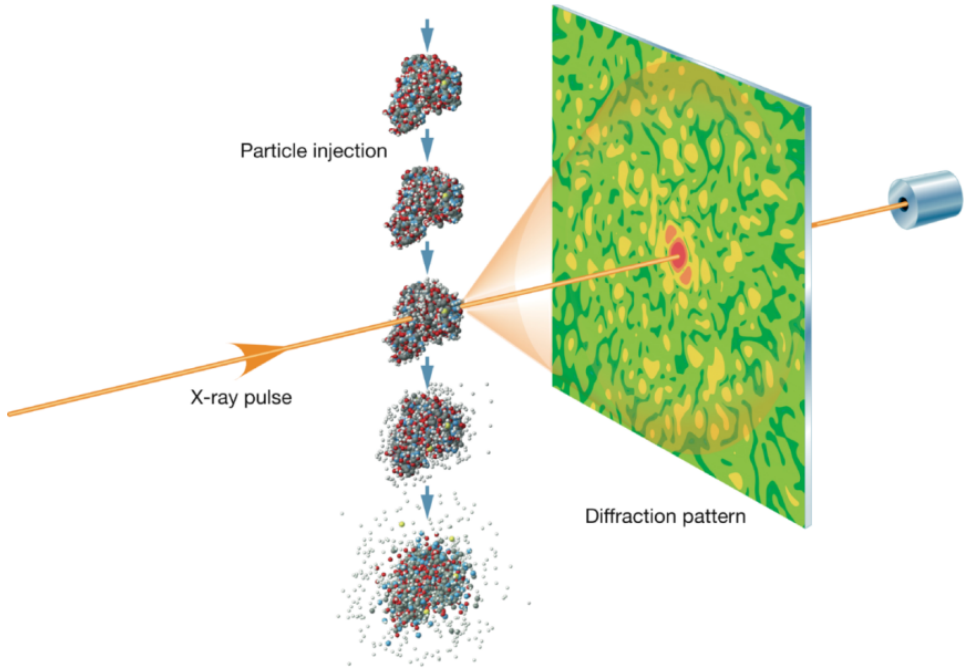
- Combination of code, output and annotation *in one document*
- If used appropriately, makes publications *reproducible*
  - For example: one notebook per figure in publication (examples: [1], [2])
- Notebooks from reproducible publications make the work *re-usable*
  - Currently, lots of time is used by researchers to repeat the work of others, before they can advance science.



[1] Appl. Phys. Lett. 109, 122401 (2016), https://doi.org/10.1063/1.4962726, https://github.com/fangohr/paper-supplement-2016-dmi-nanocylinder-hysteresis
[2] Nanotechnology 27, 455502 (2016), https://doi.org/10.1088/0957-4484/27/45/455502 https://github.com/maxalbert/paper-supplement-nanoparticle-sensing

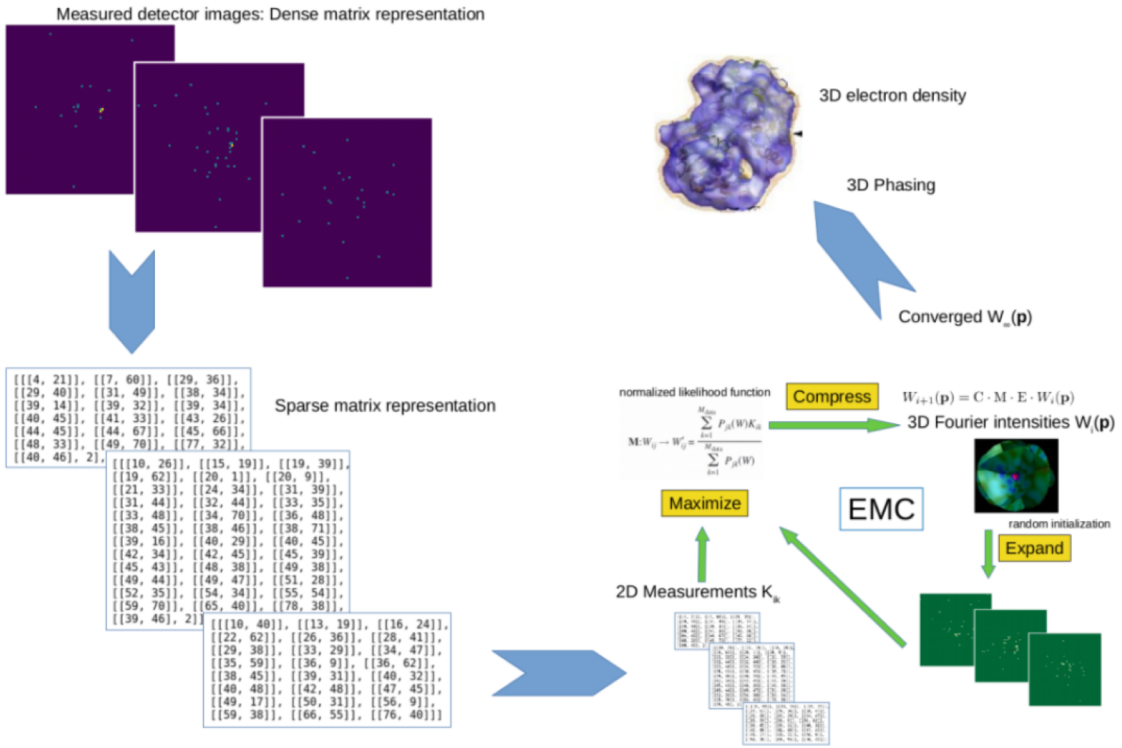
Photon and Neutron Open Science Cloud (PaNOSC)

- Research facilities using Photons and Neutrons for imaging
  - Underpins a wide range of fundamental and applied research, from basic physics to drug design
- European XFEL: use short-wavelength photons to image small things
  - Infrastructure
    - 3.4km tunnel
    - Accelerate electrons, then create photons from electrons
  - Data volume
    - Typical detector: 1 million pixels, each using 2 bytes
    - up to 27,000 X-ray pulses per second
    - → 2 byte * 1,000,000 * 27,000 / s = 54 GB/s
    - → 194 TB/h (theoretical peak)



Current state of data analysis: example European XFEL

- Data source:
  - 2d image detectors (up to 27,000 images /s)
  - Scalar values (typically 10 values per second)
  - others
- Data analysis
  - Calibration, data filtering, reduction, azimuthal integration, real space reconstruction, …
- Many steps involving different programs
  - connect `via ssh -X` to HPC cluster
  - some programs use GUIs (X display at EuXFEL)
  - some programs use command line
  - Increasingly Jupyter Notebooks



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First, let's load a run containing LPD data:

https://karabo-data.readthedocs.io/en/latest/index.html

[1]:
```
from karabo_data import RunDirectory, by_index

run = RunDirectory('fxe_example_run/')
# Using only the first three trains to keep this example light:
run = run.select_trains(by_index[:3])

run.instrument_sources
```

[1]:
```
frozenset({'FXE_DET_LPD1M-1/DET/0CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/10CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/11CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/12CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/13CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/14CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/15CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/1CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/2CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/3CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/4CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/5CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/6CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/7CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/8CH0:xtdf',
           'FXE_DET_LPD1M-1/DET/9CH0:xtdf',
           'FXE_XAD_GEC/CAM/CAMERA:daqOutput',
           'FXE_XAD_GEC/CAM/CAMERA_NODATA:daqOutput',
           'SA1_XTD2_XGM/DOOCS/MAIN:output',
           'SPB_XTD9_XGM/DOOCS/MAIN:output'})
```

Normal access methods give us each module separately:

[2]:
```
data_module0 = run.get_array('FXE_DET_LPD1M-1/DET/0CH0:xtdf', 'image.data')
data_module0.shape
```

[2]:
```
(384, 1, 256, 256)
```

The class `karabo_data.components.LPD1M` can piece these together:

[3]:
```
from karabo_data.components import LPD1M
lpd = LPD1M(run)
lpd
```

[3]:
```
<LPD1M: Data interface for detector 'FXE_DET_LPD1M-1' with 16 modules>
```

[4]:
```
image_data = lpd.get_array('image.data')
```

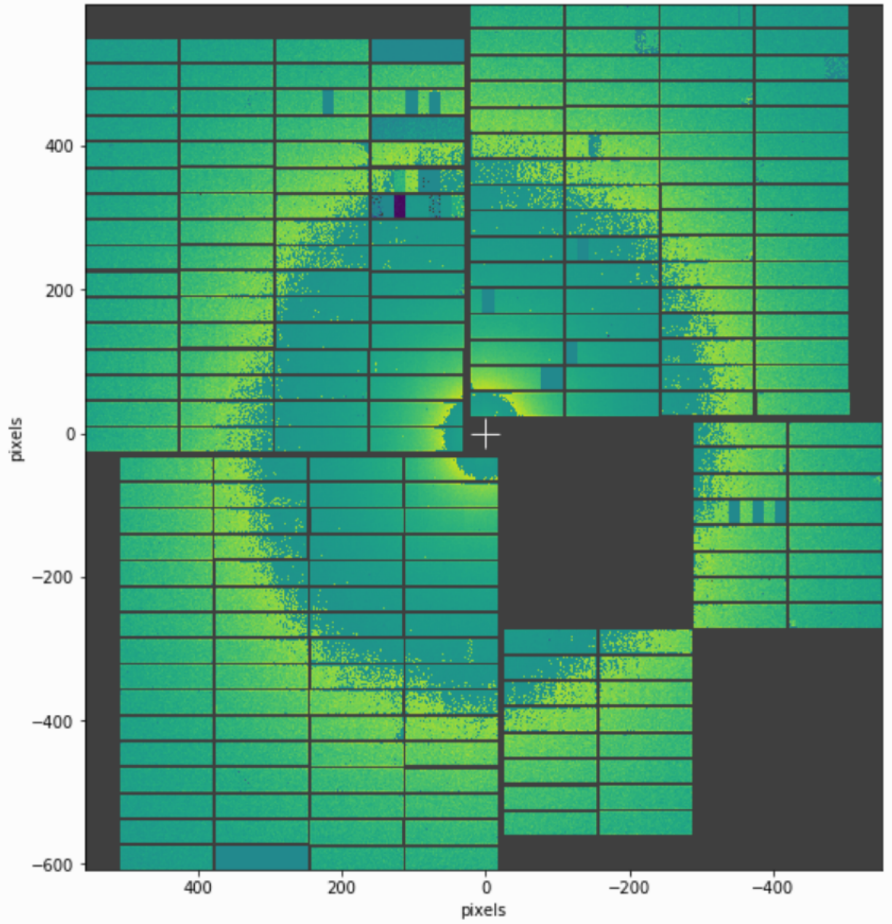
[10]:
```
# From March 18; converted to XFEL standard coordinate directions
quadpos = [(11.4, 299), (-11.5, 8), (254.5, -16), (278.5, 275)]  # mm

geom = LPD_1MGeometry.from_h5_file_and_quad_positions('lpd_mar_18_axesfixed.h5', quadpos)
```

Reassemble and show a detector image using the geometry:

[11]:
```
geom.plot_data_fast(clip(modules_data[12], max=5000))
```

[11]:



Reassemble detector data into a numpy array for further analysis. The areas without data have the special value ``*nan*`` to mark them as missing.

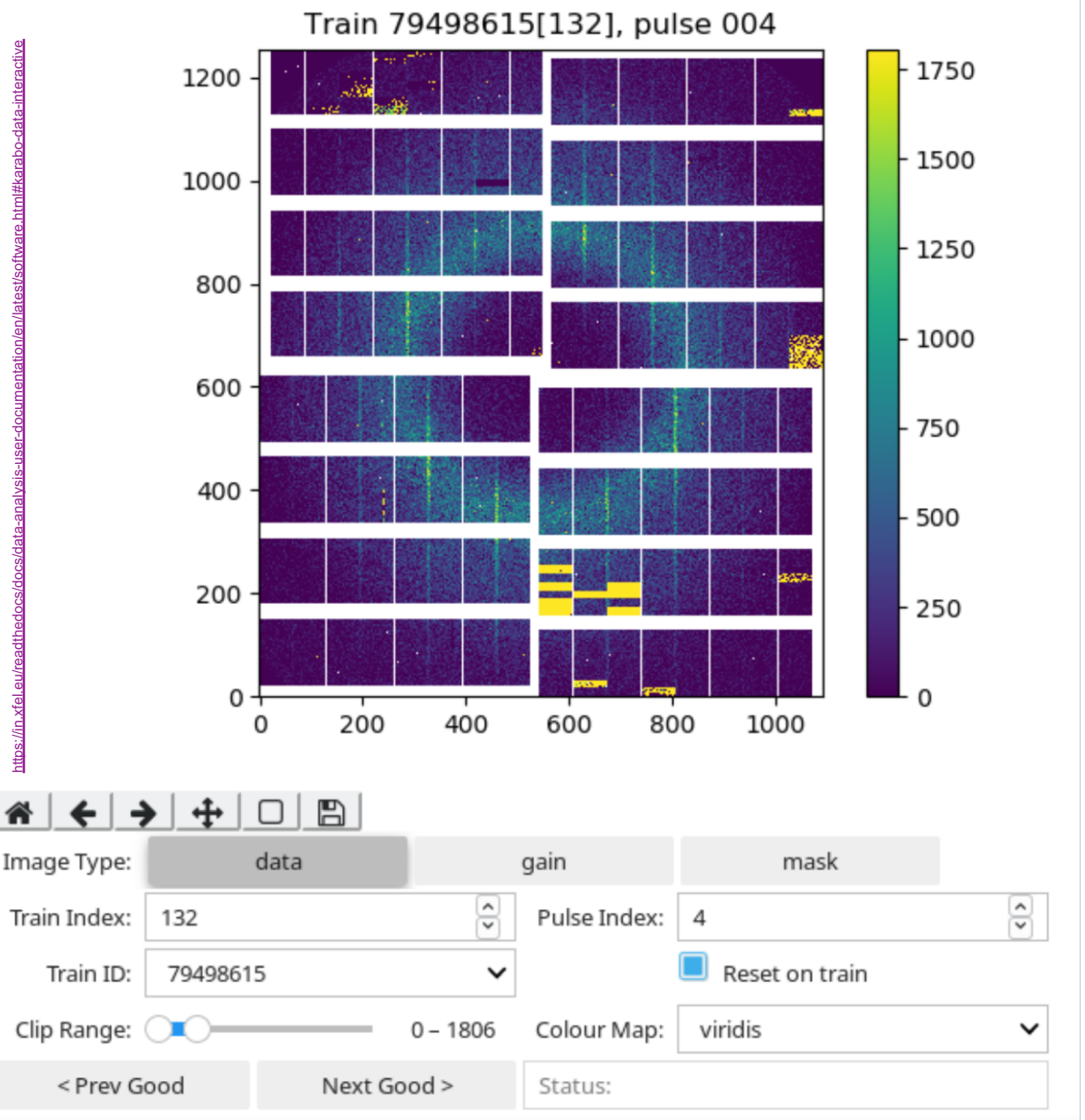
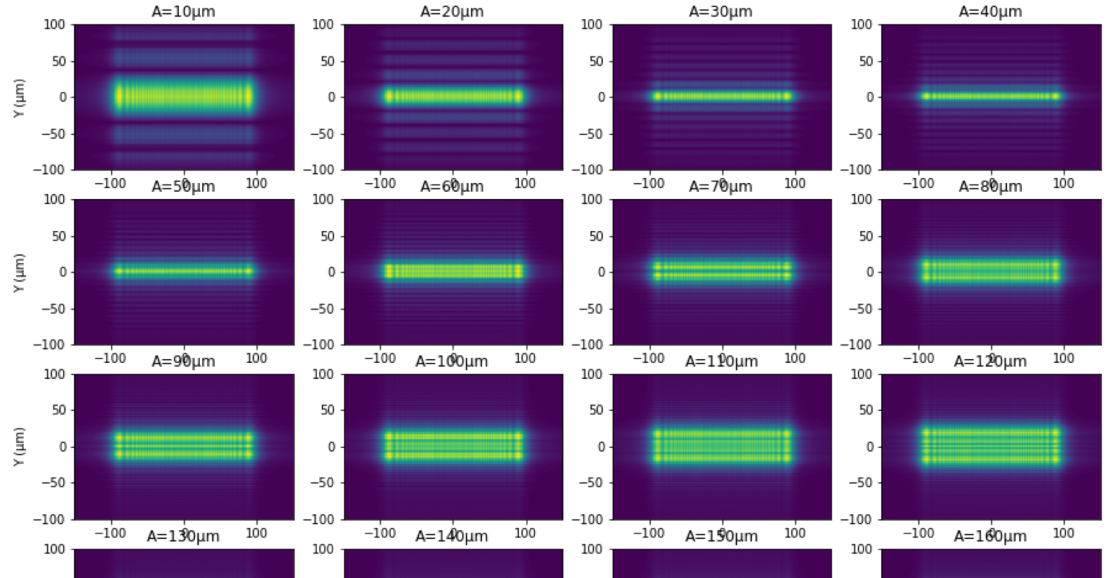


Fig. 6.2 Example image showing the karabo data interactive widget and plot layout

```
In [7]: # propagation of a stack of A x 200 microns apertures, varying A
w = Wavefront(d=np.zeros((16, 512, 512), dtype=np.complex64), pixel_size=1e-6, wavelength
=1.5e-10)
x, y = w.get_x_y()
d = w.get()
for i in range(16):
    a = 5e-6 / 2 * (i + 1)
    d[i] = ((abs(y) < a) * (abs(x) < 100e-6)).astype(np.complex64)
w.set(d)
w = PropagateFRT(1.2) * w
figure(figsize=(15, 10))
x, y = w.get_x_y()
x *= 1e6
y *= 1e6
for i in range(16):
    subplot(4, 4, i + 1)
    imshow(abs(fftshift(w.get()[i])), extent=(x.min(), x.max(), y.min(), y.max()), origin
='lower')
    title("A=%dμm" % (10 * (i + 1)))
    if i >= 12:
        xlabel('X (μm)')
    if i % 4 == 0:
        ylabel('Y (μm)')
    xlim(-150, 150)
    ylim(-100, 100)
suptitle("Fractional Fourier propagation (0.5m) of a A x 200 μm aperture")
```

```
Out[7]: <matplotlib.text.Text at 0x1141b3208>
```



Solution architecture for PaNOSC vision:

- Finding data:
  - Web interface with data base of experiment metadata
- Exploring and analysing data remotely (=in the cloud):
  - JupyterHub serving relevant notebooks
  - Move data analysis code into the notebook
  - remote desktop in browser, connected to Desktop of virtual machine

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PaNOSC Use case 1: reproducibility and re-usability published results

- For a given publication based on facility data, users can
  - Find the data (through the EOSC web portal or URL/DOI in paper)
  - Access the data through web portal
  - Inspect the data analysis (notebook) that led to key figures / statements in the publication
  - Re-execute the data analysis through (→ reproducibility)
  - Modify and extend the notebook (→ reusability)

- Users may include scientists, interested public, journal editors and reviewers, representatitves from research councils, . . .

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PaNOSC Use case 2: enable new data analysis on existing data sets

- Users can
  - Search and find data sets from experiments through web portal
  - Access the data through web portal
  - Choose from appropriate selection of data analysis tools (=Jupyter Notebook templates)
  - Execute the notebook
  - Modify and extend the notebook

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Challenges 1

- Different facilities
  - Currently 6 facilities involved
  - Generally use different ways to store meta data data
  - Common way of classifying data sets (and experiment types) ?

- Data scale
  - For some data sets, the data cannot be moved to the compute resource

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Challenges 2

- Analysis in Notebook
  - Computational environment – software (containers?)
    - Need to provide the right computational environment for each analysis type
    - How can we maintain computational environments in the future (Binder-like?)
    - Extending up to the life-time of publications and data sets
  - Which analysis is appropriate for data set → classification of data sets
  - Making analysis capabilities available in the Jupyter Notebook
    - Command line drived and Python based computation straightforward,
    - GUI-based tool more difficult / impossible
  - What to do with resulting analysis?
  - Some analysis notebooks require significant HPC resources (execute jobs from notebook?)
  - Computational environment – hardware, GPUs?

panosc

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Challenges 3

- Concurrent development with EOSC hub
- Complicated access rights for data sets
  - Data policies with embargo period
- Publication use case:
  - Requires collaboration with scientists
    - Preparation of data analysis notebooks
  - Social / cultural challenge
  - Helped by changing metrics and expectations from funding bodies and journals
  - Research facilities can lead by example

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Summary

- Introduction PaNOSC project (Photon and Neutron Open Science Cloud), http://panosc-eu.github.io
- Focus on data analysis
- Use cases
  - Make publications reproducible
    - EOSC MyBinder instance as first step?
  - Allow convenient exploration of existing data sets
- Contributions / brain storming / collaboration welcome

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