SPB/SFX Update

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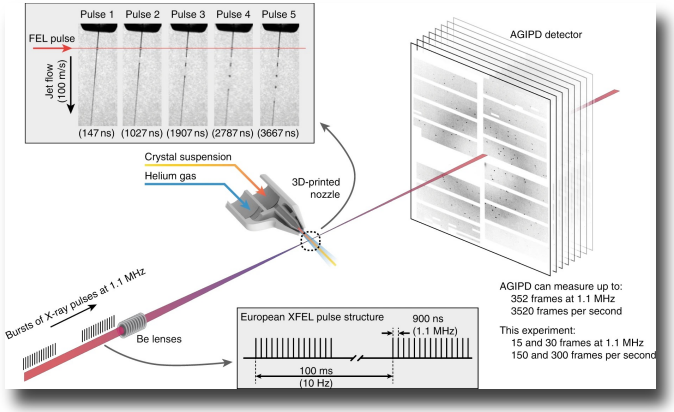
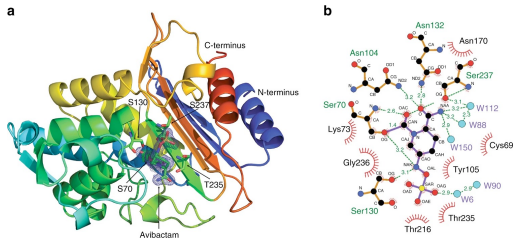
Leading Scientist

Schenefeld, 3 November 2021

Reminder: Science cases at SPB/SFX



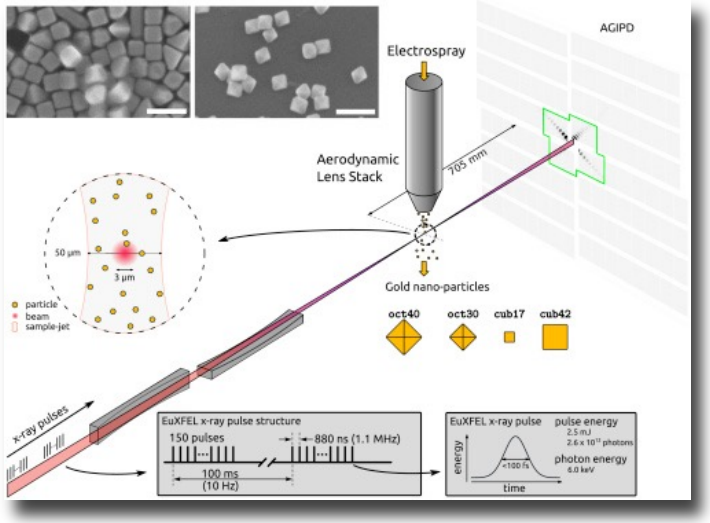


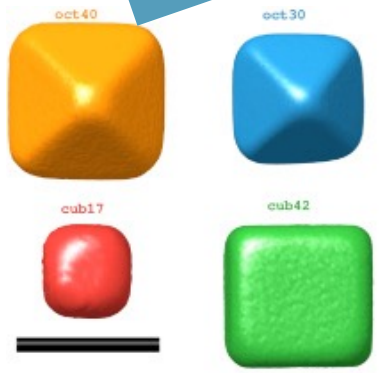
Serial Crystallography

IN PROGRESS

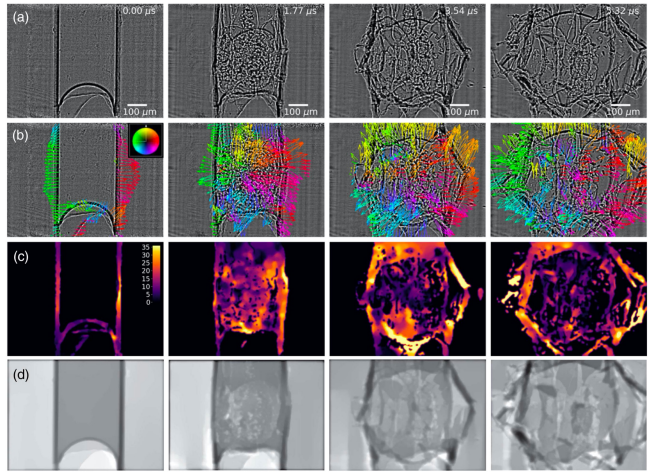
Includes time-resolved studies

Small Angle Scattering



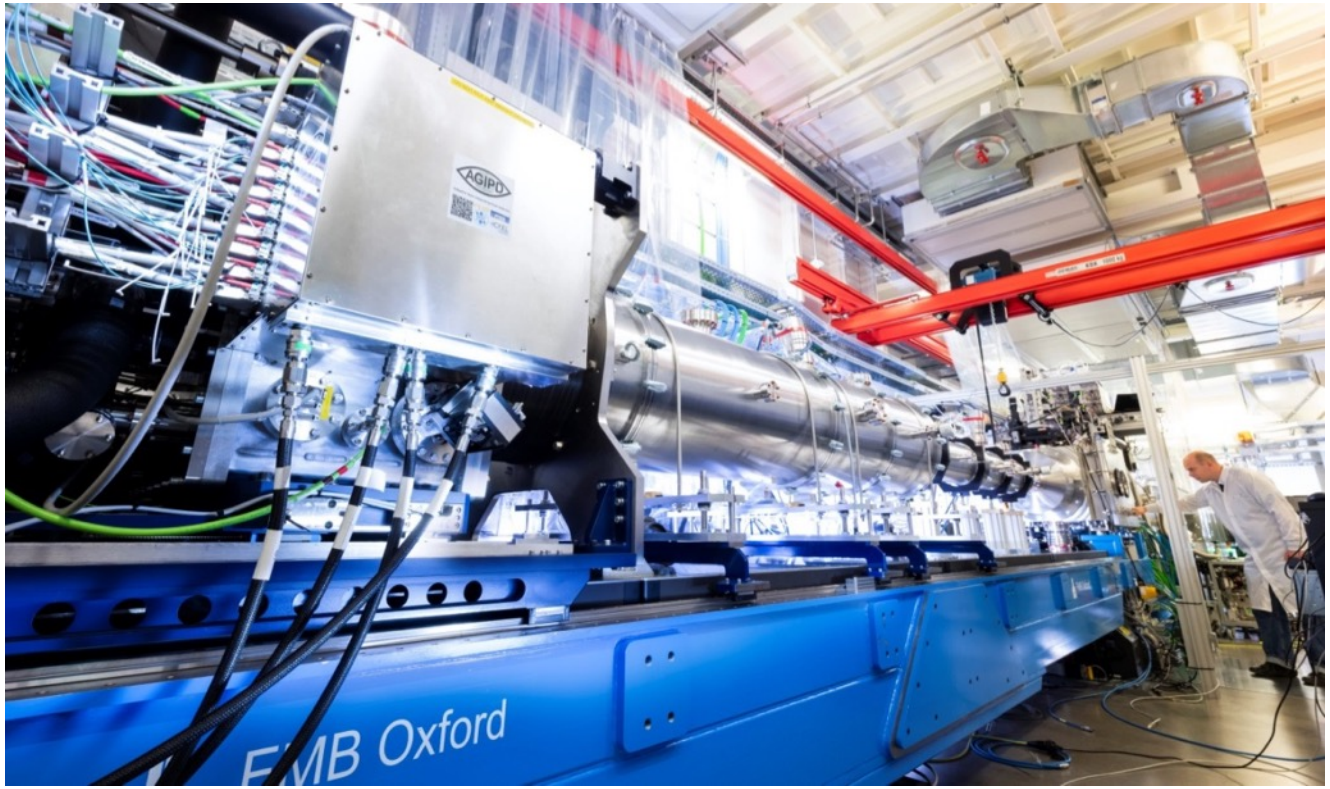


Single Particle Imaging

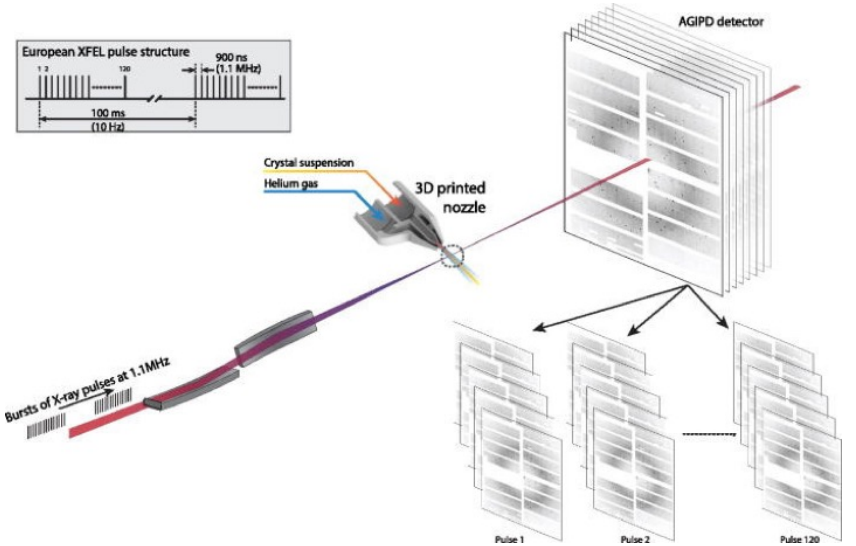


Megahertz microcopy (up to 24 keV)

Reminder: SPB/SFX Instrument layout



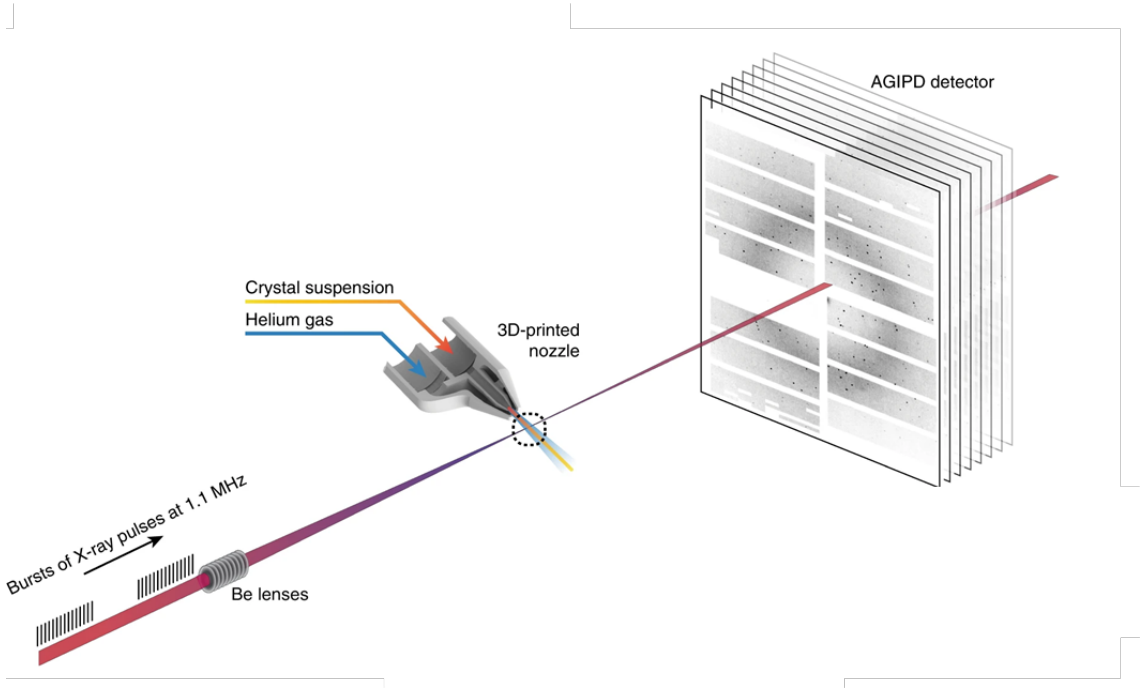
- < 6 keV to ~15 keV
- ~3 µm and 300 nm spot sizes
- 1 Mpx AGIPD
- MHz rep rate capable
- Optical pump laser
- Timing tool & more…



- Mancuso et al., The [SPB/SFX] instrument at the European XFEL: initial installation, Journal of Synchrotron Radiation, 26, pp. 660-676 (2019)

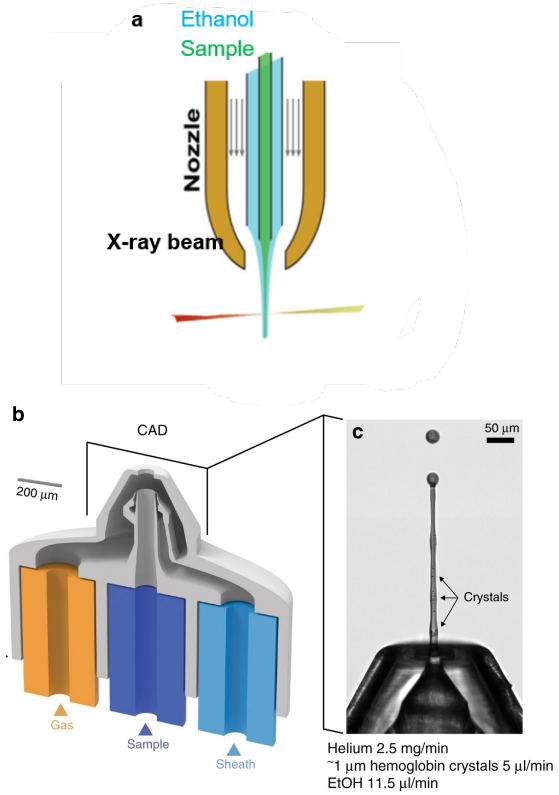
Sample delivery for SFX – 3D-printed Gas Dynamic Virtual Nozzles (GDVNs)

- Standard GDVN
  - Sample (crystal suspension) is focused by Helium gas



Modified from Wiedorn *et al* (2018). Nat. Commun. 9, 4025.

- Double-flow focusing nozzles (DFFN)
  - Outer jet (Ethanol) focused by Helium stabilizes inner jet (Sample)



Oberthuer *et al* (2017) Scientific Reports 7:44628
Knoska *et al* (2020). Nat. Commun. 11, 657.

New: Protein crystal screening (PCS) beamtimes at SPB/SFX

- Two step procedure with users on-site
  - 1. part: Injection tests in the user labs
  - 2. part: Beamtime at the SPB/SFX instrument (3 - 6 hours)
- In case sample is not jettable, sample will be considered for PCS beamtime in the next run
- Injection performed and nozzles (GDVN and DFFN) provided by SEC Group
- Data collection performed by SPB/SFX group
- Simplified proposal form
- For further information, please contact Katerina Dörner (SEC) prior to proposal submission: katerina.doerner@xfel.eu

Optical laser parameters

Optical laser system 1 properties		
Wavelength	800 nm	From 740 to 840 nm (pulse duration is longer than 15 fs)
Pulse duration	15–300 fs	
Repetition rate	4.5 MHz	Down to 100 kHz
Pulse energy	50 µJ	
Wavelength conversion	SHG, THG (no OPA)	SHG (370–420 nm), THG (246–280 nm)
Spot size	30–50 µm	Diameter (estimated, typical)

Optical laser system 2 properties	
Wavelength	1030 nm
Pulse duration	1–400 ps
Repetition rate	4.5 MHz
Pulse energy	1 mJ
Wavelength conversion	SHG, THG, FHG
Spot size	30–50 µm

Please contact us for further details:
spb.sfx@xfel.eu

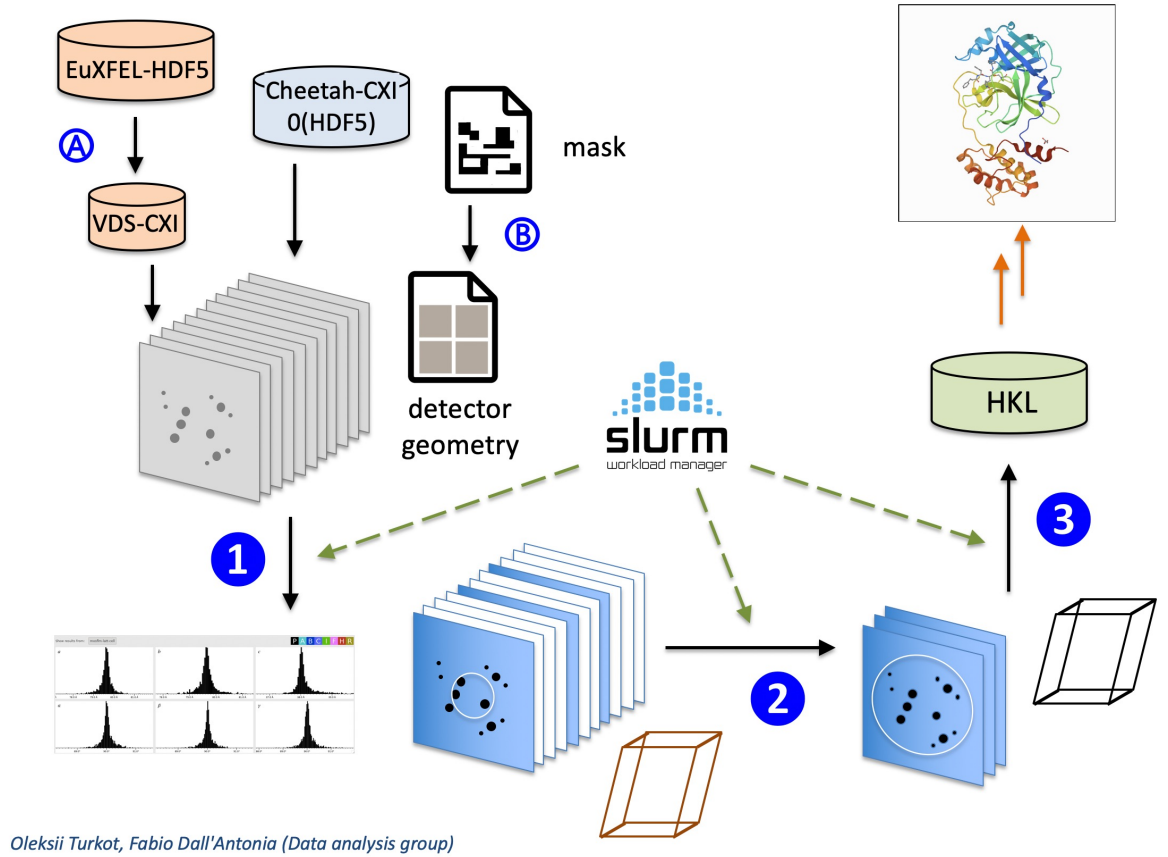
Optical laser system 3 properties (Opolette 355 HE)		
Wavelength	210 – 2400 nm	OPO output
Pulse duration	3 – 7 ns	
Repetition rate	Single shot – 20Hz	Down to 100 kHz
Pulse energy	0.5 – 9 mJ	Dependent on wavelength
Spot size	4 mm	Near field
	Three of these systems can be operated simultaneously	

Photon Arrival Monitor (PAM) timing tool available for micron beam experiments, depending on experimental configuration. TOPAS in commissioning and potentially available for experiments for run 2022-02. In Helium serial crystallography with Jungfrau 4M detector also available.

In these cases, discussion with instrument scientists before proposal submission is essential

Semi automatic SFX pipeline

- Starting from HDF5 data sets in EuXFEL or Cheetah/CXI format, diffraction images are processed in 3 steps using CrystFEL tools, embedded to a workflow with SLURM interface for distributed computing.
- (1) Initial crystallographic peak-finding and indexing of all detector images, followed by graphical determination of a crystal unit cell.
- (2) Peak-finding and indexing in a low-scattering-angle detector area using the preliminary unit cell, followed by selection of the indexable image subset ("crystal hit frames") and unit cell refinement.
- (3) Peak-finding, indexing and pixel intensity integration at predicted positions on a high-scattering-angle area using only the diffraction image subset, plus the refined unit cell. Crystallographic scaling and intensity averaging yields a unique reflection data set, suited to reconstruct the macromolecular structure (not yet part of the pipeline).
- Preparative steps like (A) automatic conversion of EuXFEL data to the required CXI format in a "virtual" data set or (B) optional import of pixel masks into the detector geometry description file are also supported.



Oleksii Turkot, Fabio Dall'Antonia (Data analysis group)

- In short, we can help go from measured data to crystallographer friendly files

Contact details

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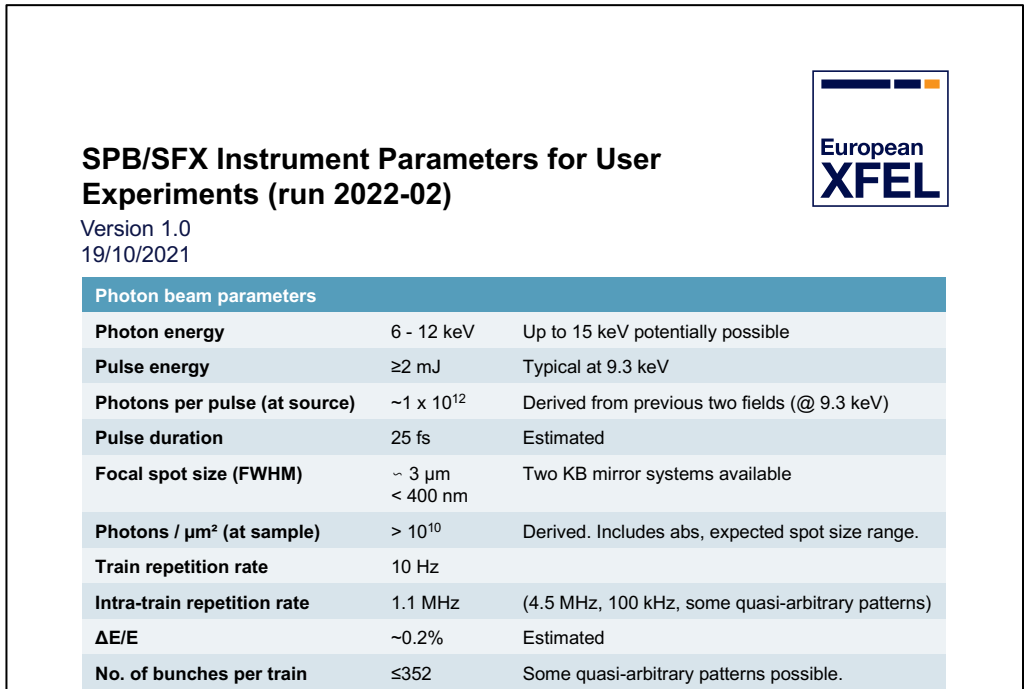
- https://www.xfel.eu/facility/instruments/spb_sfx/index_eng.html



SPB/SFX Instrument Parameters for User Experiments (run 2022-02)

Version 1.0
19/10/2021

Photon beam parameters		
Photon energy	6 - 12 keV	Up to 15 keV potentially possible
Pulse energy	≥2 mJ	Typical at 9.3 keV
Photons per pulse (at source)	~1 x 10^{12}	Derived from previous two fields (@ 9.3 keV)
Pulse duration	25 fs	Estimated
Focal spot size (FWHM)	⌣ 3 µm < 400 nm	Two KB mirror systems available
Photons / µm² (at sample)	> 10^{10}	Derived. Includes abs, expected spot size range.
Train repetition rate	10 Hz	
Intra-train repetition rate	1.1 MHz	(4.5 MHz, 100 kHz, some quasi-arbitrary patterns)
ΔE/E	~0.2%	Estimated
No. of bunches per train	≤352	Some quasi-arbitrary patterns possible.

References…

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