Data Analysis at the European XFEL using Karabo



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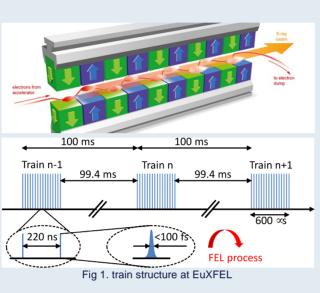
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The European XFEL has gathered about 1.5PB of raw data in the first year of operation. We describe the data analysis capabilities [1] of the Karabo distributed control system [2] and related software developed at the European XFEL to supporting scientific experiments. The range of requirements for data analysis includes near-real time during experiments and offline analysis.

Data Structure

The European XFEL facility generates coherent and intense X-ray pulses by bunches of up to 2700 pulses repeating every 100 ms.

The data generated by instruments and detectors for each of these pulses are distributed **at 10 Hz**, which corresponds to the pulses train structure. One **train data** container consist of many images taken for each pulse in a train.



Karabo Bridge

The Karabo bridge allows data analysis tools to receive data from the Karabo control system without having to be build against the framework. It uses ZeroMQ and msgpack to send data efficiently. In the future, this will be extended to send data back to Karabo as well. The European XFEL provides C++ [3] and Python [4] clients.

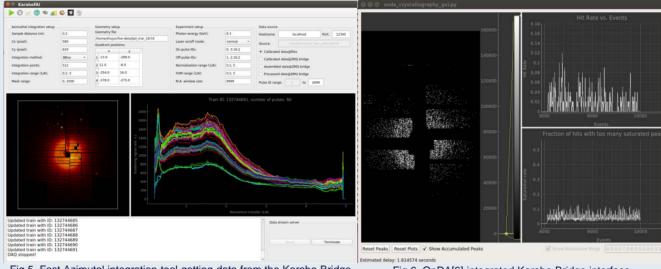


Fig 5. Fast Azimutal integration tool getting data from the Karabo Bridge

Fig 6. OnDA[6] integrated Karabo Bridge interface

The Karabo Bridge has been used to feed analysis tools such as OnDA [6], Hummingbird [7], CASS [8], Dozor [9] and PyFAI [10] based software for near-real time feedback.

Offline Processing

We develop and provide a Python package for data analysis: **Karabo-data** [5]. It is designed for **reading data** stored by the **Karabo data acquisition** service and offer a range of function and routines to **support** users **offline data analysis**.

Karabo-data is an open source project and is in active development. Feature requests and contributions are welcome. Some of the current features:

Online Processing

During experiments, **near real-time** feedback to users and beam scientists is important in order to optimize the experiment setup and collect the best data possible. We provide solutions to process data and give visualization feedback in the order of seconds.

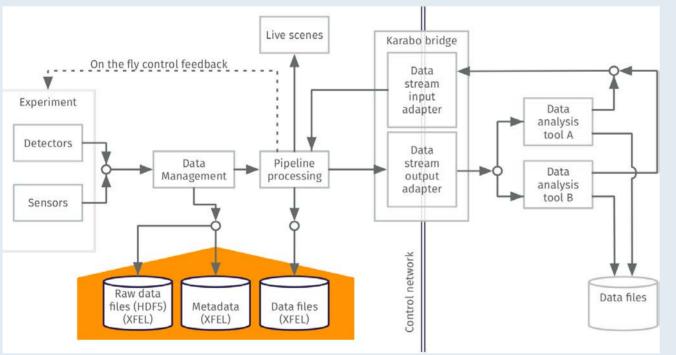
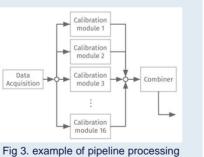


Fig 2. Schematic view of data flow for rapid feedback during experiment

Data Pipelines

The Karabo framework support **peer-to-peer** messaging between devices, allowing the implementation of processing pipelines with **high data rates**. Pipelines implemented in the Karabo environment can easily **parallelize** and **distribute** heavy processing tasks on many physical machines.



The large detectors used at the

European XFEL need

appropriate correction and

processing can be applied on

the data they produce. This is

pipelines **distributing** the data

over 8 GPU processing nodes

calibration before further

carried out using the data

on a HPC cluster.

Any processing algorithm implemented as a Karabo device can use this feature and benefit from the Karabo integration (results permanently stored via DAQ, GUI control and live view, ...)

Online Detector Calibration

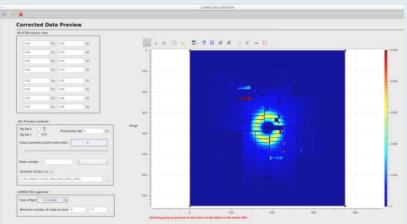
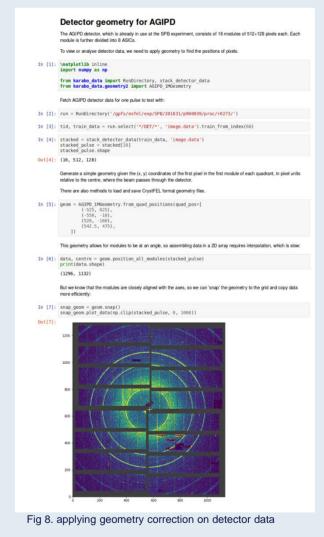


Fig 4. Live feedback of calibrated data from the LPD detector on a Karabo scene

Run data reading and exploration
Data filtering (sources, trains, ...)
Data correlation (Pandas, Xarray)
Data views to fit external tools
Stream data as the Karabo Bridge
Apply detector geometry
Data conversion (from HDF5)

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References

[1] H. Fangohr et al., "Data Analysis Support in Karabo at European XFEL", in *Proc. 16th Int. Conf. on Accelerator and Large Experimental Control Systems (ICALEPCS'17)*, Barcelona, Spain, Oct. 2017, paper TUCPA01, pp. 245-252, ISBN: 978-3-95450-193-9, https://doi.org/10.18429/JACoW-ICALEPCS2017-TUCPA01, 2018.

[2] B. Heisen, D. Boukhelef, S. Esenov, S. Hauf, I. Kozlova, L. Maia, A. Parenti, J. Szuba, K. Weger, K. Wrona *et al.*, "Karabo: An integrated software framework combining control, data management, and scientific computing tasks," in *14th International Conference on Accelerator & Large Experimental Physics Control Systems, ICALEPCS2013. San Francisco, CA*, 2013.

[3] <u>https://github.com/European-XFEL/karabo-bridge-cpp</u>
[4] <u>https://github.com/European-XFEL/karabo-bridge-py</u>
[5] <u>https://github.com/European-XFEL/karabo_data</u>
[6] <u>http://journals.iucr.org/j/issues/2016/03/00/zf5001/index.html</u>

[7] http://journals.iucr.org/j/issues/2016/03/00/zd5007/index.html
[8] http://journals.iucr.org/j/issues/2016/04/00/zw5003/index.html
[9] http://journals.iucr.org/d/issues/2015/11/00/tz5083/index.html
[10] http://journals.iucr.org/j/issues/2015/02/00/fv5028/index.html

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