The common goal of the PaNOSC and ExPaNDS projects is to make scientific FAIR data (Findable, Accessible, Interoperable and Reproducible) a reality and support the advancement of open science through the development of high-value-added services leveraging that data that will also be available from the European Open Science Cloud.

Cloud-based Data Analysis Services for Photon and Neutron Science

PaNOSC has been developing the **Common Portal for Data Analysis Services** to facilitate starting a data analysis session after a dataset of interest has been collected. The Portal aims to provide access to both remote desktop environments and Jupyter Notebooks, enabling users to **remotely analyse data** from PaN facilities, such as synchrotrons and neutron sources.

After initial deployment at facilities to provide remote analysis services to local data, the Portal will be deployed as part of the EOSC to provide federated data analysis of data across the facilities.

This poster aims to present a selection of use cases of the data analysis services developed in the projects.

Typical workflow for Common Portal usage

User authentication using Umbrella ID

↓

Search for datasets (for which the user has been a proposal member, thus requiring authenticated access)

↓

Selection of an analysis environment (in either a remote desktop, or Jupyter Notebook environment)

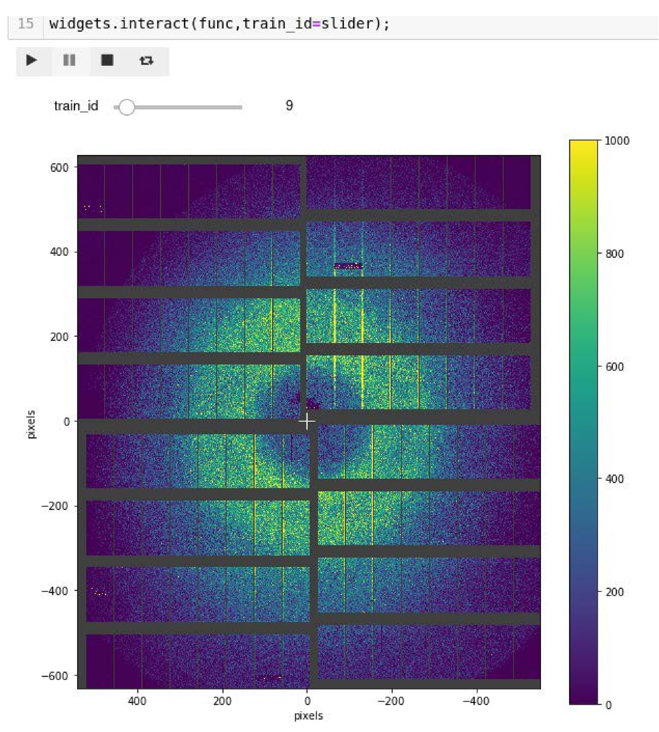
↓

Spawn the chosen analysis environment and link it to the chosen datasets (if the analysis environment is not physically located with the data, data transfer protocols will be active)

↓

Access the environment via the Portal and perform data analysis

EuXFEL Data in NeXus Golden Standard



There were great efforts put in the last two decades in the research community to elaborate a common standard for high data-rate macromolecular crystallography (HDRMX). This agreed "Gold Standard" builds on the NeXus/HDF5 NXmx application definition and the International Union of Crystallo-graphy (IUCr) imgCIF/CBF dictionary, and it is compatible with major data-processing programmes and pipelines. Here we demonstrate the EuXFEL data packed into a NeXus file, which is fully compliant with the Gold Standard by design, since it is built directly from HDRMX NeXus definitions. We use open-source software developed both by community (cctbx) and in-house (extra-data).

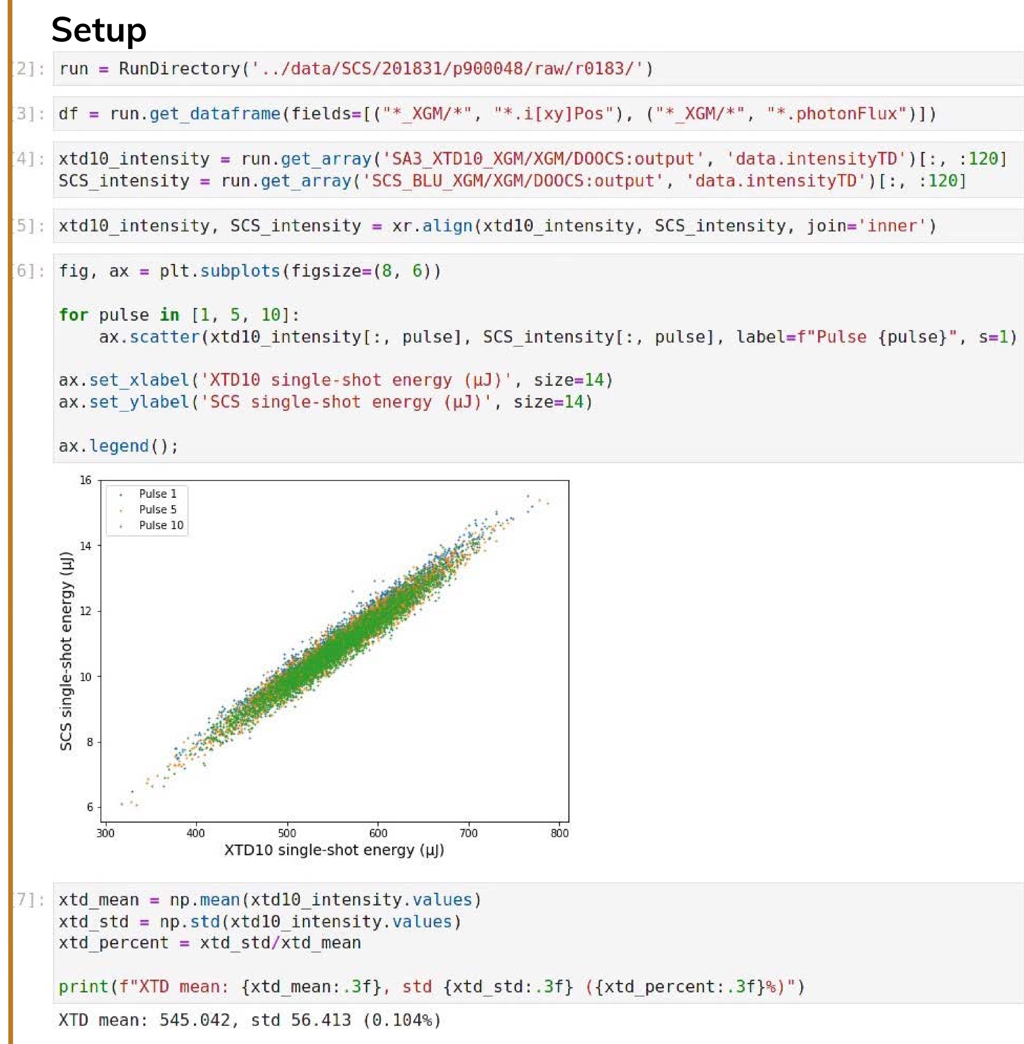
Developers:
Herbert Bernstein, Andreas Förster, Asmit Bhowmick, Aaron Brewster, Sandor Brockhauser, Luca Gelisio, David Hall, Filip Leonarski, Valerio Mariani, Gianluca Santoni, Clemens Vonrheink, Graeme Winter, Anton Barty, Thomas Kluyver, Fabio Dall'Antonias, Yury Kirienko

References:
[1] Bernstein, H. J., Förster, A., Bhowmick, A., Brewster, A. S., Brockhauser, S., Gelisio, L., ... & Winter, G. (2020). Gold Standard for macromolecular crystallography diffraction data. IUCrJ, 7(5), DOI: https://doi.org/10.1107/S2052252520008672
[2] CXI DB #80, DOI: https://dx.doi.org/10.11577/1464101
[3] A. Brewster, M. Wang, H. Bernstein. (2019). 68 image lysozyme dataset recorded on the Jungfrau 16M detector at SwissFEL and formatted as a NeXus file (Version 3) [Data set]. DOI: https://doi.org/10.5281/zenodo.3834335

More: https://github.com/European-XFEL-examples/panosc-nexus

Operation of X-ray gas monitors at the European XFEL

Setup



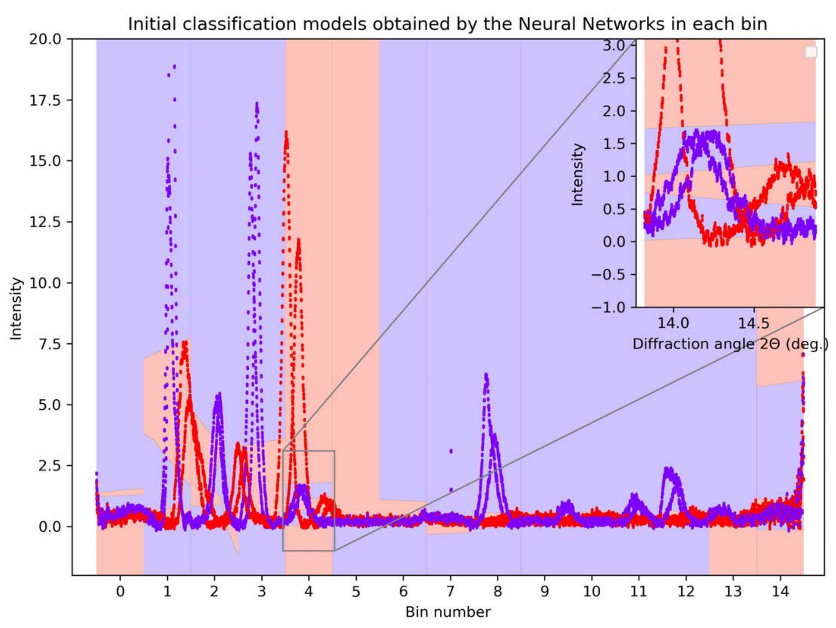
X-ray gas monitors (XGMs) are operated at the European XFEL for non-invasive single-shot pulse energy measurements and average beam position monitoring. They are used for tuning and maintaining the self-amplified spontaneous emission (SASE) operation and for sorting single-shot experimental data according to the pulse-resolved energy monitor data. The XGMs were developed at DESY based on the specific requirements for the European XFEL. In total, six XGM units are continuously in operation. Here, the main principle and experimental setup of an XGM are summarized, and the locations of the six XGMs at the facility are shown. Pulse energy measurements at 0.134 nm wavelength are presented, exceeding 1 mJ obtained with an absolute measurement uncertainty of 7–10%; correlations between different XGMs are shown, from which a SASE1 beamline transmission of 97% is deduced. Additionally, simultaneous position measurements close to the undulator and at the end of the tunnel are shown, along with the correlation of beam position data simultaneously acquired by an XGM and an image

Developers:
T. Maltezopoulos, F. Dietrich, W. Freund, U. F. Jastrow, A. Koch, J. Laksman, J. Liu, M. Planas, A. A. Sorokin, K. Tiedtke and J. Grünert, R. Rosca

References: [1] J. Synchrotron Rad. (2019). 26, 1045-1051, DOI: doi.org/10.1107/S1600577519003795

More: https://github.com/European-XFEL-examples/jsr-operation-xgm-euxfel-paper

Machine Learning Based Spectra Classification



At the European XFEL, X-ray pulses can be generated with only 220ns separation in time and a maximum of 27000 pulses per second. In experiments at European XFEL, spectral changes can indicate the change of the system under investigation and so the progress of the experiment. An immediate feedback on the actual status (e.g., time resolved status of the sample) would be essential to quickly judge how to proceed with the experiment. The two major spectral changes that we aim to capture are either the change of intensity distribution (e.g., drop or appearance) of peaks at certain locations, or the shift of those on the spectrum. Machine Learning (ML) opens up new avenues for data-driven analysis in spectroscopy by offering the possibility to quickly recognize such specific changes on-the-fly during data collection.

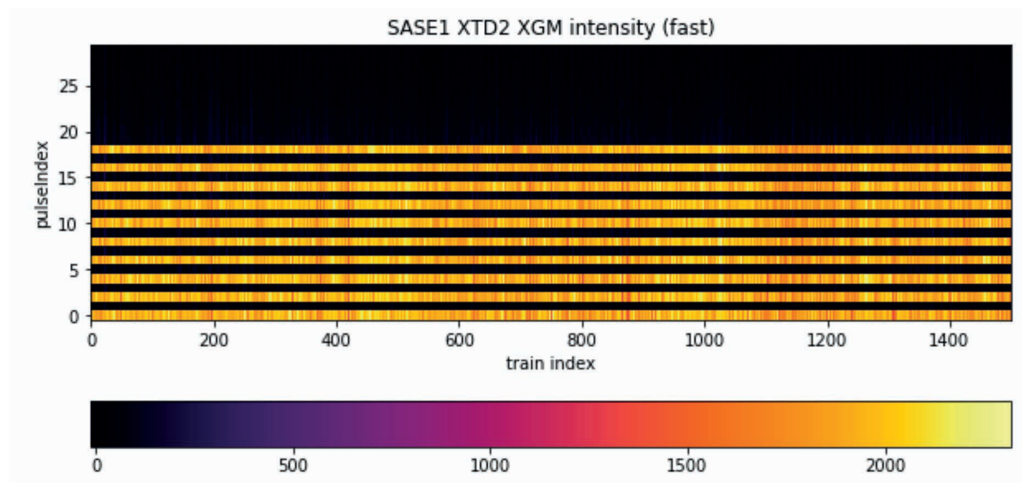
ML requires lots of data which are clearly annotated. Hence, it is important that research outputs align with the FAIR principles. In case of XFEL experiments, it is suggested to introduce NeXus data format standards in future experiments. In this work an example is presented, of a possible use of Neural Network based ML for accurately classifying the system state if data is properly provided. A solution is shown, to automatically find the regions (or bins) with high separability where the spectra classes differ significantly. By teaching individual neural networks for each bin, and by combining them with a weighting technique, a robust classification of any new spectral curve can be quickly obtained.

Developers: Christian Plueckthun; Zuzana Konopkova; Sandor Brockhauser; Yue Sun

References:
[1]. Pennicard, D., Smoljanin, S., Pithan, F., Sarajlic, M., Rothkirch, A., Yu, Y., Liermann, H.P., Morgenroth, W., Winkler, B., Jenei, Z. and Stawitz, H., 2018. LAMBDA 2M GaAs—A multi-megapixel hard X-ray detector for synchrotrons. Journal of Instrumentation, 13(01), p.C01026, DOI: 10.1088/1748-0221/13/01/C01026

More: https://github.com/European-XFEL-examples/panosc-ml-spectra-classification

SASE Pulse Delivery Analysis



An analysis workflow implemented to a Jupyter notebook was used to look at XGM (X-ray Gas Monitor) data that was recorded in the same time interval, but in different parts of European XFEL. In essence, pulse energy (intensity) values from one XGM in SASE1 were compared to another set from an XGM in SASE3. This data stems from alternating X-ray pulses sent through one or the other tunnel and recorded separately. The aim was to determine the suppression rate for intensity from unwanted residual photons in each "non-pulse" time interval.

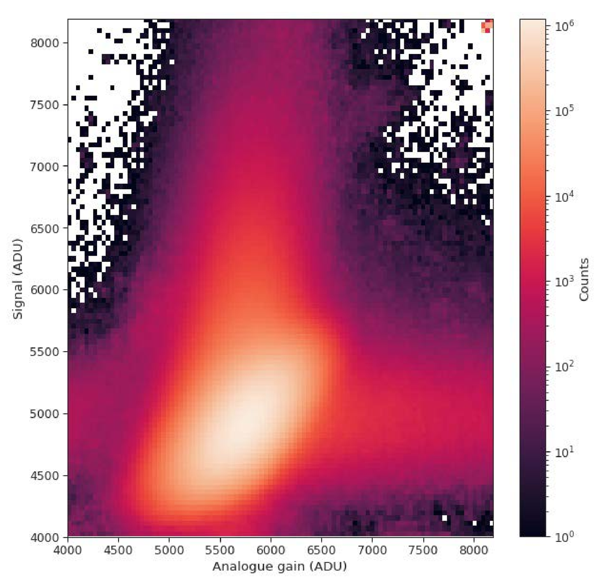
Conceptually and technically, this analysis makes use of the data-object xarray.DataArray within the EXtra-data framework and implements a simple form of error propagation. It is already public as example notebook in the EXtra-data documentation: https://extra-data.readthedocs.io/en/latest/xpd_examples2.html, and could be of value to PaNOSC due to its transferability to the general case of data comparison and/or error determination.

Developers:
Theophilos Maltezopoulos, Jan Grünert, Thomas Kluyver, Fabio Dall'Antonia

References:
[1] Tiedtke et al., Gas-detector for X-ray lasers , J. Appl. Phys. 103, 094511 (2008) - DOI 10.1063/1.2913328
[2] Sorokin et al., J. Synchrotron Rad. 26 (4), DOI 10.1107/S1600577519005174 (2019)
[3] Th. Maltezopoulos et al., J. Synchrotron Rad. 26 (4), DOI 10.1107/S1600577519003795 (2019)

More: https://github.com/European-XFEL-examples/panosc-sase-pulse-delivery-analysis

Detector Calibration



European XFEL uses a range of pixel detectors, including some which are custom built to cope with the high pulse rate. The raw data recorded from these detectors needs various corrections applied as a first step in analysing it. The workflows for applying corrections and for creating the calibration constants they use are implemented in a collection of Jupyter notebooks. Detector experts can conveniently work with a small amount of data to develop these notebooks interactively. A supporting software infrastructure runs the notebooks in parallel on the Maxwell cluster as new runs are saved, to create corrected data. The notebooks also generate plots and summary statistics to monitor the calibration quality, and the notebooks used for each run are converted into a PDF report saved alongside the data.

Developers: M. Kuster, J.-S. Dambietz, S. Hauf, T. Kluyver, R. Rosca, Y. Kirienko

References
[1] M. Kuster, D. Boukhelef, M. Donato, J.-S. Dambietz, S. Hauf, L. Maia, N. Raab, J. Szuba, M. Turcato, K. Wrona & C. Youngman (2014) Detectors and Calibration Concept for the European XFEL, Synchrotron Radiation News, 27:4, 35-38, DOI: 10.1080/08940886.2014.930809
[2] H. Fangohr, S. Brockhauser, et al. (2020) Data Exploration and Analysis with Jupyter Notebooks. Proc. ICALEPCS'19, 799--806. doi:10.18429/JACoW-ICALEPCS2019-TUCPR02

More: https://github.com/European-XFEL-examples/panosc-detector-calibration

CALL FOR USE CASES

Call for Use Cases of the data management and analysis services being developed.

Users of photon and neutron(PaN) facilities and their data, are invited to submit their use case(s)* for data treatment or data management needs.

*Submitted Use Cases must be related to one of the data services being developed by PaNOSC.

SUBMIT YOUR USE CASE

https://www.panosc.eu/submit-your-use-case/

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