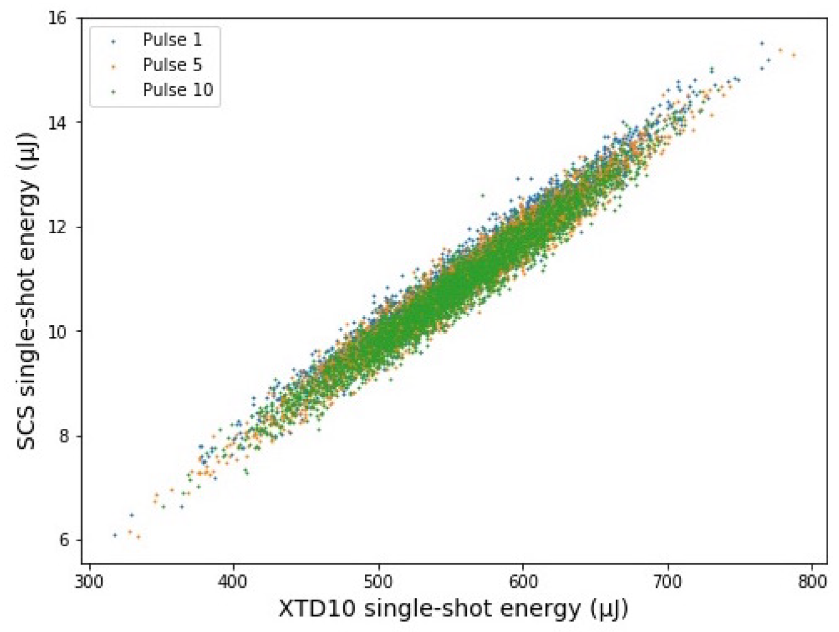
The common goal of the PaNOSC and ExPaNDS projects is to make scientific FAIR data (Findable, Accessible, Interoperable and Reproducible) a reality and support the advancement of open science through the development of high-value-added services leveraging that data that will also be available from the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

Cloud-based Data Analysis Services for Photon & Neutron Science

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

Setup

```
[2]: run = RunDirectory('../data/SCS/201831/p900048/raw/r0183/')

[3]: df = run.get_dataframe(fields=[("*_XGM/*", "*.i[xy]Pos"), ("*_XGM/*", "*.photonFlux")])

[4]: xtd10_intensity = run.get_array('SA3_XTD10_XGM/XGM/DOOCS:output', 'data.intensityTD')[:, :120]
     SCS_intensity = run.get_array('SCS_BLU_XGM/XGM/DOOCS:output', 'data.intensityTD')[:, :120]

[5]: xtd10_intensity, SCS_intensity = xr.align(xtd10_intensity, SCS_intensity, join='inner')

[6]: fig, ax = plt.subplots(figsize=(8, 6))

     for pulse in [1, 5, 10]:
         ax.scatter(xtd10_intensity[:, pulse], SCS_intensity[:, pulse], label=f"Pulse {pulse}", s=1)

     ax.set_xlabel('XTD10 single-shot energy (μJ)', size=14)
     ax.set_ylabel('SCS single-shot energy (μJ)', size=14)

     ax.legend();
```




```
[7]: xtd_mean = np.mean(xtd10_intensity.values)
     xtd_std = np.std(xtd10_intensity.values)
     xtd_percent = xtd_std/xtd_mean

     print(f"XTD mean: {xtd_mean:.3f}, std {xtd_std:.3f} ({xtd_percent:.3f}%)")

     XTD mean: 545.042, std 56.413 (0.104%)
```

Operation of X-ray gas monitors at the European XFEL

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 imager.

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

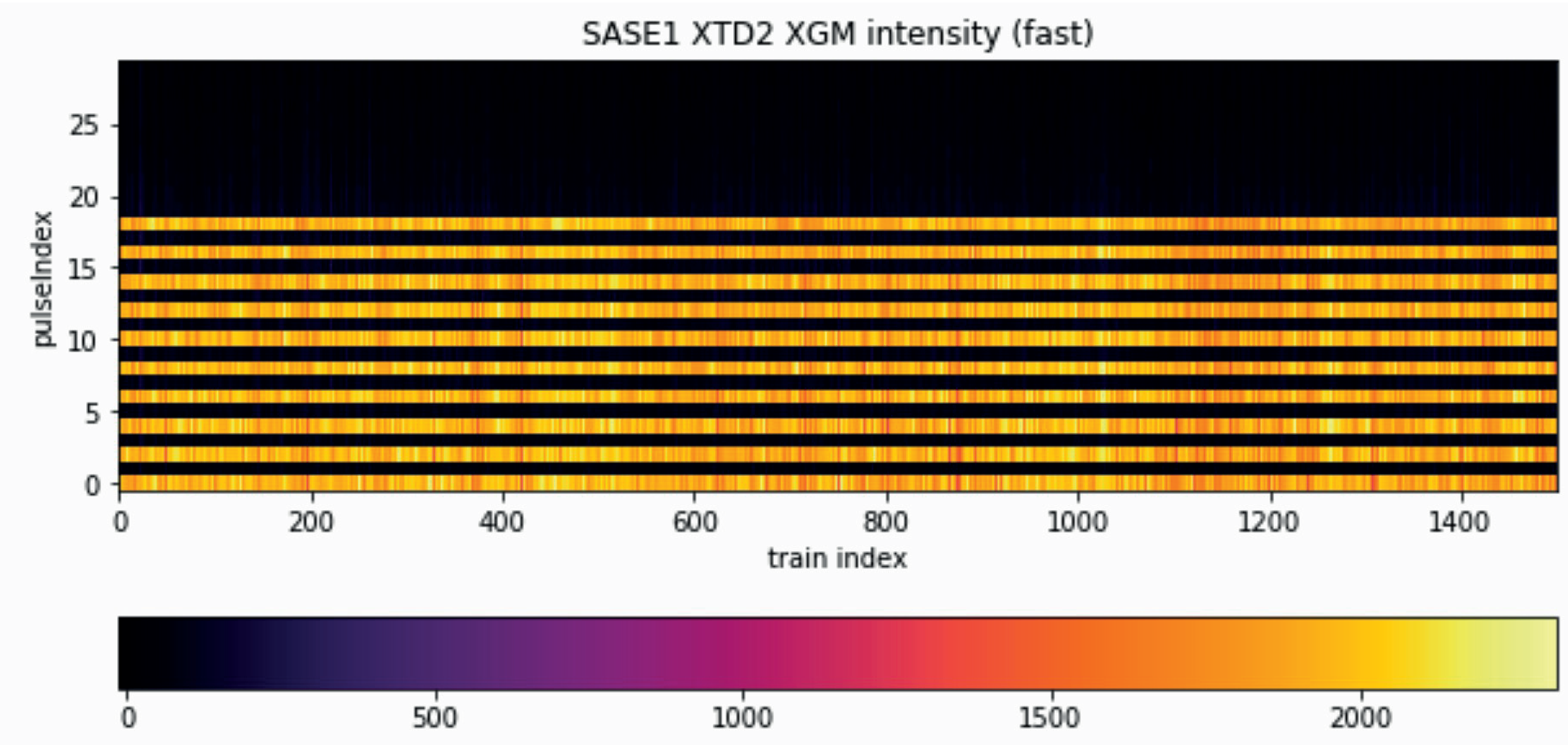
References:

[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

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.



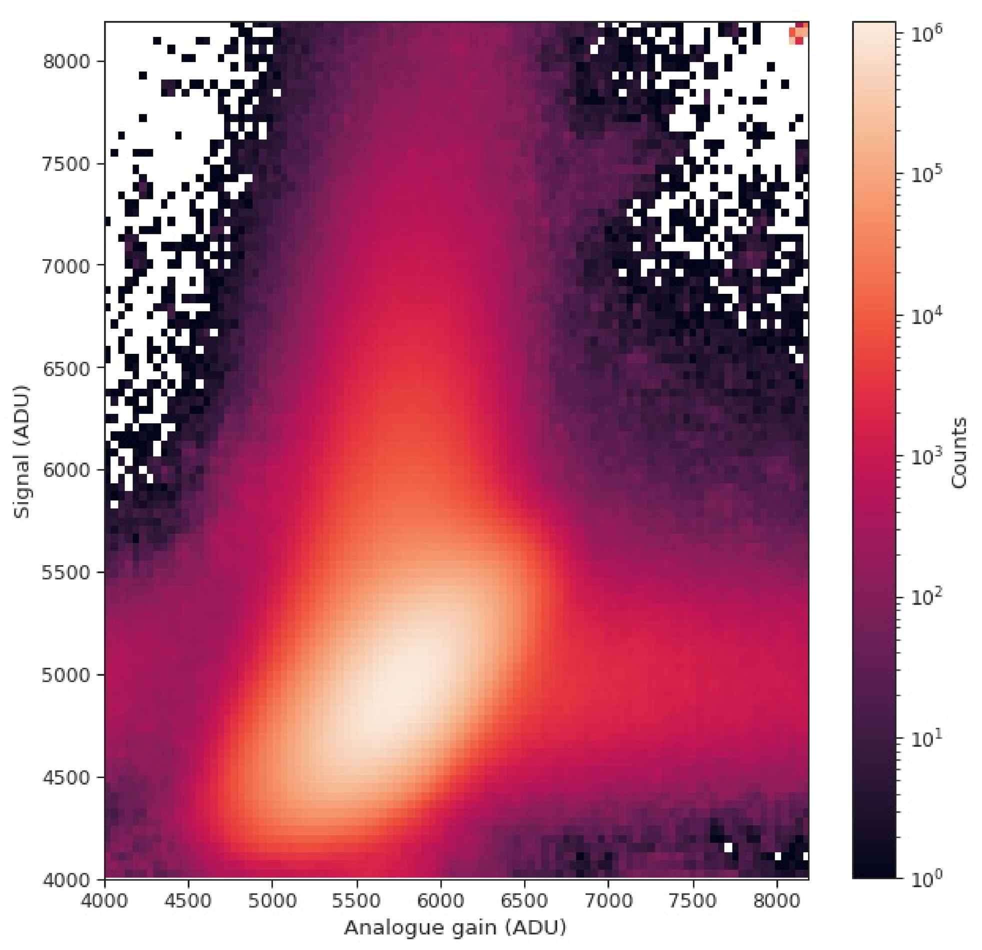
Developers:
Theophilos Maltezopoulos, Jan Grünert, Thomas Kluyver, Fabio Dall'Antonia

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

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)

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

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