DAMNIT **A Tool for Automated Experiment Overviews**

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Introduction

The Data And Metadata iNspection Interactive Thing (DAMNIT^[1]) is a software developed by the Data Analysis group at European XFEL (EuXFEL) that automates the creation of experimental overviews for beamline scientists and users.

At EuXFEL, experimental tracking has traditionally relied on manually filled spreadsheets and electronic logbooks to record experimental settings, metadata, and analysis results. This approach is time-consuming, error-prone, and challenges reproducibility. DAMNIT replaces these manual processes with an automated solution.

Toward standardized analysis

Fully integrated with the EuXFEL data system, DAMNIT automatically collects metadata and manages data analysis workflows during experiments, providing users with real-time progress monitoring. Users can configure complex data analysis workflows running on the Maxwell^[2] computing cluster through the Slurm scheduling system, with results automatically saved and displayed in the overview table.



Runs while data is collected

- Automatically creates run table
- Automated processing
- Distributed

- Table overview
- Explore analysis results Edit analysis code
- Integrated with facility services
- Electronic logbook

Interested in learning more? Want to test and use it on your experiments? Get in touch at da@xfel.eu and check the documentation at damnit.rtfd.io

Tailored to your experiment

DAMNIT enables a wide range of application, spanning from basic metadata collection to advanced data analysis processing and final result generation. Users can incorporate custom code by defining Python functions, simplifying the integration of external tools.

A Variable generates a column in the table Integration Run Detector preview @Variable(title="Detector preview") def detector(run): 0.2655 agipd = AGIPD1M(run) accessible [3] image = _some_processing(agipd) through return image Defined summary data to be displayed @Variable(title="Integration", summary="max") def integration(run, image: "var#detector"): I, q = integrate1D(image) return xr.DataArray(I, dims=["q"], coords=[q]) and explore Data analysis results

Functions are interconnected as a Directed Acyclic Graph (DAG) that automatically manages the execution order.





)	•	Metadata catalog
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Results are systematically saved in structured formats: SQLite^[4] for summaries, HDF5^[5]/NetCDF^[6] for data. A Python API enables result retrieval, allowing users to read the generated data for validation, visualization or further analysis through any tool.

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The tool includes a user-friendly **frontend** built with Qt^[7] featuring a **tabular interface** that displays tracked quantities for each measurement, allowing users to explore interactively data and helps them steer the experiment as data is being collected.

It also includes a code editor allowing to quickly modify the analysis software, (re)process data and explore logs from the code execution.



HERFD-XAS and WAXS at FXE (p004507 / Christopher Milne)

Coming soon

• Web-based interface for access from any location



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- Enhance reproducibility by
- Versioning the analysis code
- Keeping result history
- Grouping: aggregation of statistics, plots, and other data from various measurements



Sample database: integrate and interact with sample information

References

[1] github.com/European-XFEL/DAMNIT	
[2] docs.desy.de/maxwell	

- [5] hdfgroup.org/solutions/hdf5/ [6] https://www.unidata.ucar.edu/software/netcdf
- [7] riverbankcomputing.com/software/pyqt [3] github.com/European-XFEL/EXtra-data

[4] <u>sqlite.org</u>

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