European XFEL data workshop

Report of Contributions

https://indico.desy.de/e/data_2026

Contribution ID: **1** Type: **not specified**

Welcome

Friday 23 January 2026 10:00 (15 minutes)

Presenters: WRONA, Krzysztof (Eur.XFEL (European XFEL)); GELISIO, Luca (European XFEL)

Contribution ID: **2** Type: **not specified**

Data orientation

Friday 23 January 2026 10:15 (30 minutes)

This session for new & less experienced European XFEL users is a brief summary of the systems & infrastructure which you'll use to work with data produced at a beamtime. We'll talk about how to prepare for data collection, and show some of the tools you might be using to analyse data during & after your experiment.

Presenter: KLUYVER, Thomas (Eur.XFEL (European XFEL))

Contribution ID: **3** Type: **not specified**

News & highlights

Friday 23 January 2026 10:45 (45 minutes)

This talk will cover new developments from the Data department in addition to highlighting notable achievements in 2025. The past year saw many new additions to our data analysis software suite, EXtra. There is now a new GUI interface (extra.gui) which features a graphical tool to calibrate 2D spectrometers in Jupyter and a couple of widgets for ROI and peak selection. Another big addition is the extra.applications module where multi-step specialized analyses built on the EXtra library can be implemented; the calibration of the photo-electron spectrometer is such an application. The talk will also discuss many more smaller changes (some of them break backward compatibility), and new helper functions for plotting and more. Another new development is the release of the web interface of the DAMNIT, our interactive experiment overview tool. The talk will also give a quick overview of the policy along with the newly created data local contact (DLC) role. Finally, the talk will cover some highlights from experiments as well as from data science and machine learning activities in the department.

Presenter: BISHARA, Fady Adibsamy (Eur.XFEL (European XFEL))

Contribution ID: **5** Type: **not specified**

Data management plans & data reduction: a practical demonstration

Friday 23 January 2026 11:45 (45 minutes)

The new Scientific Data Policy takes effect for all user proposals starting in 2026, which includes the introduction of data management plans and data reduction as an integral part of the proposal lifecycle. Over the past two years, the necessary workflows have been developed as part of pilot programs in conjunction with users of select experiments.
Here we present a practical end-to-end demonstration of how this process looked like for a typical experiment, as well as some examples of how it can benefit in the case of more special requirements.

Presenters: SOBOLEV, Egor (Eur.XFEL (European XFEL)); SCHMIDT, Philipp (Eur.XFEL (European XFEL))

Contribution ID: **9** Type: **not specified**

First insights to refined results: mapping charge transfer in dissociating molecules

Friday 23 January 2026 13:30 (30 minutes)

Charge transfer is essential to many complex chemical processes and thus a thorough understanding at the molecular level is desired. One particular aspect concerns the interplay between the positions of nuclei and the probability of charge transfer. During a beamtime at EuXFEL's SQS instrument, we studied how the ability to transfer electrons in dissociating molecules with a rotating fragment changes throughout the dissociation process.
Beyond the fundamental physics, this talk highlights the data analysis journey. We demonstrate how preliminary online and first offline feedback enabled us to steer the experiment, yet how it differs from the post-beamtime refined results. We discuss the role of the EuXFEL data analysis ecosystem using tools such as EXtra-metro, DAMNIT and EXtra in different stages of that journey.

Presenter: SENFFTLEBEN, Bjoern (ETH Zurich)

Contribution ID: **10** Type: **not specified**

Reduction and analysis of time resolved solution scattering data measured with non-standard excitation patterns

Friday 23 January 2026 14:00 (30 minutes)

I will introduce Time resolved X-ray solutions scattering as a technique and outline some of the challenges associated with measuring at ~100 kHz X-ray repetition rate.
I will discuss the data pipeline that we have developed in conjunction with the data analysis group and outline how that helped solve these challenges.

Presenter: HAUBRO, Morten (Technical University of Denmark)

Contribution ID: **11** Type: **not specified**

Automating Talbot phase imaging at HED

Friday 23 January 2026 14:30 (30 minutes)

High rep-rate data requires high rep-rate solutions, where human-in-the-loop decision making no longer sufficient to manage many experiments efficiently. Simultaneously, the requirement for high-level, (near-) online analysis to manage experiments is often explicitly at odds with their goal: to do something new where you don't know exactly what you'll see. I'll walk through how HED have built from early, often user-provided notebooks/codebases, toward (more) robust, adaptable analysis deployed across many experiments - making use of DAMNIT and extra-metro frameworks at European XFEL - focusing on the example of Talbot phase imaging.

Presenter: HUMPHRIES, Oliver (Eur.XFEL (European XFEL))

Contribution ID: **12** Type: **not specified**

Data quality enhancement

Friday 23 January 2026 15:00 (30 minutes)

Research done at European XFEL takes advantage of both high-throughput data, as well as the enhanced data quality. Different research topics are being explored to ensure that we continue to deliver increasingly high-quality data. The presentation expands on selected projects and research topics within three main areas. One topic includes beam automation and instrument alignment automation, which reduce the time spent in this task during the beam time, leading to a larger time budget spent on the data collection. Another avenue being explored consists of improving the quality of the diagnostics provided, combining information from multiple sources. A final research topic includes the provision of quality labels to the acquired data, and its correction, when needed.

Presenter: FERREIRA DE LIMA, Danilo Enoque (Eur.XFEL (European XFEL))

Contribution ID: **13** Type: **not specified**

Wrap-up

Friday 23 January 2026 15:30 (15 minutes)

Presenters: WRONA, Krzysztof (Eur.XFEL (European XFEL)); GELISIO, Luca (European XFEL)

Contribution ID: **14** Type: **not specified**

Breakout room 1. Feedback & discussion: Data management plans & data reduction

Friday 23 January 2026 16:00 (1 hour)

Join this breakout room to discuss the data reduction topic, as well as data management plans.

Contribution ID: **15** Type: **not specified**

Breakout room 2. Feedback & discussion: Data access & data analysis

Friday 23 January 2026 16:00 (1 hour)

Join this breakout room to discuss tools and methods to access and analyze data at European XFEL.