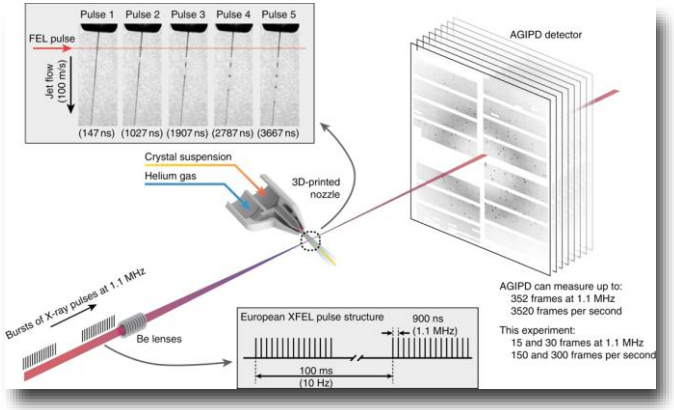
SPB/SFX Instrument Update
EuXFEL Proposal Call 10

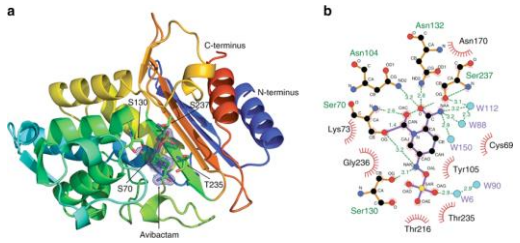
Richard Bean
SPB/SFX Interim Group Leader

10.11.2022

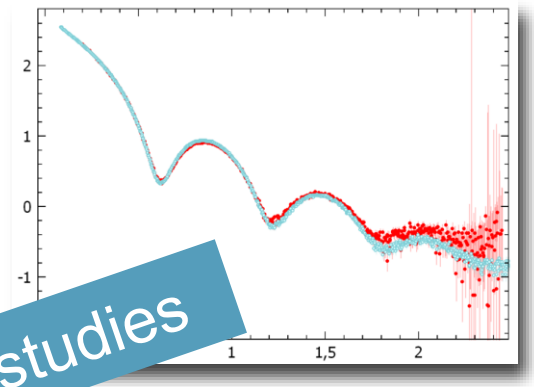
SPB / SFX

Reminder: Science cases at SPB/SFX



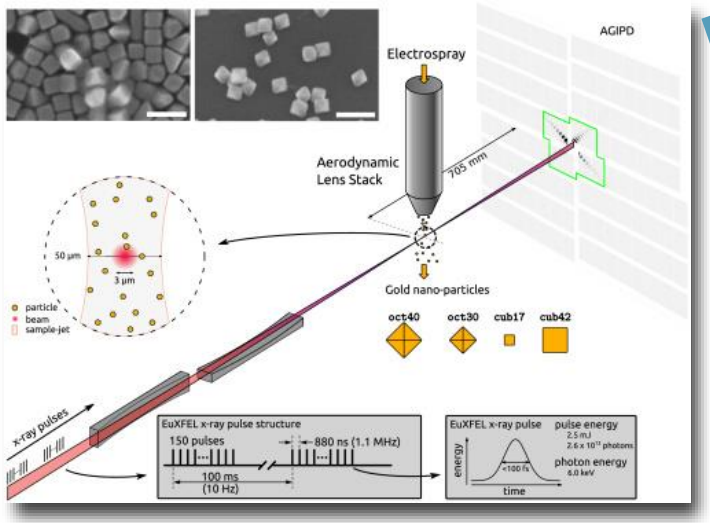


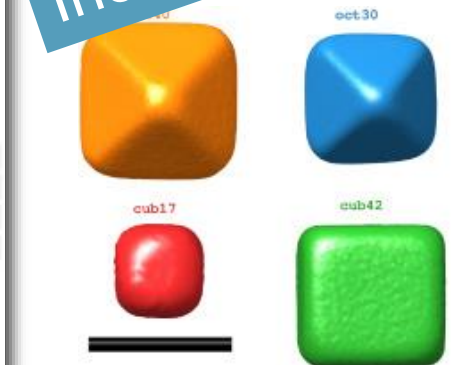
Serial Crystallogra



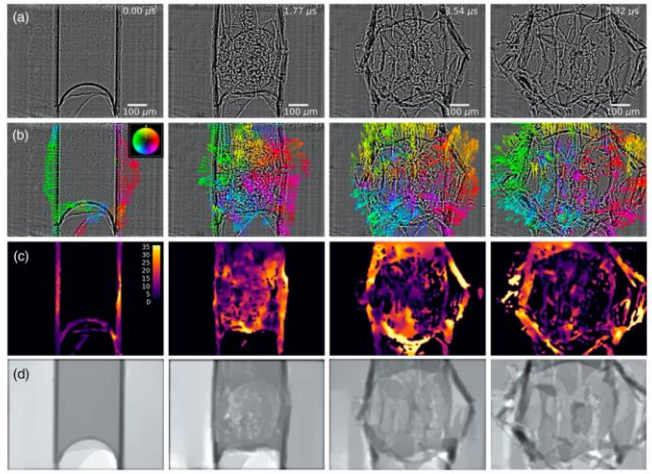
Small Angle Scattering

Includes time-resolved studies



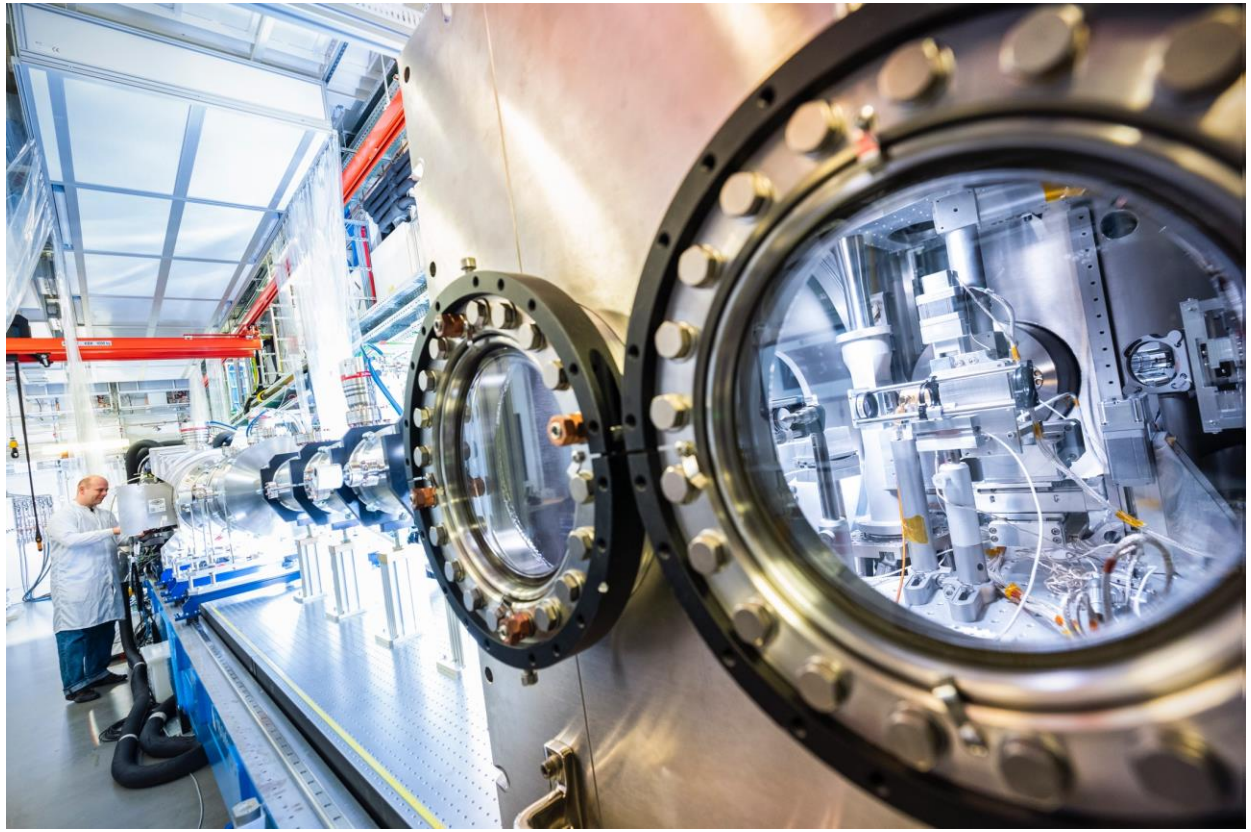


Single Particle Imaging

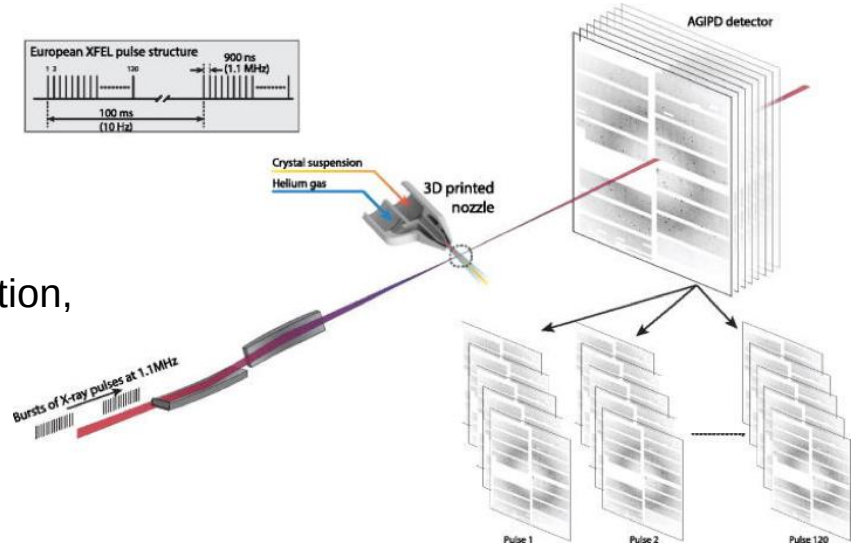


Megahertz microscopy (up to 24 keV)

Reminder: SPB/SFX Instrument layout (SFX, SPI, Small angle)



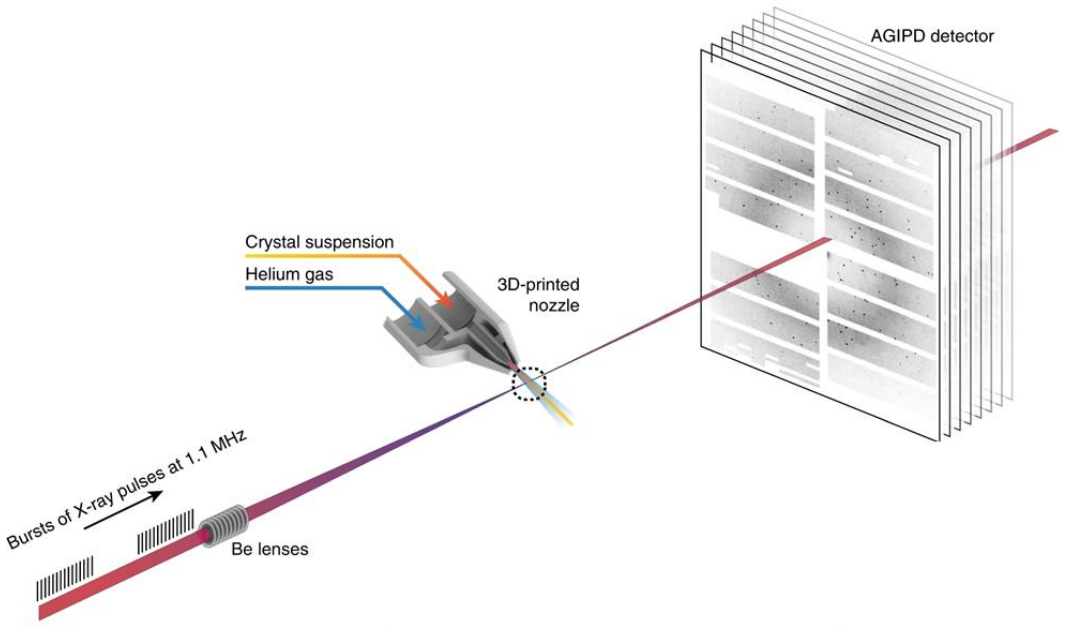
- ~ 6 keV to ~15 keV
- ~3 µm and 300 nm spot sizes
- 1 Mpx AGIPD
- MHz rep rate capable
- Optical pump laser
- Timing tool & more…



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

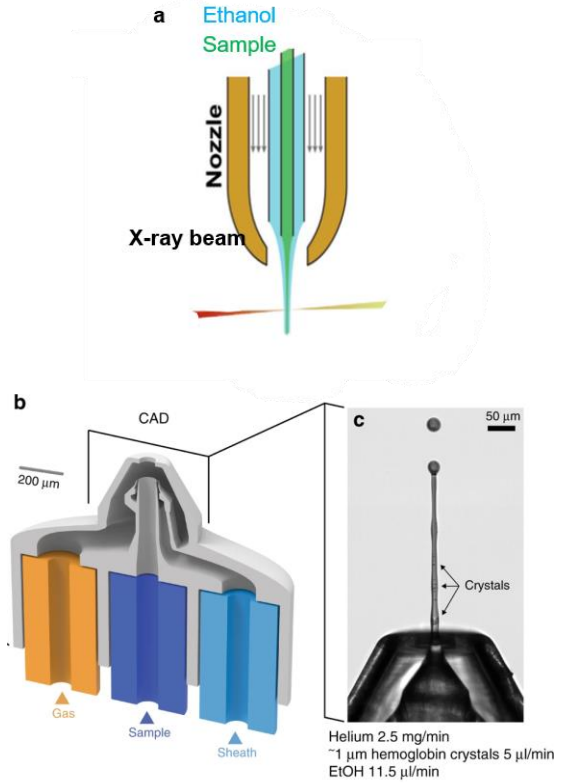
Sample delivery for SFX – 3D-printed Gas Dynamic Virtual Nozzles (GDVNs)

- 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)



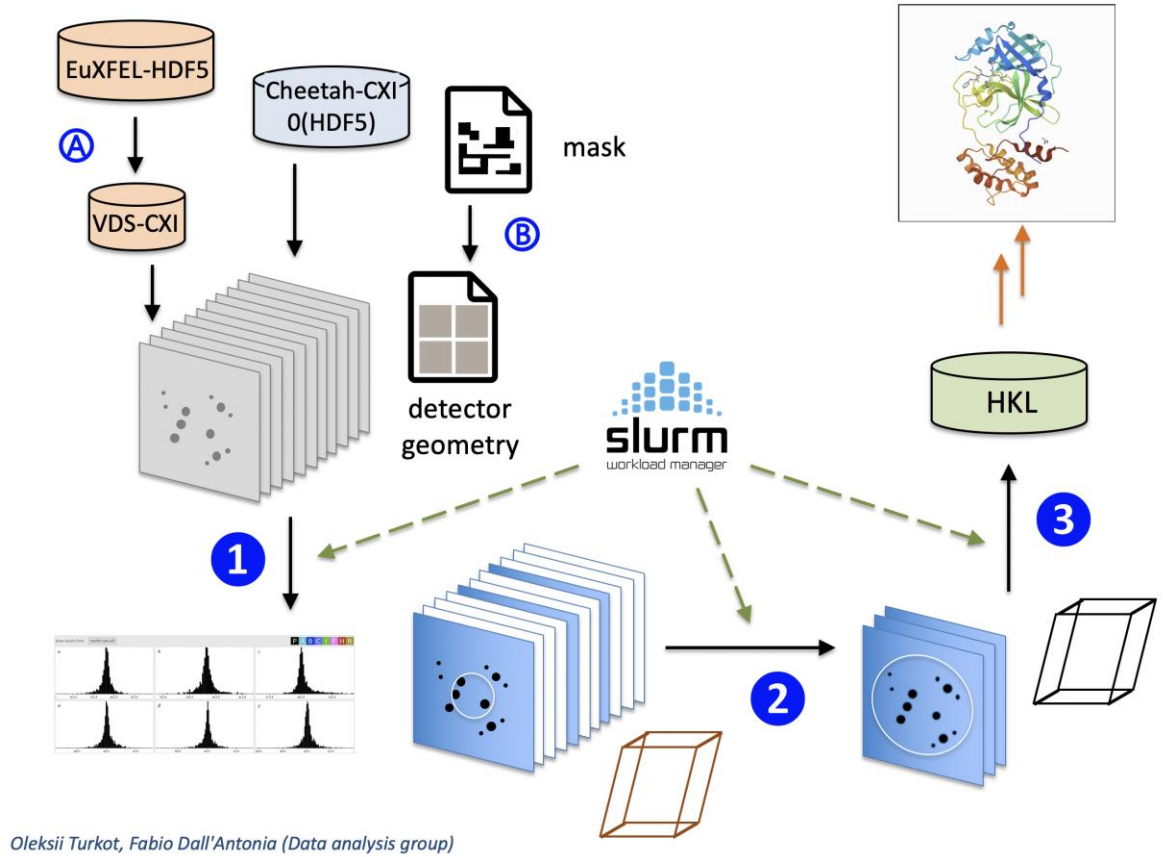
Oberthuer *et al* (2017) Scientific Reports 7:44628
Knoska *et al* (2020). Nat. Commun. 11, 657.

Protein crystal screening (PCS) beamtime at SPB/SFX

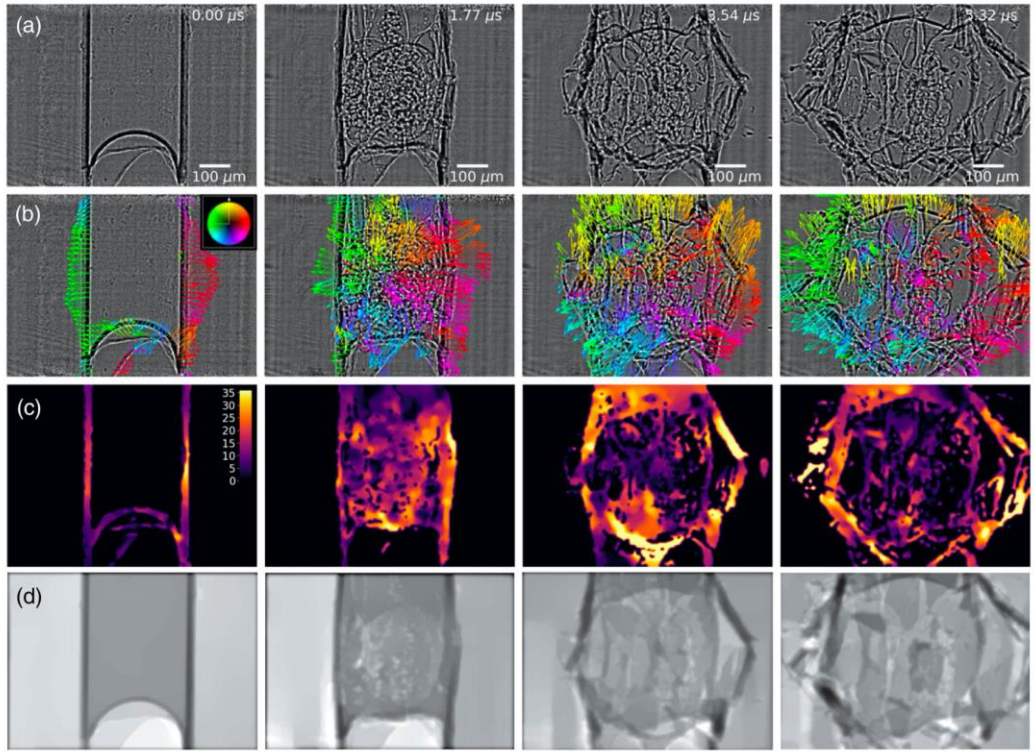
- Two step procedure with users on-site
  - 1. part: Injection tests / sample verification in the user labs
  - 2. part: Beamtime at the SPB/SFX instrument (~3 hours)
- In case sample is not jettable, sample will be considered for PCS beamtime in the next run
- Injection performed and nozzles (GDVN and 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

Semi automatic SFX pipeline

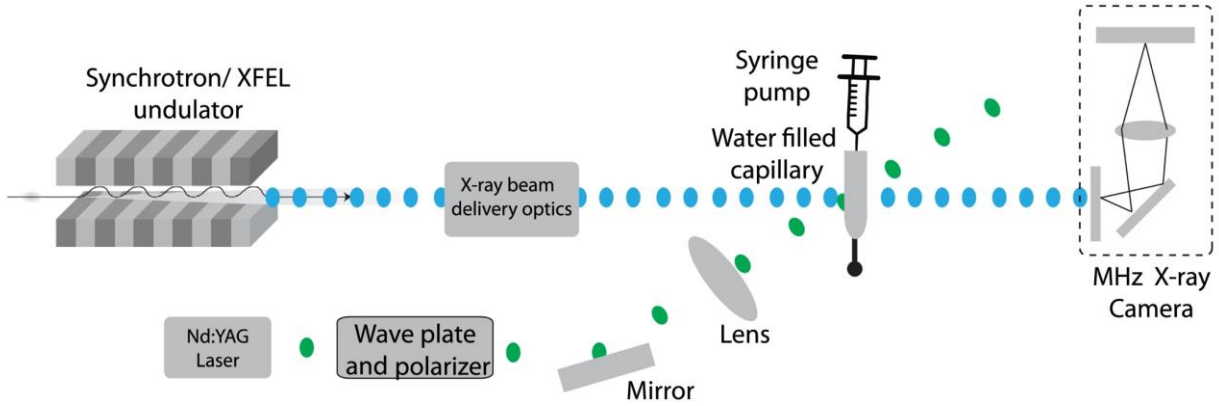
- Starting from HDF5 data sets in EuXFEL or Cheetah/CXI format, diffraction images are processed in 3 steps using CrystFEL tools, embedded to a workflow with SLURM interface for distributed computing.
- (1) Initial crystallographic peak-finding and indexing of all detector images, followed by graphical 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.



Reminder: SPB/SFX Instrument layout (MHz microscopy)



- ~12 keV to ~24 keV
- ~1mm beam size
- MHz train capable Shimadzu cameras
- Flexible sample environment



Optical laser parameters

Optical laser system 1 properties		
Wavelength	800 nm	Tuneable from 750 to 850 nm (pulse duration is longer than 15 fs)
Pulse duration	15, 50 or 300 fs	
Repetition rate	1.1 MHz	Some quasi-arbitrary patterns possible.
Pulse energy	250 µJ	
Wavelength conversion	SHG, THG, OPA	SHG: 375–425 nm, THG: 250–283 nm, OPA: 400–2600 nm
Spot size (FWHM)	≥ 40 µm	
Optical laser system 2 properties		
Wavelength	1030 nm	No wavelength tuneability
Pulse duration	0.85 or 400 ps	
Repetition rate	1.1 MHz	Some quasi-arbitrary patterns possible.
Pulse energy	4 mJ	
Wavelength conversion	SHG, THG, FHG	SHG: 515 nm, THG: 343 nm, FHG: 258 nm
Spot size (FWHM)	≥ 40 µm	

Optical laser system 3 properties (Opolette 355 HE)		
Wavelength	210 – 2400 nm	OPO output
Pulse duration	3 – 7 ns	
Repetition rate	Single shot – 20Hz	
Pulse energy	0.5 – 5 mJ	Dependent on wavelength
Spot size (FWHM)	≥ 100 µm	
	Three of these systems can be operated simultaneously	

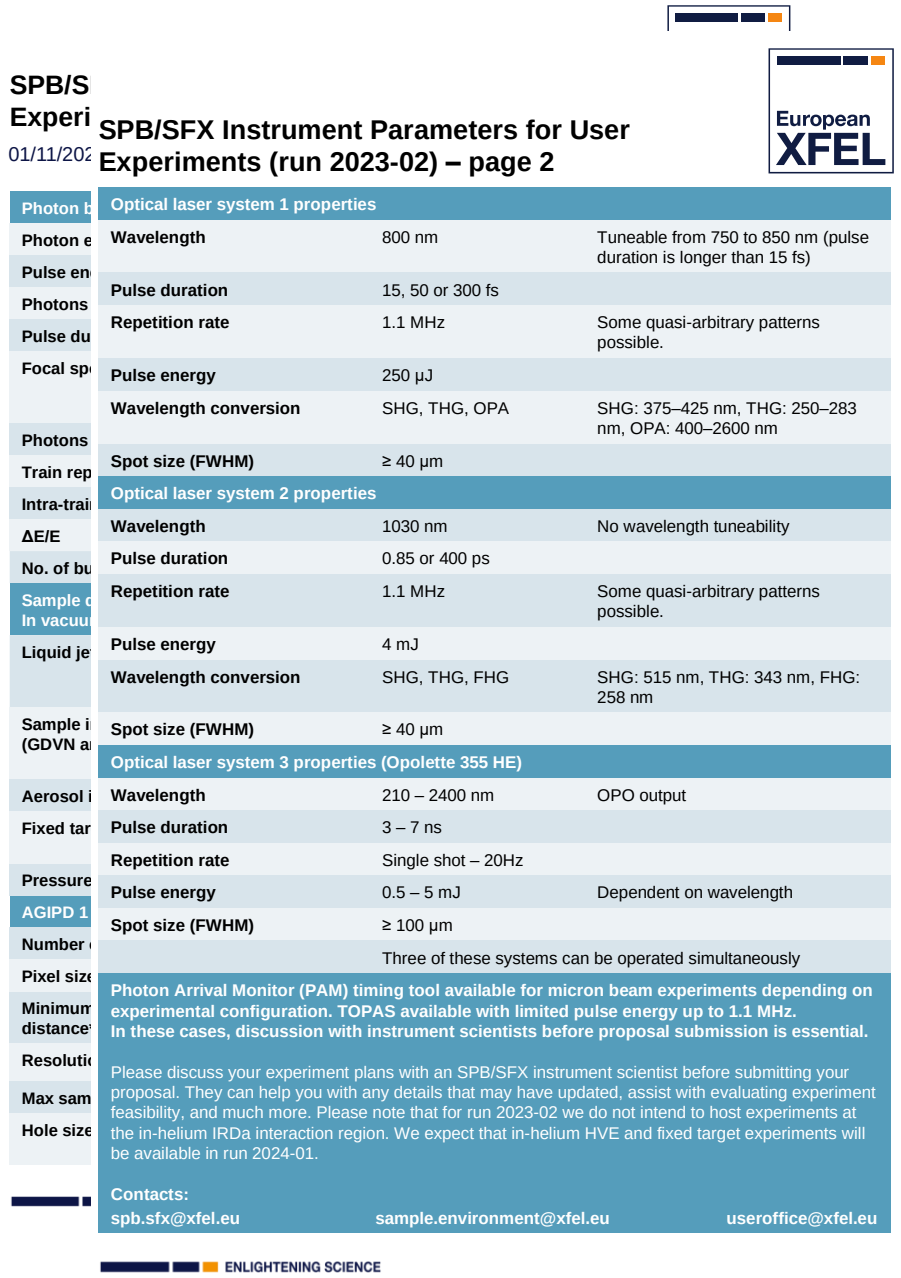
Photon Arrival Monitor (PAM) timing tool available for micron beam experiments depending on experimental configuration. TOPAS available with limited pulse energy up to 1.1 MHz.
In these cases, discussion with instrument scientists before proposal submission is essential.

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

Further details

- For run 2023-02 we do not intend to host experiments at the in-helium IRDa interaction region
- We expect that in-helium HVE and fixed target experiments will be available in run 2024-01

- richard.bean@xfel.eu
- spb.sfx@xfel.eu
- https://www.xfel.eu/facility/instruments/spb_sfx/index_eng.html



SPB/S
Experi
01/11/202

SPB/SFX Instrument Parameters for User Experiments (run 2023-02) – page 2

European XFEL

Photon b	**Optical laser system 1 properties**	
Photon e	**Wavelength**	800 nm	Tuneable from 750 to 850 nm (pulse duration is longer than 15 fs)
Pulse en	**Pulse duration**	15, 50 or 300 fs	
Photons	**Repetition rate**	1.1 MHz	Some quasi-arbitrary patterns possible.
Pulse du	**Pulse energy**	250 µJ	
Focal sp	**Wavelength conversion**	SHG, THG, OPA	SHG: 375–425 nm, THG: 250–283 nm, OPA: 400–2600 nm
Photons	**Spot size (FWHM)**	≥ 40 µm	
Train rep	**Optical laser system 2 properties**		
Intra-trai	**Wavelength**	1030 nm	No wavelength tuneability
ΔE/E	**Pulse duration**	0.85 or 400 ps	
No. of bu	**Repetition rate**	1.1 MHz	Some quasi-arbitrary patterns possible.
Sample c In vacuu	**Pulse energy**	4 mJ	
Liquid je	**Wavelength conversion**	SHG, THG, FHG	SHG: 515 nm, THG: 343 nm, FHG: 258 nm
Sample i (GDVN a	**Spot size (FWHM)**	≥ 40 µm	
	Optical laser system 3 properties (Opolette 355 HE)		
Aerosol i	**Wavelength**	210 – 2400 nm	OPO output
Fixed tar	**Pulse duration**	3 – 7 ns	
	Repetition rate	Single shot – 20Hz	
Pressure	**Pulse energy**	0.5 – 5 mJ	Dependent on wavelength
AGIPD 1	**Spot size (FWHM)**	≥ 100 µm	
Number		Three of these systems can be operated simultaneously	
Pixel size	**Photon Arrival Monitor (PAM) timing tool available for micron beam experiments depending on experimental configuration. TOPAS available with limited pulse energy up to 1.1 MHz. In these cases, discussion with instrument scientists before proposal submission is essential.**		
Minimum distance	Please discuss your experiment plans with an SPB/SFX instrument scientist before submitting your proposal. They can help you with any details that may have updated, assist with evaluating experiment feasibility, and much more. Please note that for run 2023-02 we do not intend to host experiments at the in-helium IRDa interaction region. We expect that in-helium HVE and fixed target experiments will be available in run 2024-01.		
Resoluti	**Contacts:**		
Max sam	**spb.sfx@xfel.eu**	**sample.environment@xfel.eu**	**useroffice@xfel.eu**
Hole size			

ENLIGHTENING SCIENCE

References...

Ayyer et al., 3D diffractive imaging of nanoparticle ensembles using an x-ray laser, Optica 8(1), 15 (2021)
Bielecki et al., Perspectives on single particle imaging with x rays at the advent of high repetition rate x- ray free electron laser sources, Structural Dynamics, 7, 040901 (2020)
Dallari et al., M 2021)
Doppler et al., 22)
Echelmeier et a , 11, 4511 (2020)
Gisriel et al., M
Gorel et al., Sh 10 (12), 1145 (2020)
Grünbein et al. 018)
Grünbein et al.
Hadian-Jazi et
Kirkwood et al.
Kirkwood et al. (2022)
Lehmkühler et
Mancuso et al. FELL: initial installation,
Journal of Syn
Mills et al., Firs
Pandey et al.,
Pandey et al., stallography, IUCrJ
8(6) (2021)
Sato et al., Fer (2020)
Sobolev et al.,
Vagovič et al.,
Vakili et al., 3D printed devices and infrastructure for liquid sample delivery at the European XFEL, J. Synchrotron Radiation, 29(2) (2022)
Wiedorn et al., Megahertz serial crystallography, Nature Communications, 9, 4025 (2018)
Yefanov et al., Evaluation of serial crystallographic structure determination within megahertz pulse trains, Structural Dynamics, 6, 064702 (2019)
Zhuang et al., Unsupervised learning approaches to characterize heterogeneous samples using X-ray single particle imaging, IUCrJ, 9(2) (2022)