SPB/SFX Instrument Update
EuXFEL Proposal Call 12

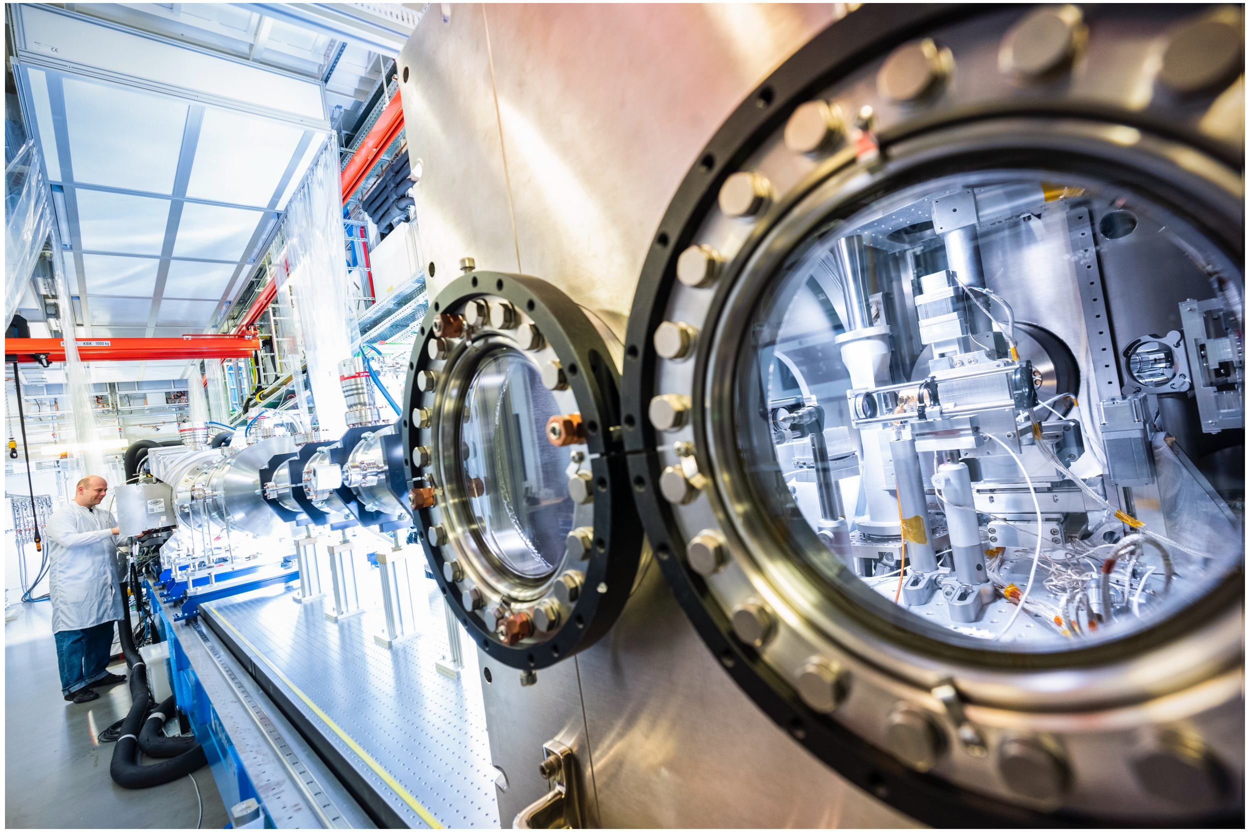
Richard Bean
SPB/SFX Instrument Group Leader

10.10.2023

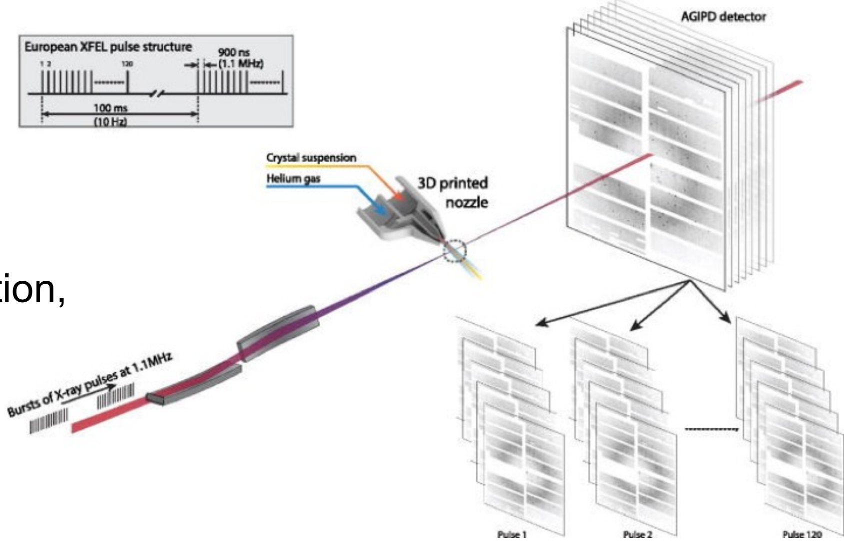
European XFEL

SPB / SFX

SPB/SFX Instrument basic parameters



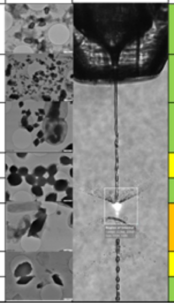
- ~ 6 keV to ~15 keV (focused beam)
- ~3 µm and 200 nm spot sizes
- 1 Mpx AGIPD
- MHz rep rate capable
- Optical pump laser (variable colour / rate)
- up to 10mJ/um^2 flux density

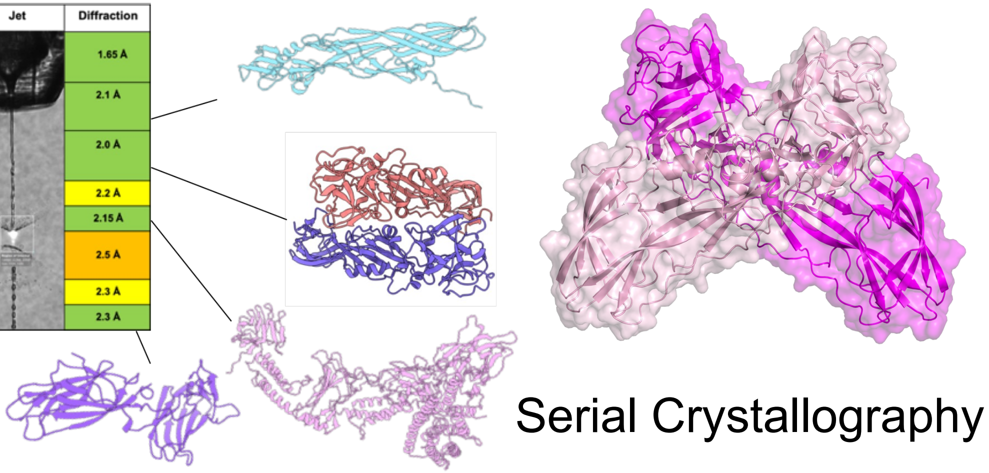


- Mancuso et al., The [SPB/SFX] instrument at the European XFEL: initial installation, Journal of Synchrotron Radiation, 26, pp. 660-676 (2019)

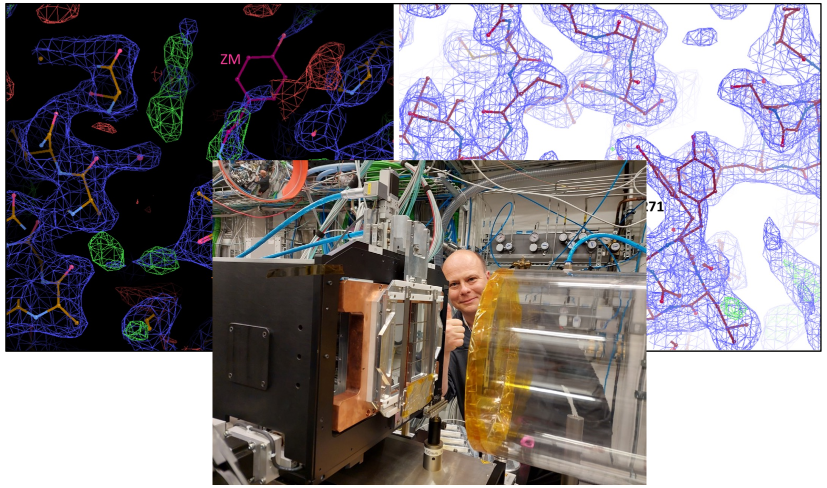
Experimental modes supported at SPB/SFX

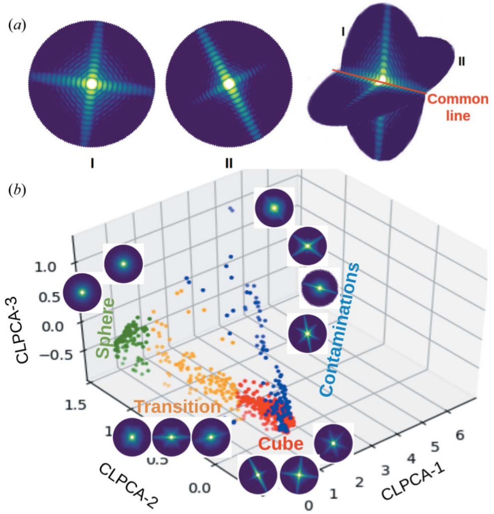
Serial Crystallography

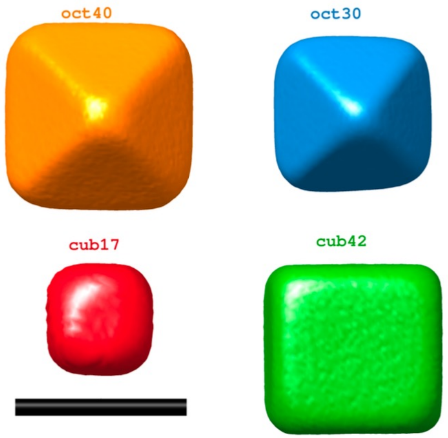
sample	Indexed/hits	Crystals	Jet	Diffraction
CpGV (for calibration)	40072 / 215964			1.65 Å
1	64305 / 127726			2.1 Å
2	70295 / 91488			2.0 Å
3a	30165 / 73100			2.2 Å
3b	33552 / 73100			2.15 Å
4	1409 / 3159			2.5 Å
5a	10069 / 63443			2.3 Å
5b	17662 / 63443			2.3 Å



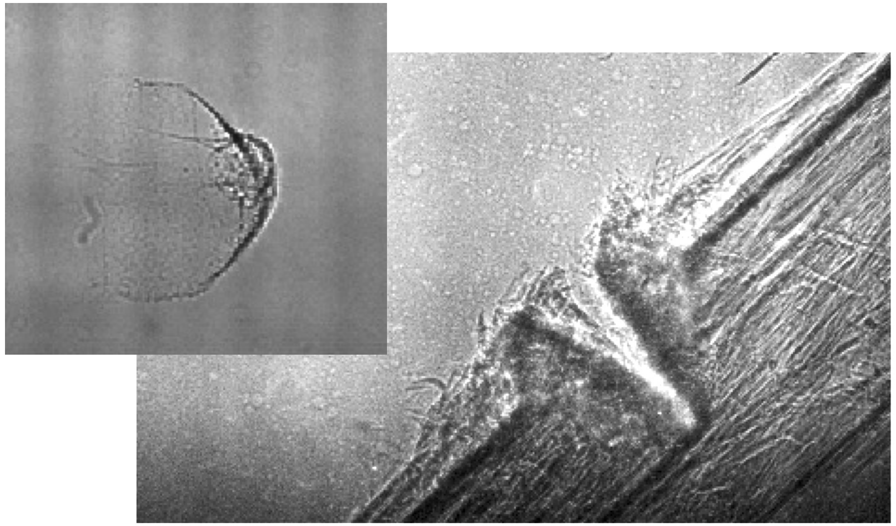
HVE injection SFX







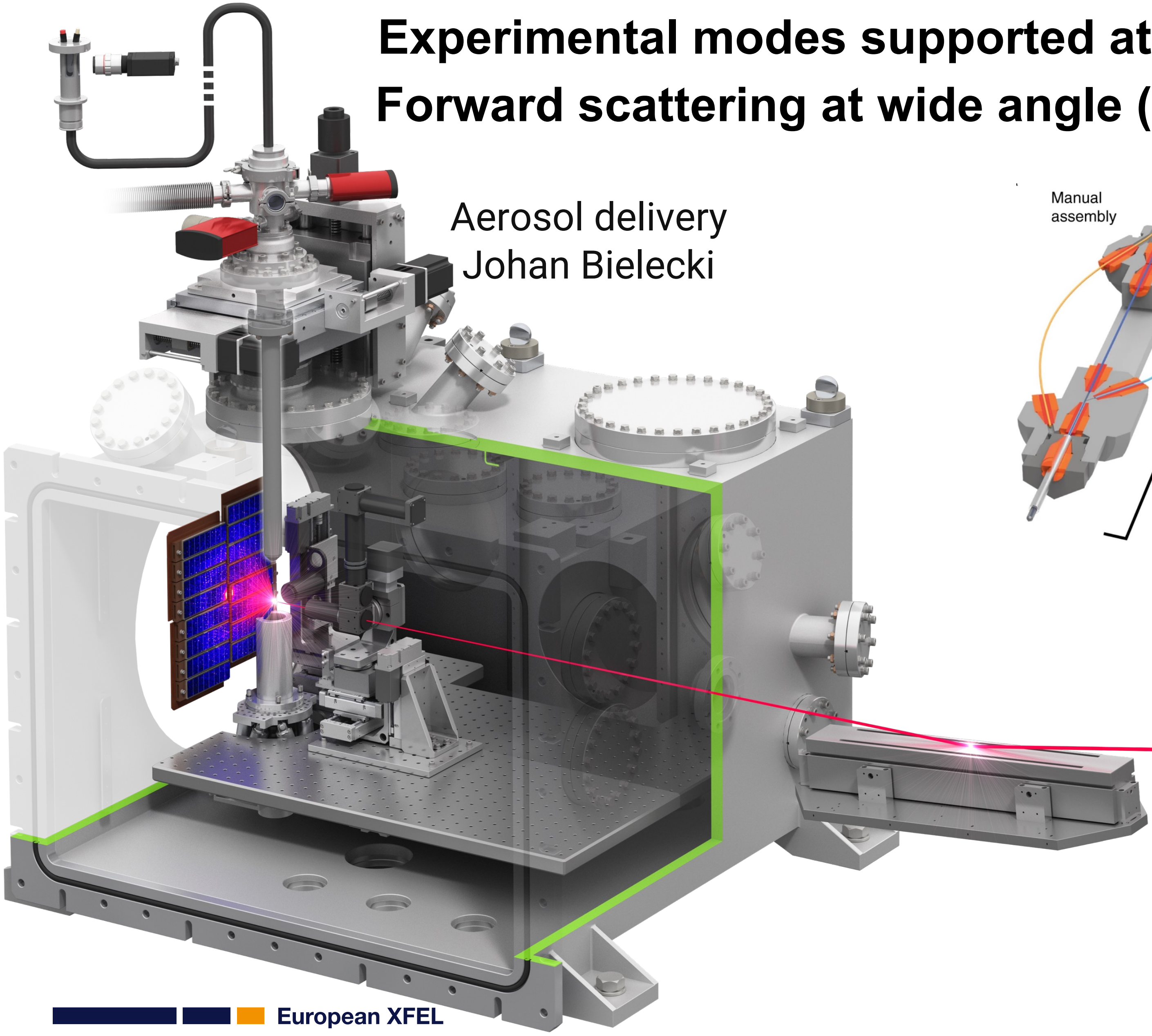
Materials Single Particle Imaging



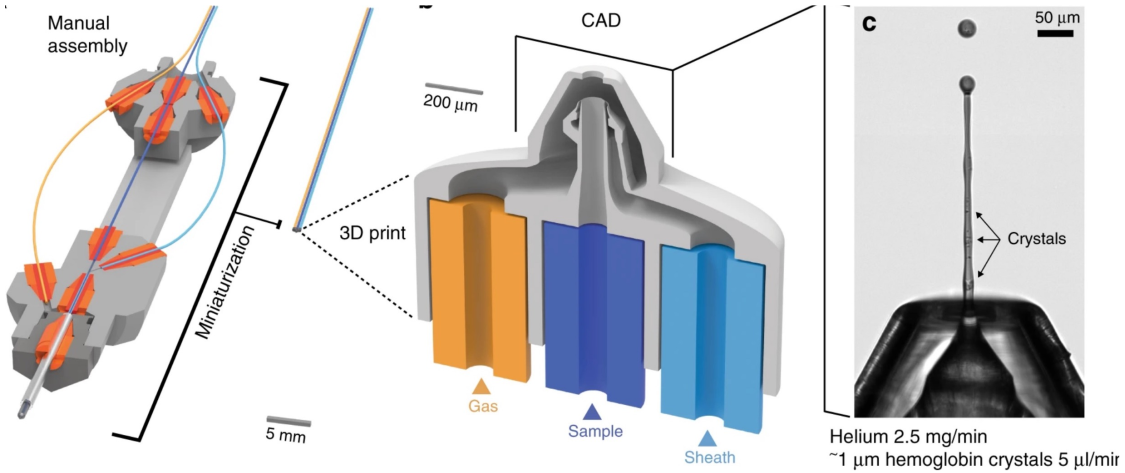
Megahertz rate Microscopy

Experimental modes supported at SPB/SFX

Forward scattering at wide angle (Materials SPI, SFX)

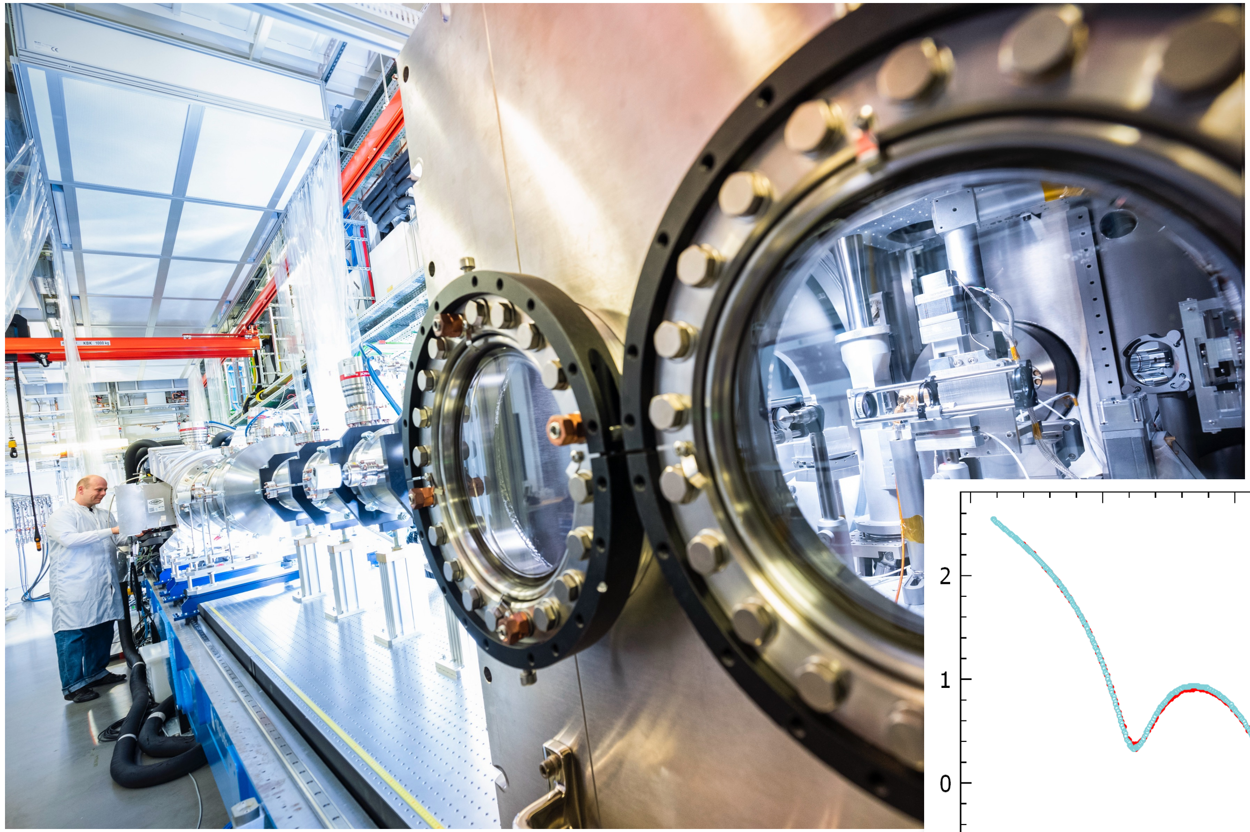


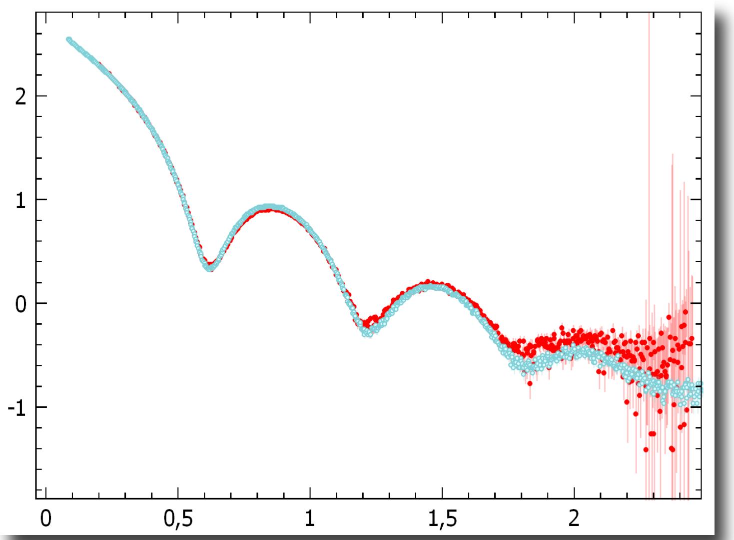
Aerosol delivery
Johan Bielecki



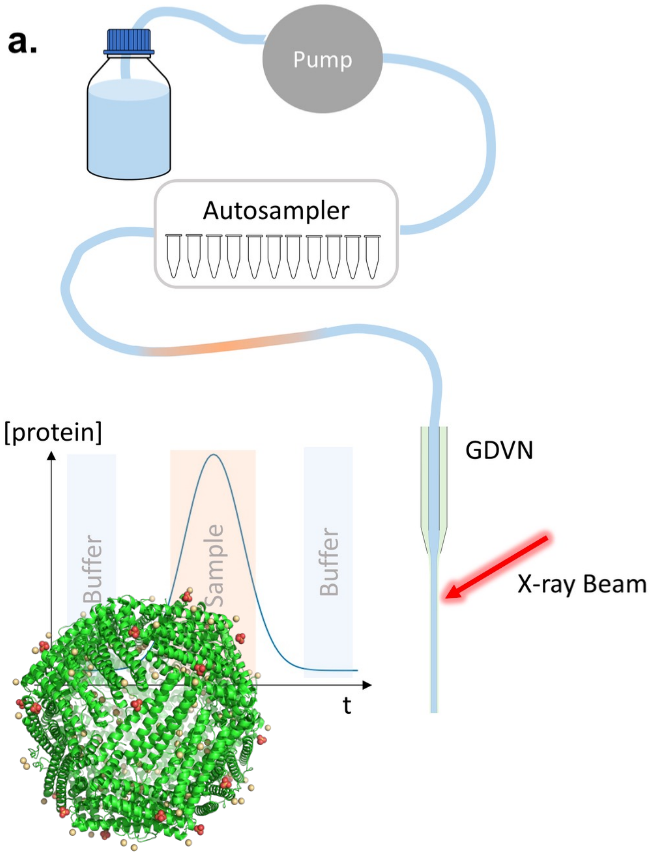
Sample nozzle designs: J Knoška (CFEL) Mo Vakili (now CFEL)
In production with SEC group

Experimental modes supported at SPB/SFX
Forward scattering at lower angle (SPI, SAXS)



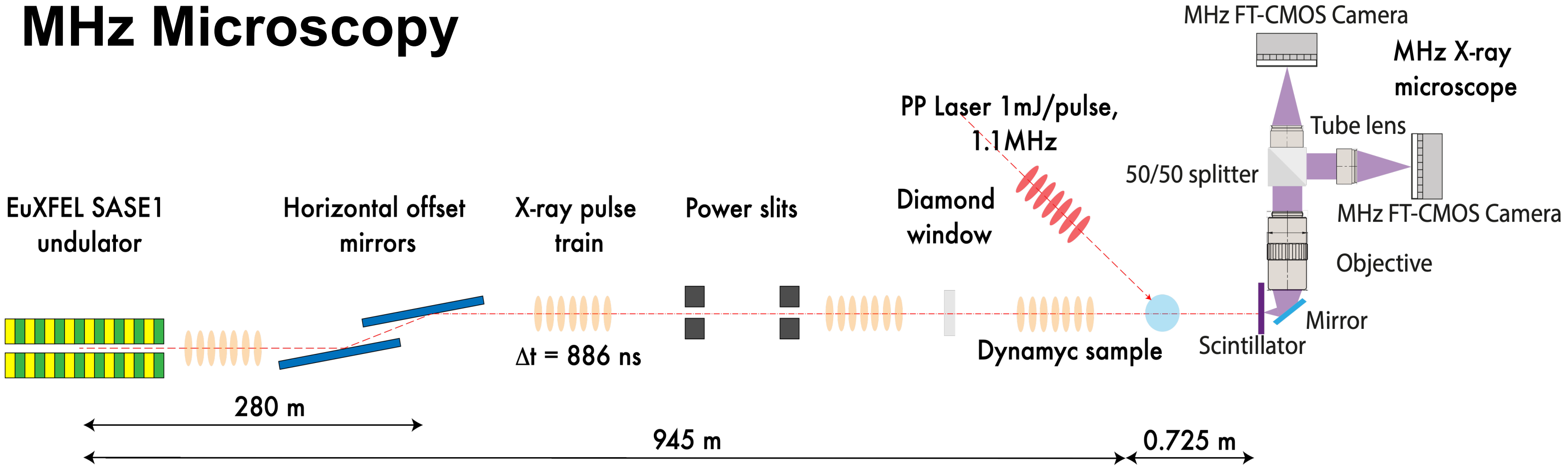


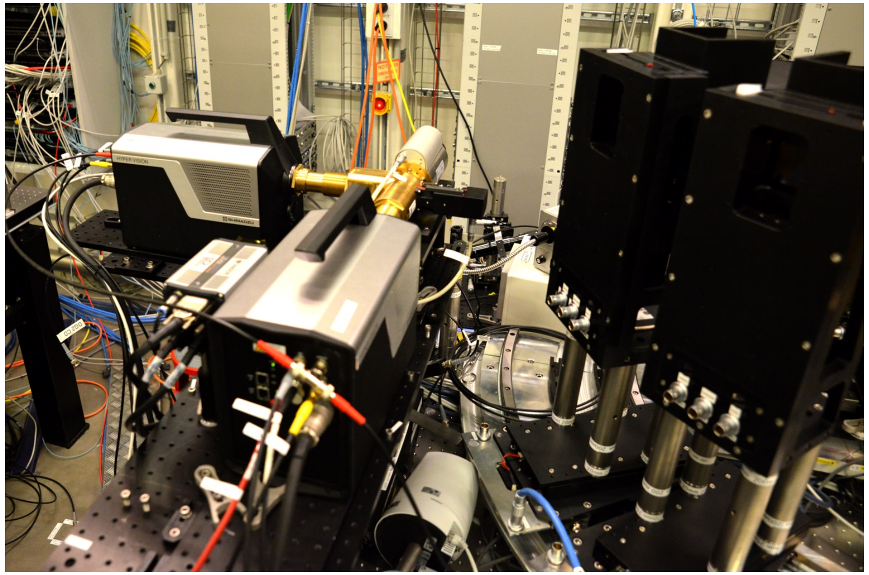
Small Angle Scattering



Experimental modes supported at SPB/SFX

MHz Microscopy

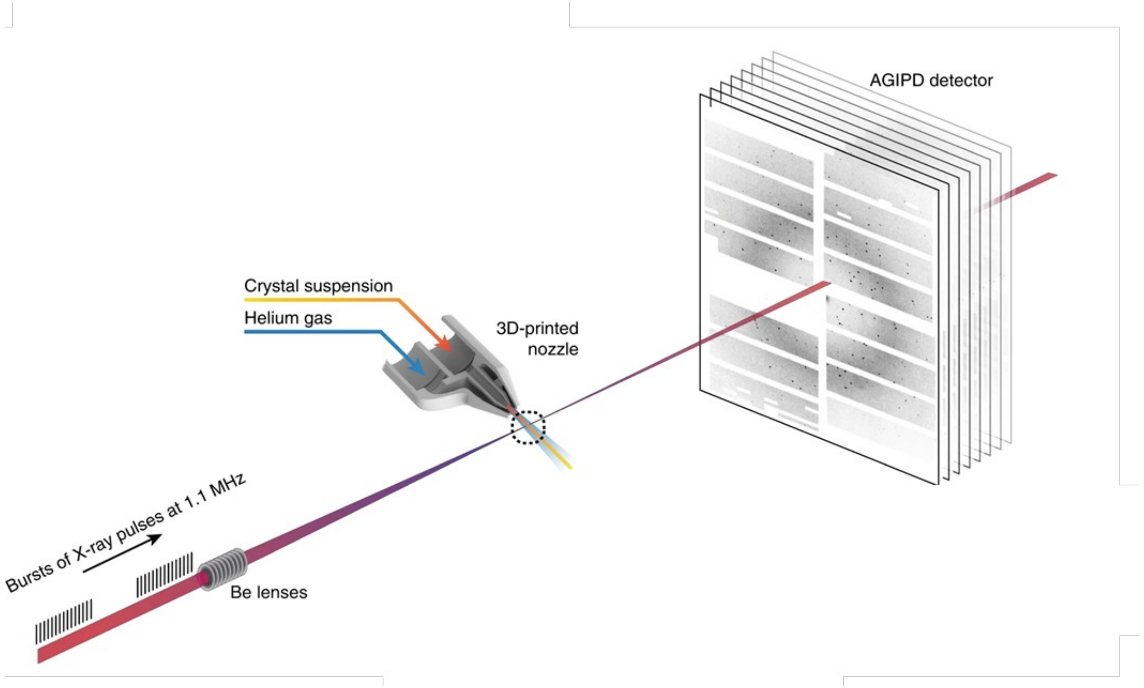




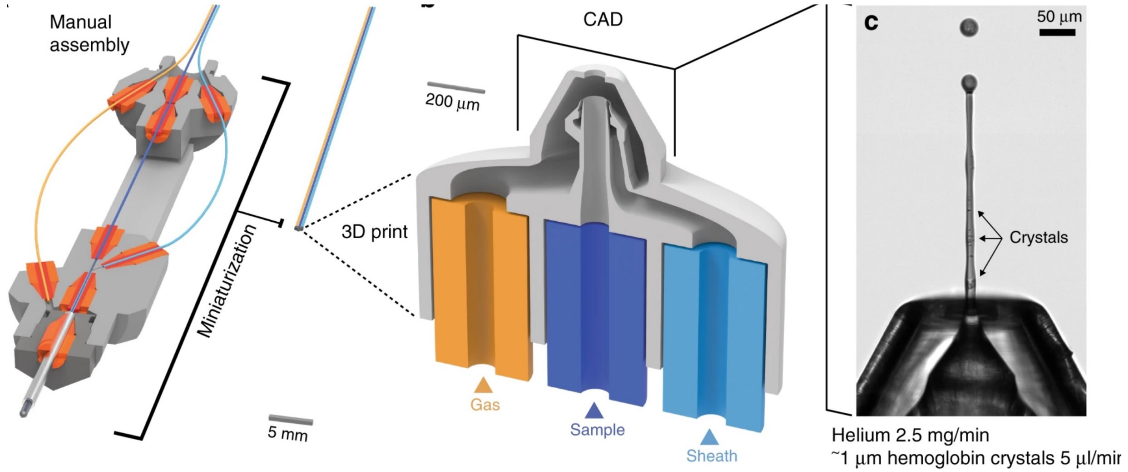
- ~12 keV to ~24 keV (direct beam)
- ~1.5 mm beam size
- MHz train capable Shimadzu cameras
- Flexible sample environment
- Optical pump laser (variable colour / rate)

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

- Standard GDVN
  - Sample (crystal suspension) is focused by Helium gas
- Double-flow focusing nozzles (DFFN)
  - Outer jet (Ethanol) focused by Helium stabilizes inner jet (Sample)



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



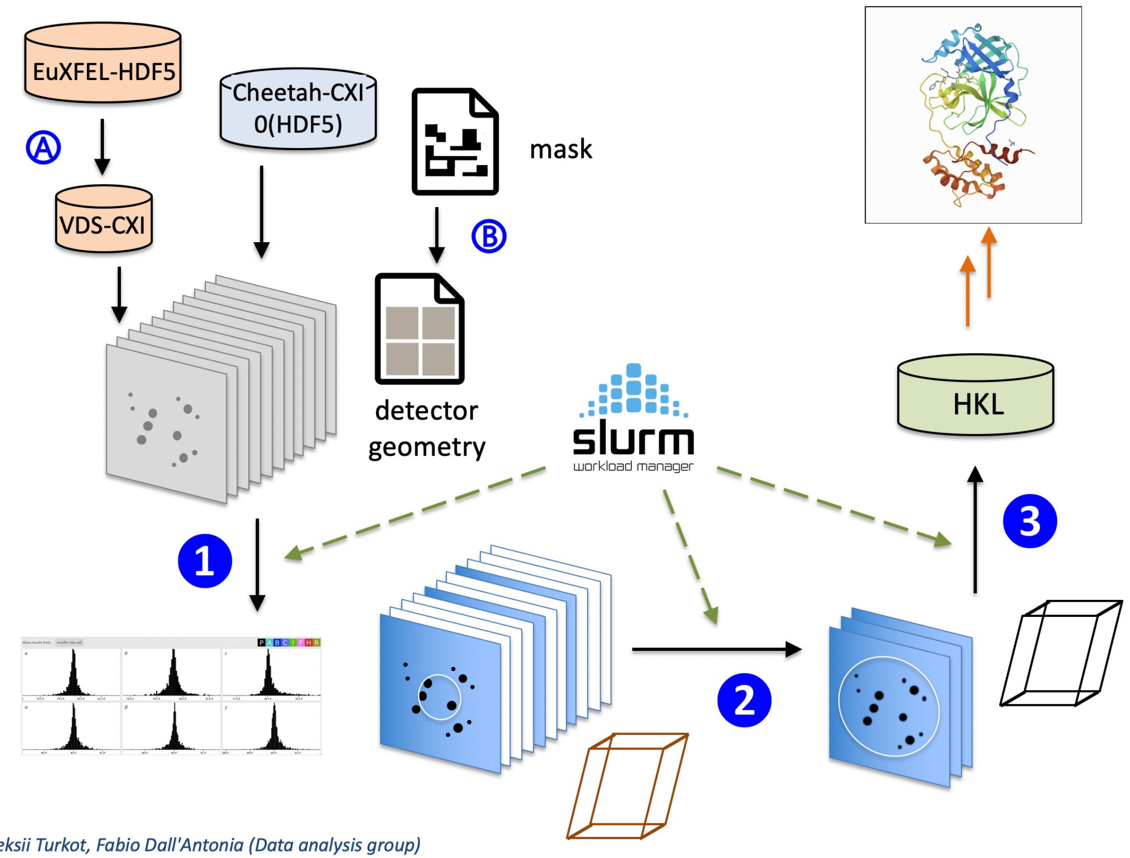
Oberthuer *et al* (2017) Scientific Reports 7:44628
Knoska *et al* (2020). Nat. Commun. 11, 657.

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.



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

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 (see footnote)	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	3 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 at a maximum repetition rate of 564 kHz.
In these cases, discussion with instrument scientists before proposal submission is essential.

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

Further details

- In-helium HVE, low viscosity jets, and fixed target experiments possible at our downstream interaction region

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

SPB/SFX Instrument Parameters for User Experiments Call

04/10/2023

Photon beam parameters
Photon energy
Pulse energy
Photons per pulse (at sour
Pulse duration
Focal spot size (FWHM)
Photons / µm² (at sample)
Train repetition rate
Intra-train repetition rate
ΔE/E
No. of bunches per train
Sample delivery systems: In vacuum (upstream, 1 Mp
Liquid jet injector rod
Sample injection nozzles (GDVN and DFFN)
High viscosity liquid jet
Aerosol injector
Fixed target sample holder
Pressure systems
AGIPD 1 Mpx detection pro
Number of pixels
Pixel size
Minimum sample–detector distance
Resolution at edge @ 9.3 k
Max sample-detector distai
Hole size

SPB/SFX Instrument Parameters for User Experiments Call 12 (run 2024-02) – page 2

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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.

Contacts:
spb.sfx@xfel.eu
sample.environment@xfel.eu
useroffice@xfel.eu

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