Data analysis support in Karabo at European XFEL

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Joint effort

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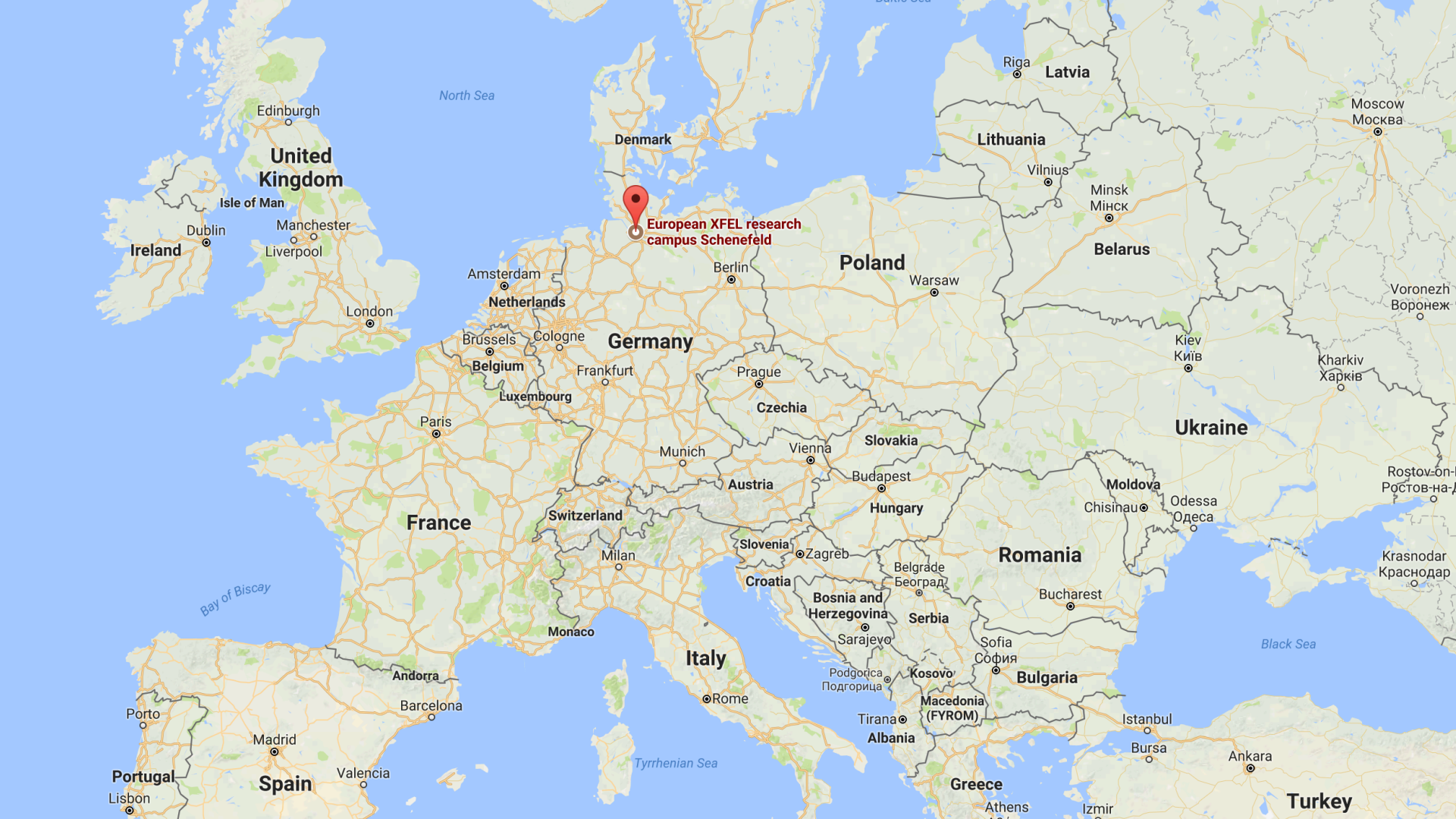
Outline

- European XFEL – current status
- Data analysis infrastructure
- Online data analysis
- Offline data analysis
- Summary


European XFEL research campus Schenefeld
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Liverpool
London
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Izmir

European XFEL – current status

- European XFEL, Northern Germany
  - Official opening 1 September 2017
- 2 of 6 scientific instruments live
- First experiments started 14 Sept 2017
- X-rays
  - 10 trains per second
  - Up to 2700 pulses (222 ns separation) per train

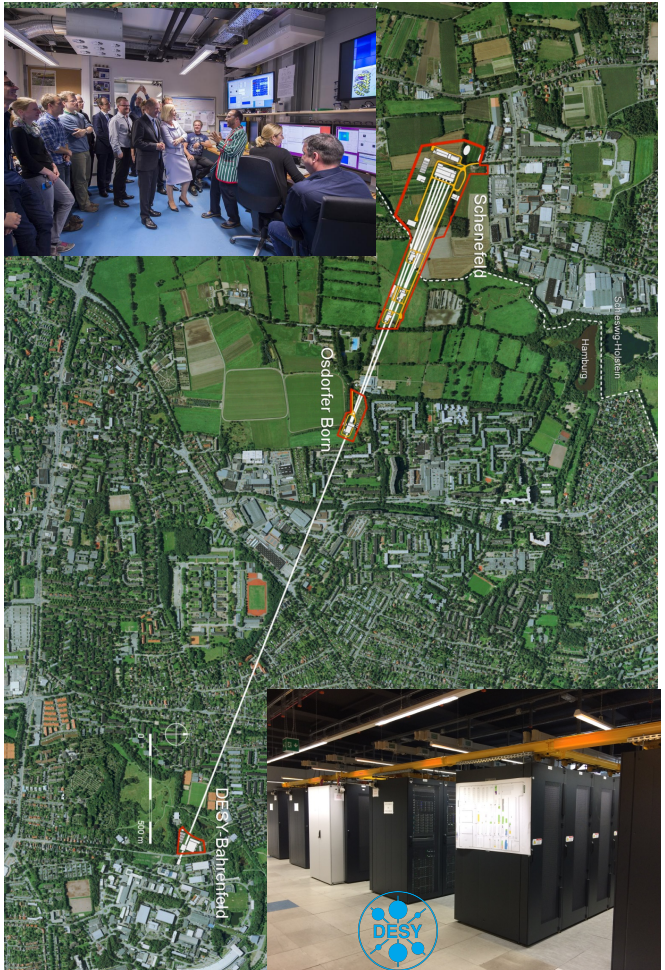

Hamburg
Schenefeld
Osdorfer Born
3400m
DESY-Bahrenfeld
0
500 m

Data analysis infrastructure

- Hardware: “Online cluster”,
  - 8 nodes x 20 cores, 256GB RAM dedicated to users
  - Additional nodes for control and XFEL provided calibration and processing

- Hardware: “Offline cluster” = Maxwell cluster (DESY)
  - 80 nodes/3200 cores (Intel Xeon E5-2698v4)
  - ~112 TFlops
  - 512GB RAM each node
  - +20 nodes with other spec

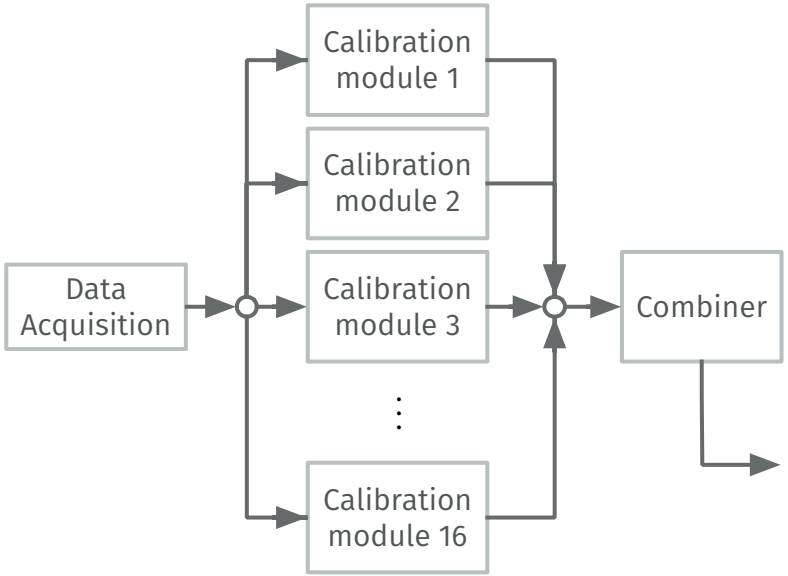
- Software: Karabo [1]



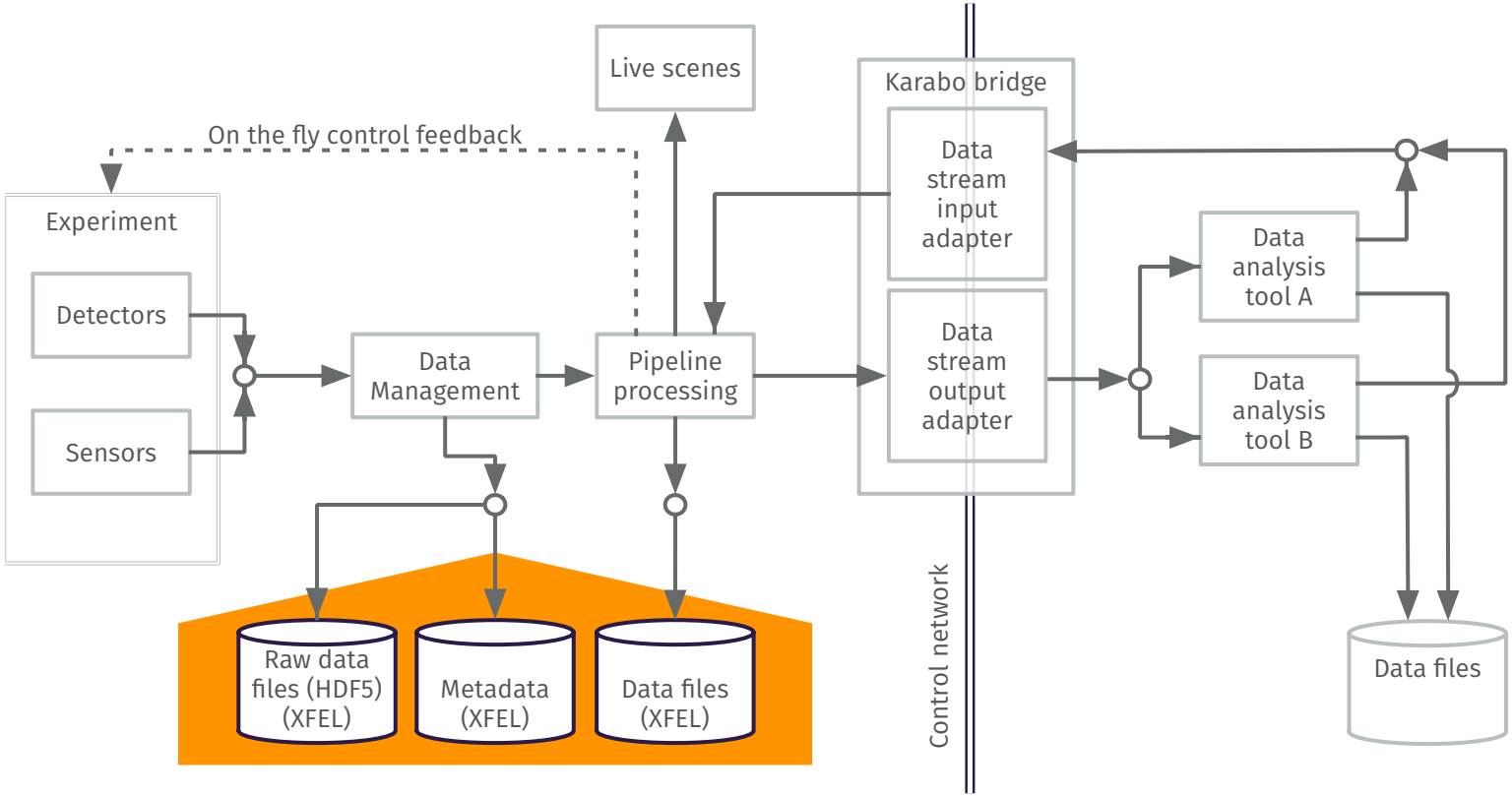
[1] B. Heisen et al: “Karabo: An integrated software framework combining control, data management, and scientific computing tasks,” in14th ICALEPCS2013. San Francisco, CA, 2013.

Karabo processing pipeline example

- Data tokens pass through pipeline
- Processing units called “devices”
- Devices can be distributed over hardware
- Example: calibration done for 16 detector panels in 16 pipelines, distributed over 8 nodes
- Different protocols what to do with data if listening device cannot keep up

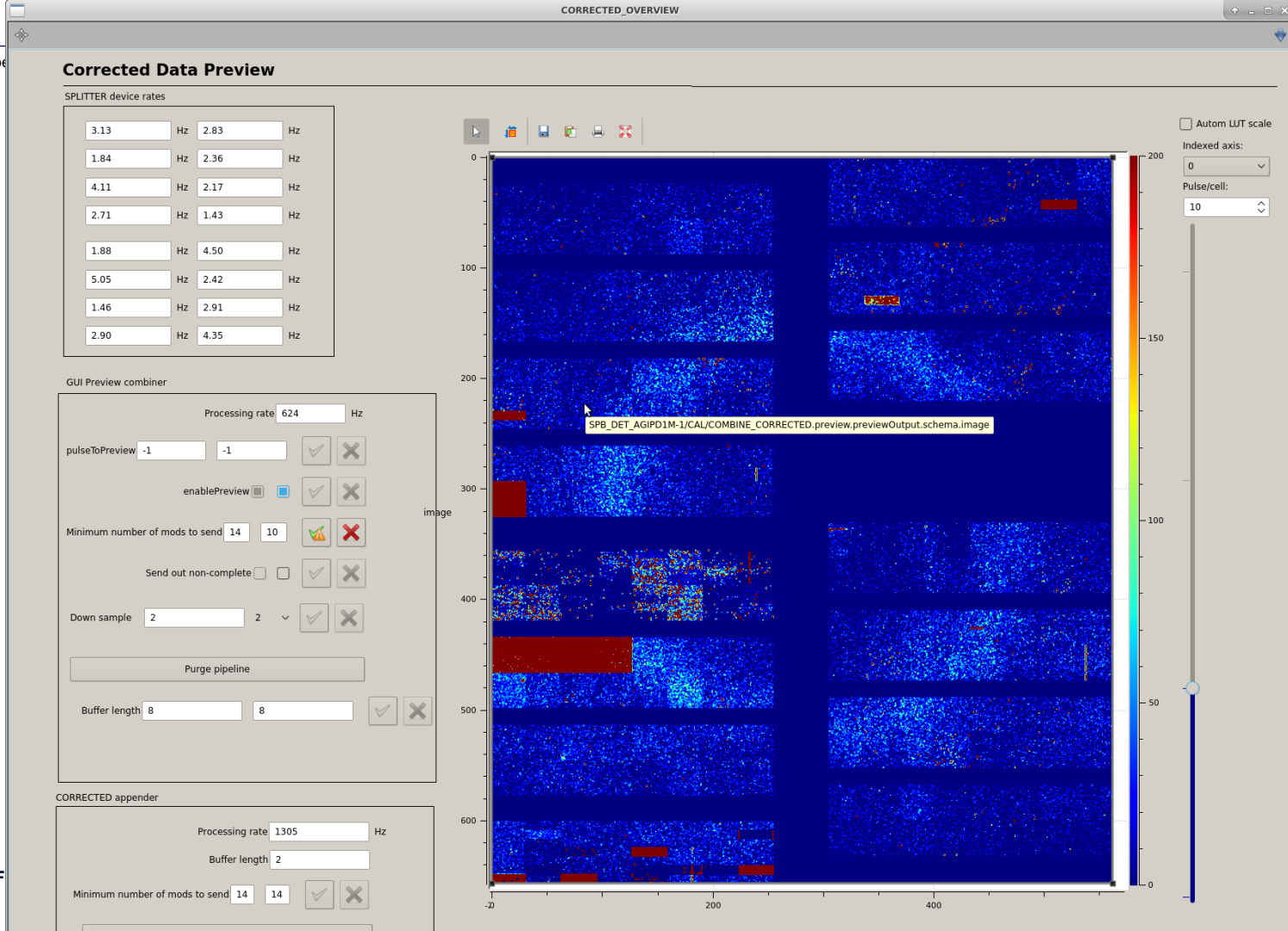


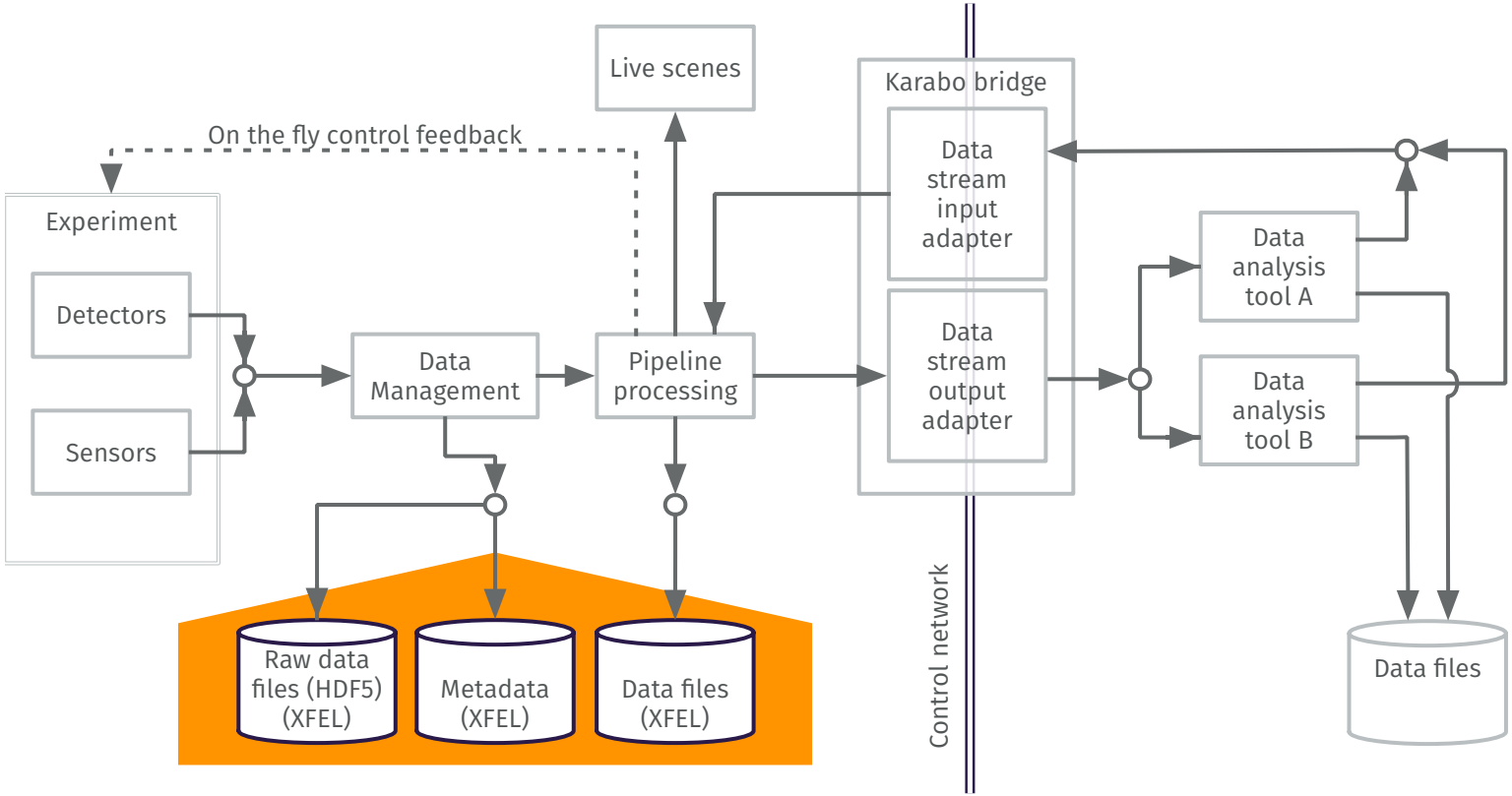
Online data analysis



Online data analysis

Rapid feedback through GUI





Online data analysis

Karabo bridge

- Provide “receiving client code templates”
  - Python
  - C++
- Karabo bridge tested with OnDA [1] during first experiments
- Latency
  - 2.5 seconds corrected
  - 1.5 seconds uncorrected
- Provide test data set

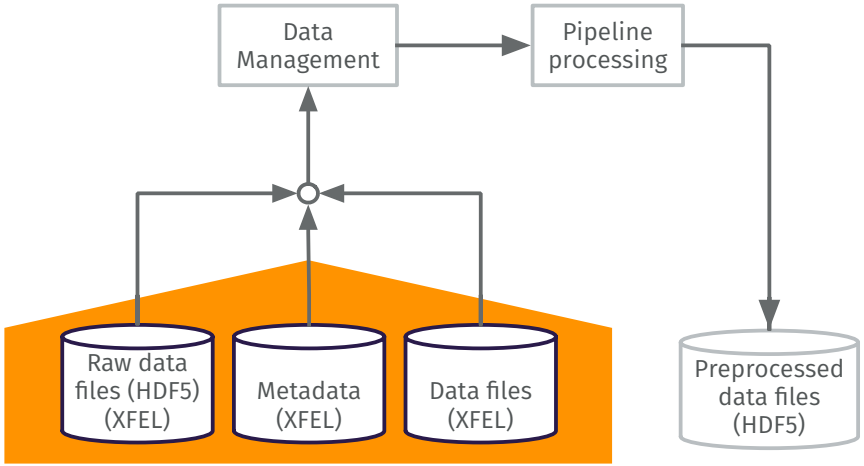
- Implementation:
  - ZeroMQ as the network connection
  - Protocol for serialised data under investigation. Candidates:
    - Pickled Python dictionaries
    - MessagePack
    - ProtoBuf

[1] OnDA: online data analysis and feedback for serial X-ray imaging,” Journal of Applied Crystallography, vol. 49, no. 3, pp. 1073–1080, Jun 2016

Offline data analysis

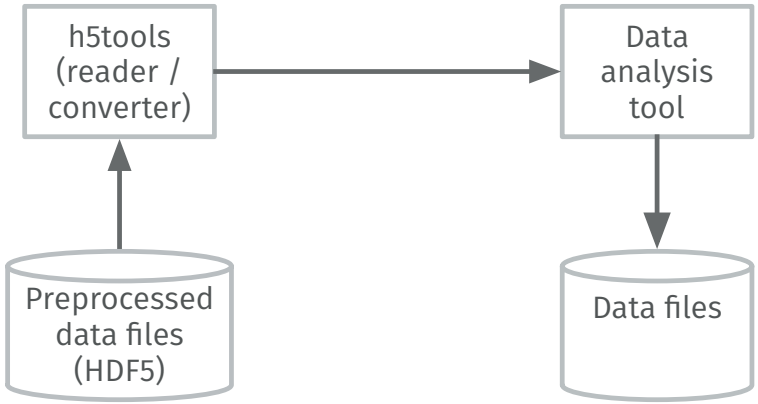
Offline data access

- Preprocessed data files can be requested on demand
- During experiment preprocessed files become available automatically on offline cluster (a few minutes after run stops)

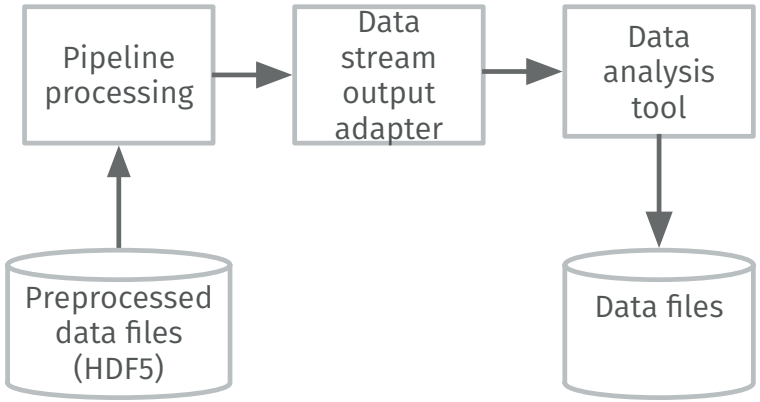


Offline: Two ways of using preprocessed files

- Processing HDF5 files
  - Using European XFEL's h5tools
  - Or directly

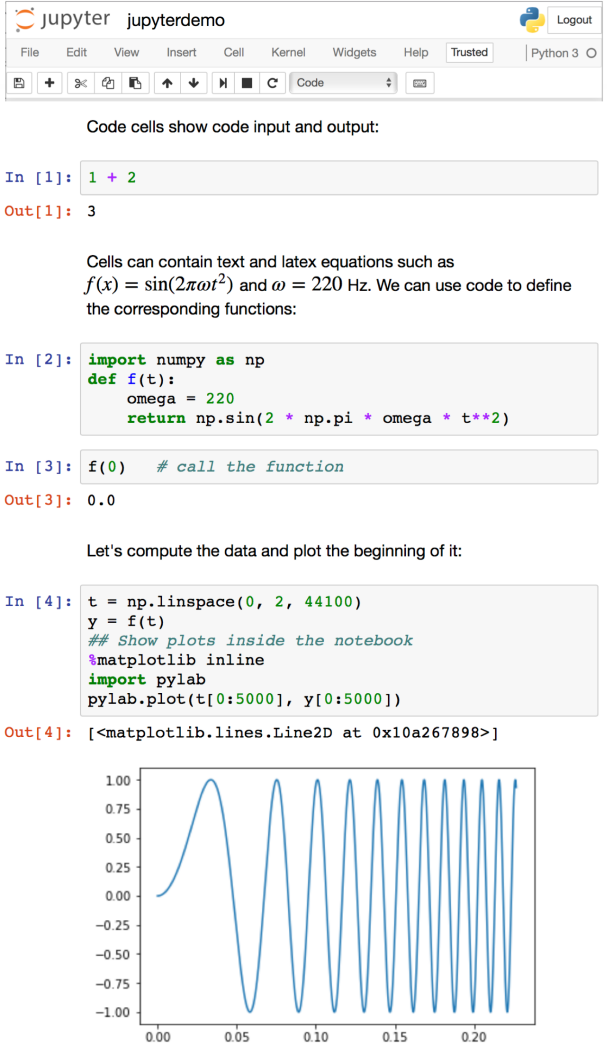


- Sending HDF5 files through the Karabo bridge
  - Imitates online setup
  - Good for re-use of interface
  - Can test in advance of experiment



Reproducible Science and Jupyter Notebook

- Jupyter Notebook
  - Executable document
  - Code, output, interpretation
- Integrate (Python) tools in Notebook
  - h5reading tools [1]
  - Example notebooks [2]
  - Pydetlib [3]
- Hope to grow library of analysis recipes with community
- [1, 2] http://github.com/European-XFEL
  [3] https://in.xfel.eu/readthedocs/docs/pydetlib/en/latest/index.html



Summary

- Online: GUI & Karabo bridge (& HDF5)
- Offline: HDF5 file based & Karabo bridge
- User support
  - Online documentation (http://tinyurl.com/ybx29ryt)
  - Growing set of open source tools (http://github.com/European-XFEL)
  - Access to Maxwell cluster (DESY)
  - Jupyter Notebook
  - Docker
  - Support before, during and after experiment
- Collaboration with users and other facilities desired

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