Automatic data processing and results overview during SFX experiments

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Serial Femtosecond Crystallography (SFX)

Crystallography at European X-ray free electron laser (XFEL):

- Photon pulses are bright enough to observe diffraction from extremely small crystals;
- Femtosecond duration of individual pulses;
- Sample gets destroyed shortly after diffraction;
- Experiments are performed serially with a continuously resupplied sample;
- Still images from the randomly oriented crystals;
- Goal reconstruct the electron density distribution corresponding to the atomic structure.

EXtra-Xwiz

EXtra-Xwiz^[1] is a pipeline tool for streamlining SFX analysis:

- Abstracts the complexity of data at EuXFEL;
- Utilizes programs from the the *CrystFEL*^[2] framework;
- Has been integrated into *DAMNIT*.



Structure factor intensities

Real space electron density map

DAMNIT

The Data And Metadata iNspection Interactive Thing (DAMNIT^[3]):

- Executes code in a *context file* as soon as new data arrives;
- Displays the results in a GUI as shown below;
- A web interface will soon be released.

					Data And Metadata iNspect	tion Interactive Thing	(on max-exfl461.desy.de	2)					~
Table													
un table	Context file												
Run 🔺	Run length	Run type	Sample Name	Requested geometry	Input geometry	Requested xwiz_config	Input xwiz_config	Hit rate, %	Indexing rate, %	N crystals	Cell parameters	Peakogram	Peak count
4 104	0:00:54	LPD dark	No Sample										
3 103	0:11:10	SFX	Cl-rsEGFP2		sam_geom_21_11.geom		xwiz_RSEGFP2_v0.toml						
2 102	0:06:15	SFX	Cl-rsEGFP2		sam_geom_21_11.geom		xwiz_RSEGFP2_v0.toml	3.1590	3.4003	2170	ETH	A. A.	44))
1 101	0:08:44	SFX	Cl-rsEGFP2		sam_geom_21_11.geom		xwiz_RSEGFP2_v0.toml	5.8868	6.5170	5812	111 111	۵. 🗮	프네크)
0 100	0.00.12 Export table t	SEX o the Logbook	Cl-rsEGFP2		sam_geom_21_11.geom		xwiz_RSEGFP2_v0.toml			0			
99	View processi	ng logs	I-rsEGFP2		sam_geom_21_11.geom	xwiz_RSEGFP2_v1.toml	xwiz_RSEGFP2_v1.toml						
98	0:01:19	SFX	Cl-rsEGFP2		sam_geom_21_11.geom		xwiz_RSEGFP2_v0.toml	3.6488	3.7299	506	111	1 <u>4.</u> (81	
97	0:03:38	SFX	Cl-rsEGFP2	sam_geom_21_11.geom	sam_geom_21_11.geom	xwiz_RSEGFP2_v0.toml	xwiz_RSEGFP2_v0.toml	9.2487	10.0506	3735	222	۵. 🛋	
96	0:01:27	LPD Darks Parallel gain mode	Lysozyme										
95	0:12:12	SFX	Lysozyme		sam geom with masks 19 11.geom		xwiz lyso 01.toml	36.1195	0.0844	99	EXE:	t sul	

A glimpse into the run's data quality

Results of processing SFX data by *EXtra-Xwiz* are displayed in the *DAMNIT* table to provide an overview of the run's data quality. They include an overall hit rate, indexing rate, number of indexed crystals, as well as several new features:

Cell parameters

Peakogram

Peak count

DAMNIT plotting indexing rate

... and many more

The DAMNIT context file allows to extend the table with many more values or figures suitable for each individual experiment.

Would you like to learn more about DAMNIT?

Visit a poster "DAMNIT: A Tool for Automated Experiment Overview" by Thomas Michelat

References

1. "EXtra-Xwiz: A Tool to Streamline Serial Femtosecond Crystallography Workflows at European XFEL", Crystals 2023, 13, 1533 (2023): https://www.mdpi.com/2073-4352/13/11/1533

- 2. "CrystFEL: a software suite for snapshot serial crystallography",
- J. Appl. Cryst. 45(2), 335–341 (2012): https://journals.iucr.org/paper?S0021889812002312
- 3. "Data And Metadata iNspection Interactive Thing user documentation": https://damnit.readthedocs.io/en/latest/

