

Advancing FAIR principles for MHz-XPCS data from XFEL experiments within the DAPHNE4NFDI project

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Introduction

X-ray Photon Correlation Spectroscopy (XPCS) is an experimental technique used to study protein and molecular dynamics on length scales ranging from angstroms to micrometers [1]. The unique properties of the pulses from the European X-ray Free Electron Laser (EuXFEL), such as exceptional transverse coherence and megahertz (MHz) repetition rate, have made it possible to investigate the collective diffusive dynamics of such systems with (sub-) microsecond temporal resolution. Although XPCS has become a routine technique at storage-ring sources, its implementation at EuXFEL is still in progress.

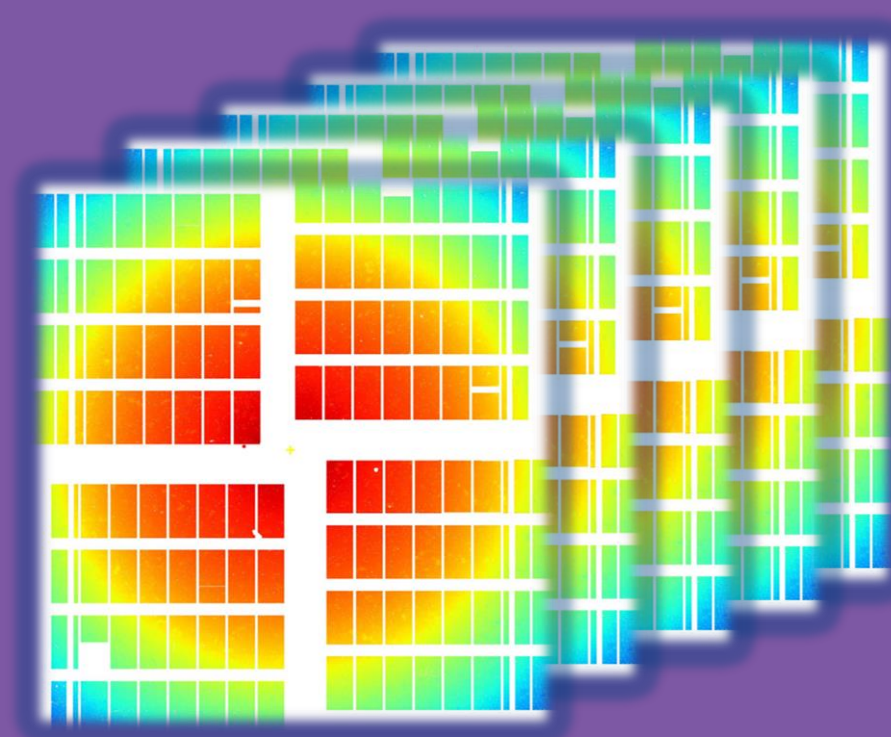
We aim at developing the MHz-XPCS at EuXFEL as a routine technique guided by the FAIR principles [2], the implementation of which is actively progressing within the DAPHNE4NFDI project [3]. In our poster, we discuss possible strategies to achieve this goal, covering stages from initial near-online data processing to the uploading of the refined "Top Level" data on the dedicated DAPHNE web platform.

Making MHz-XPCS Data/Metadata FAIR

EuXFEL

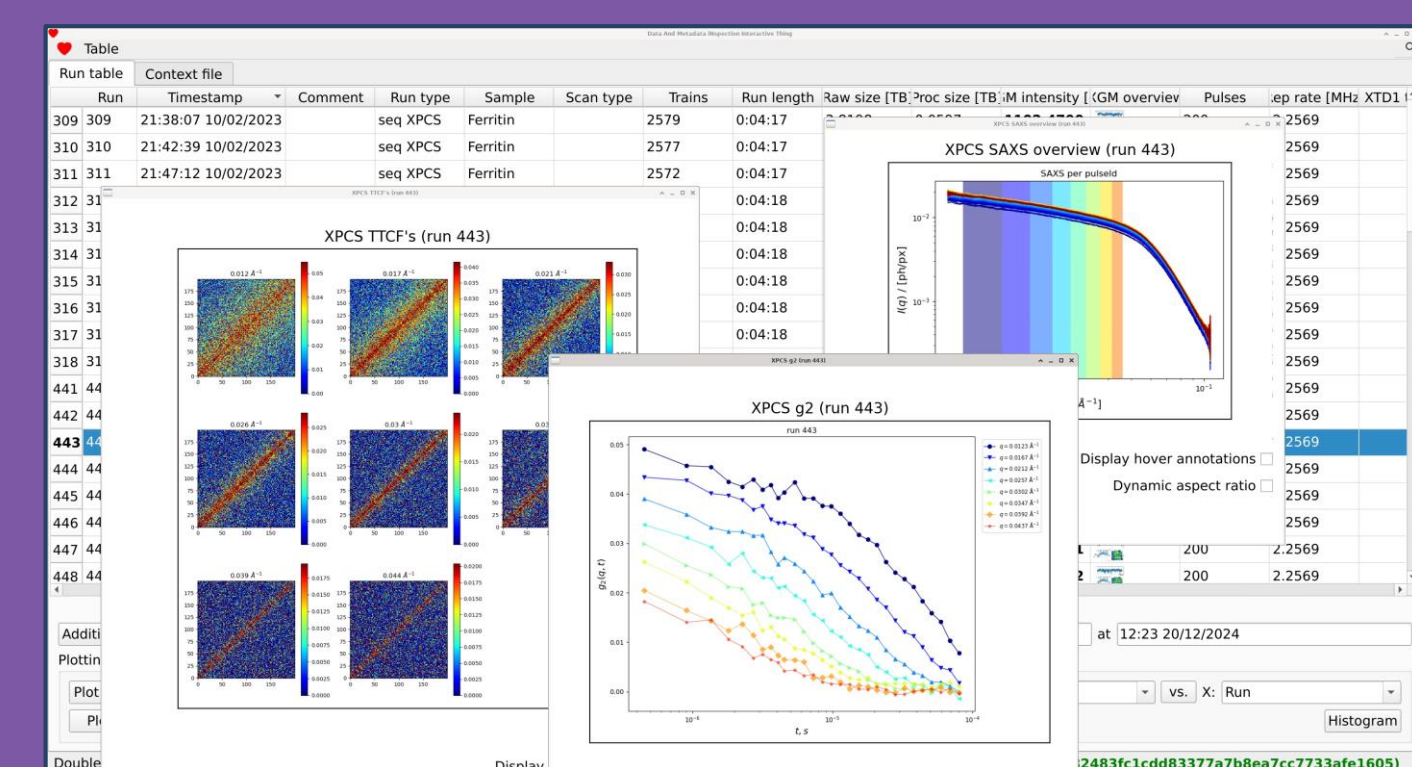
MHz-XPCS Experiment / MID instrument

- Data acquisition / correction



DAMNIT Tool

- Robust near-online / offline analysis
- Collecting necessary "Variables"
- "Short" SQLite + "Full" HDF5 output



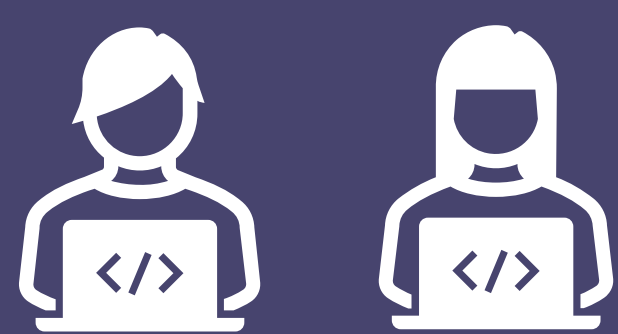
EXtra-speckle (pipeline)

- statistics / filtering
- TTCF / off-correlation
- g2 / fitting, SAXS

EuXFEL myMdc portal

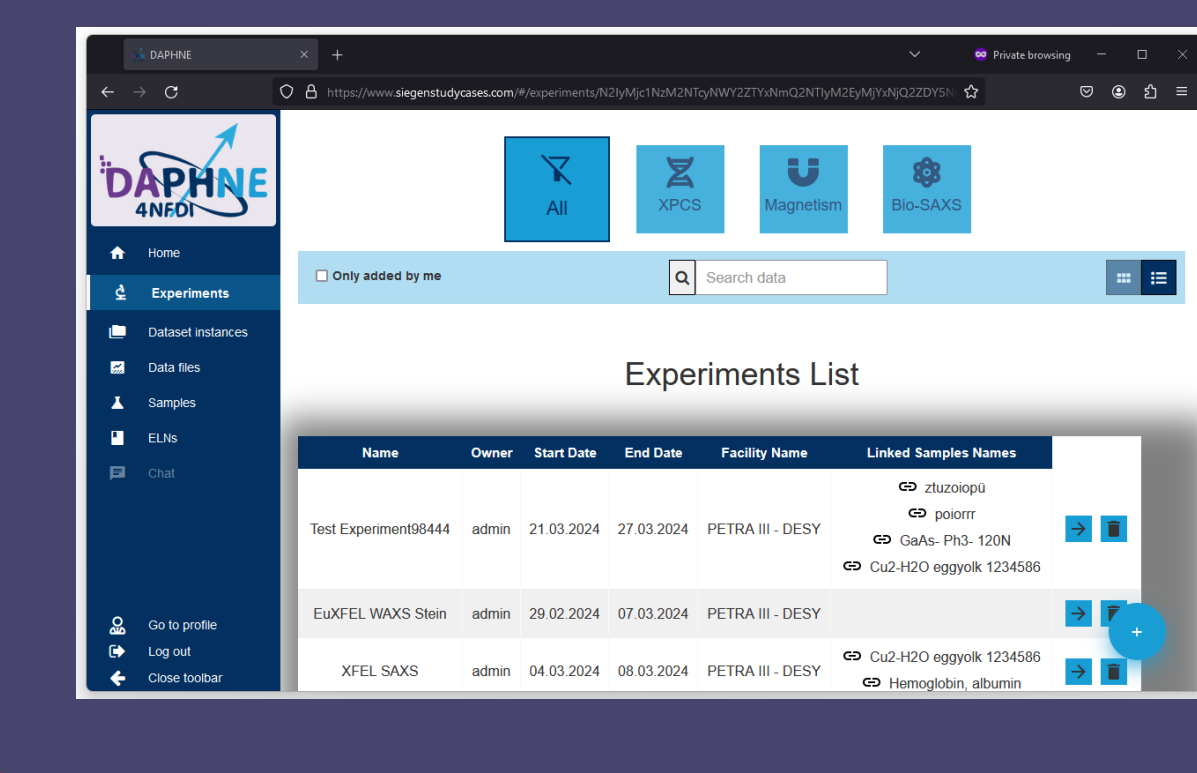
- Proposal Data / Metadata
- Electronic logbook

FAIR Data Users



Export to DAPHNE Platform

- "Top Level" Data / Metadata
- Attachments (images, codes)



Additional Metadata

- Manual input by the user at the DAPHNE platform

Open questions



Defining
"Top Level"
Data



Bridging
DAMNIT and XPCS
platform



Secure
User
authentication



FAIR XPCS
Data
Policy

Images created by AI

References

- [1] F. Perakis, C. Gutt, *Towards molecular movies with X-ray photon correlation spectroscopy*, PCCP **22**, 19443-19453 (2020)
- [2] B.M. Murphy, et al., *FAIR data – the photon and neutron communities move together towards Open Science*, IUCrJ **12**, 8-15 (2025)
- [3] A. Barty, et al., DAPHNE4NFDI – Consortium Proposal, DOI: 10.5281/zenodo.8040605
- [4] EXtra-speckle, <https://git.xfel.eu/dataAnalysis/extra-speckle>
- [5] DAMNIT, <https://damnit.readthedocs.io/en/latest/>

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