PAUL SCHERRER INSTITUT

PSI

John Beale :: SLS User Meeting :: Paul Scherrer Institut

Serial crystallography at SLS and SwissFEL

01.03.2022

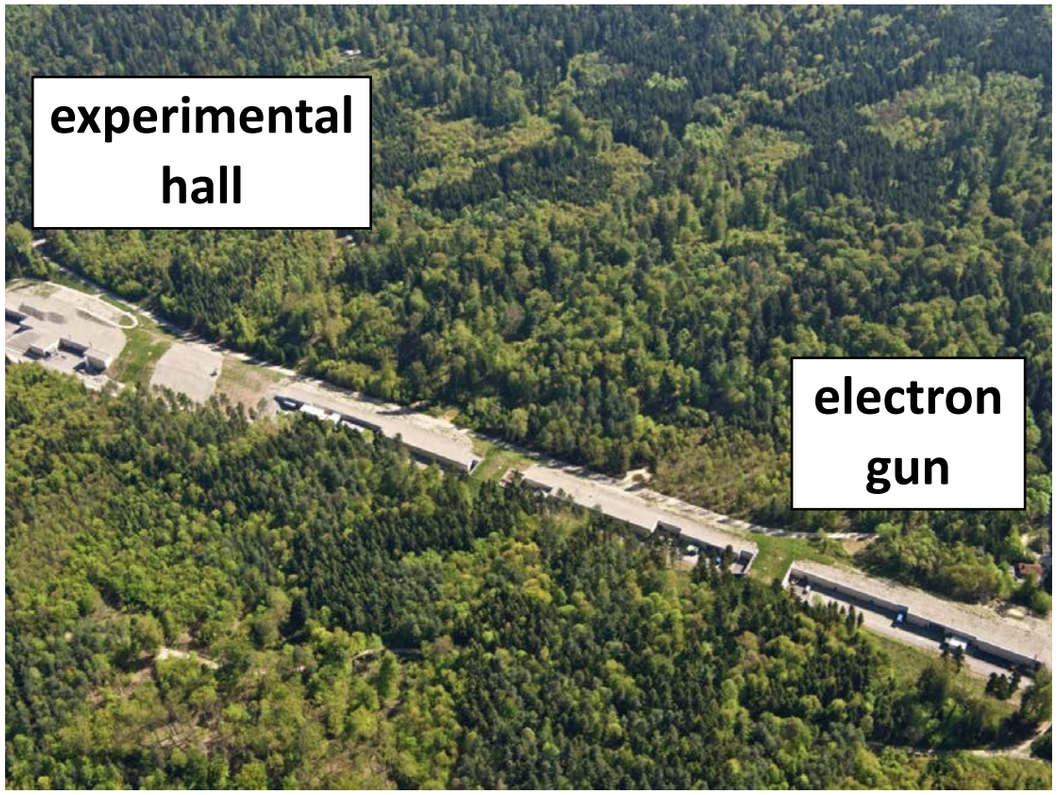
Overview

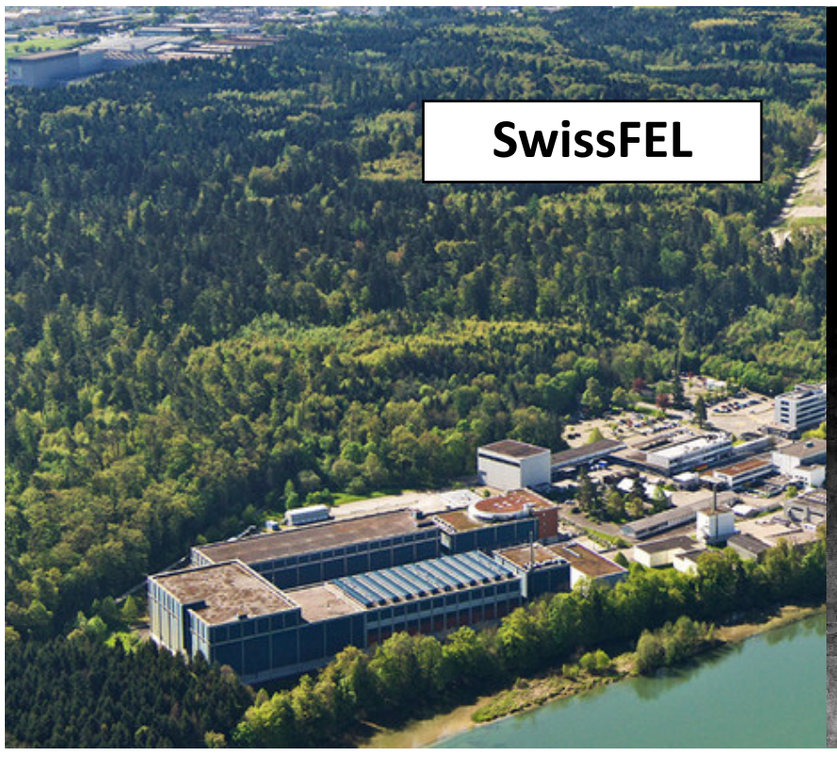
- Summary of serial crystallography at PSI:
  - SwissFEL - ALvra and Cristallina
  - SLS
- Current developments
- Vision for the future

SwissFEL overview

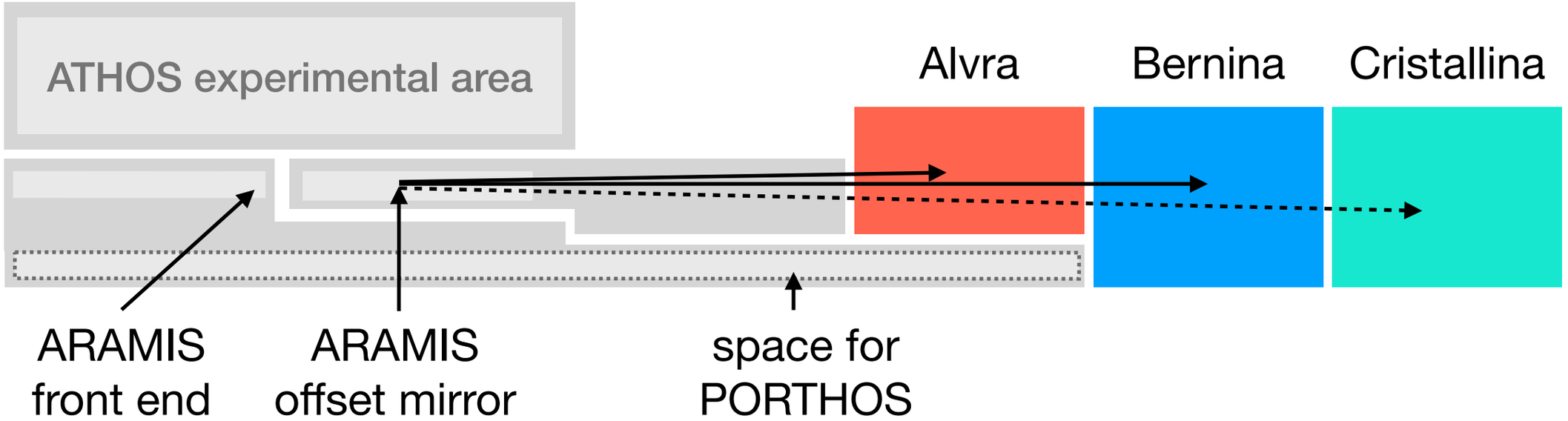
- ARAMIS
  - hard X-ray (1.8 - 12.4 keV)
  - 300 - 600 µJ per pulse
  - first users 2018

- ATHOS
  - soft X-ray (240 - 1,930 eV)
  - first users 2021



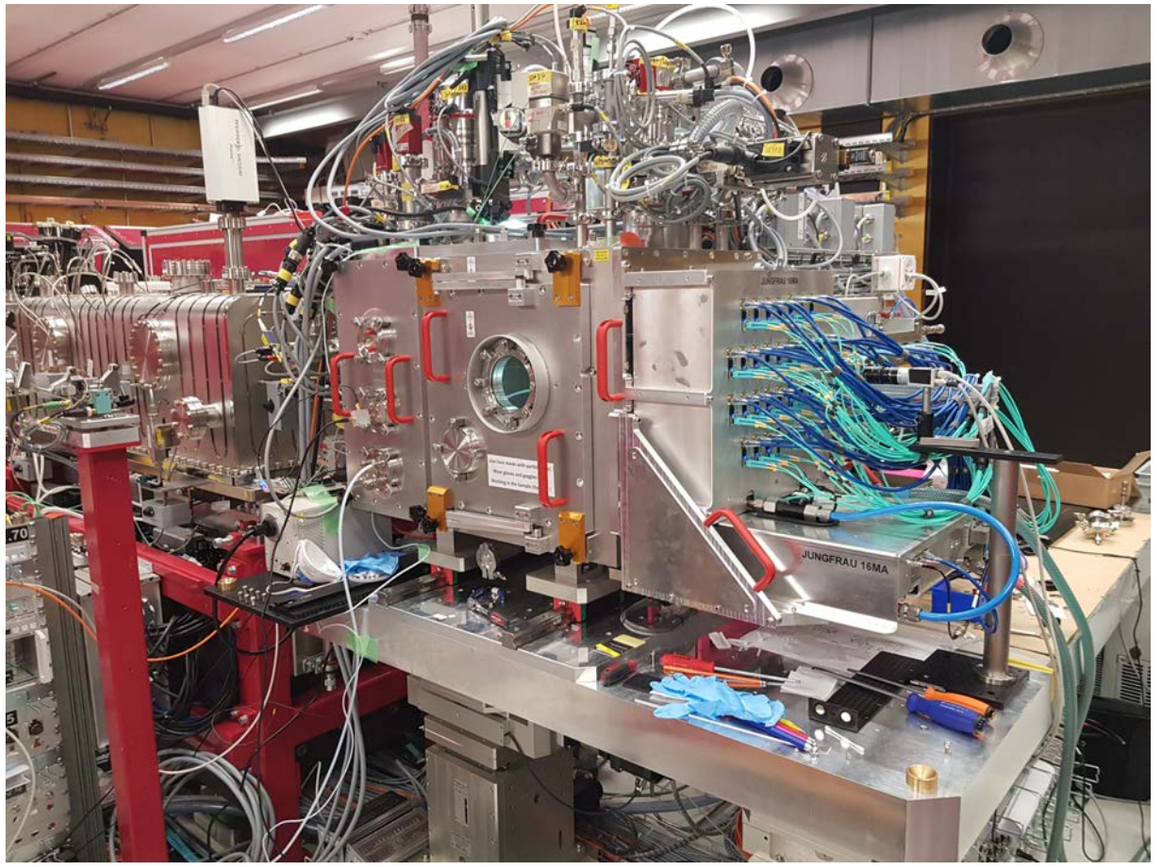


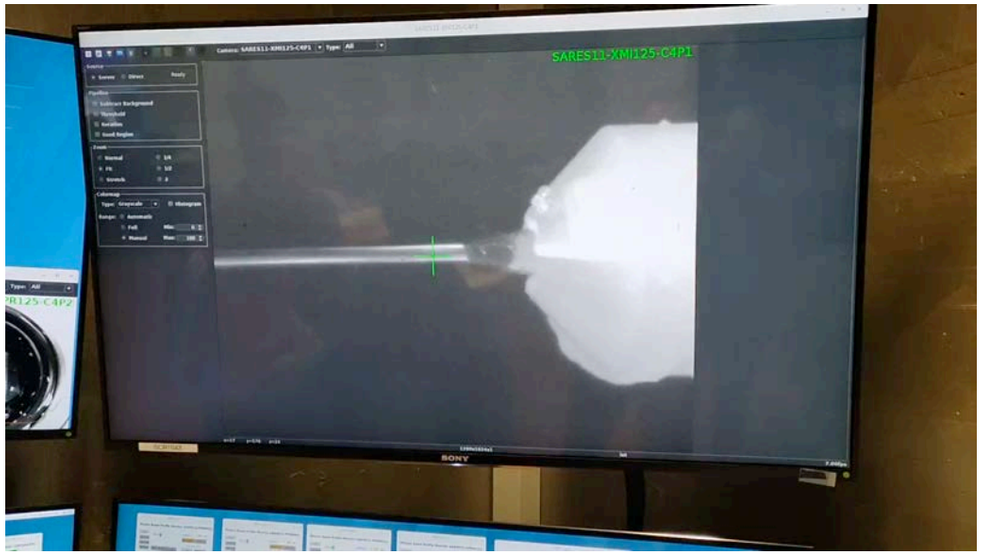
SwissFEL overview - ARAMIS beamline



- ARAMIS is the SwissFEL hard X-ray beamline and delivers beam to three endstations: Alvra, Bernina and now, Cristallina.
- Alvra has been the primary site of SFX experiments at SwissFEL where the endstation is shared between SFX and spectroscopy users.
- Cristallina will be shared between SFX and quantum technologies.

SwissFEL overview - Alvra: fs time-resolved SFX using extruders and jets

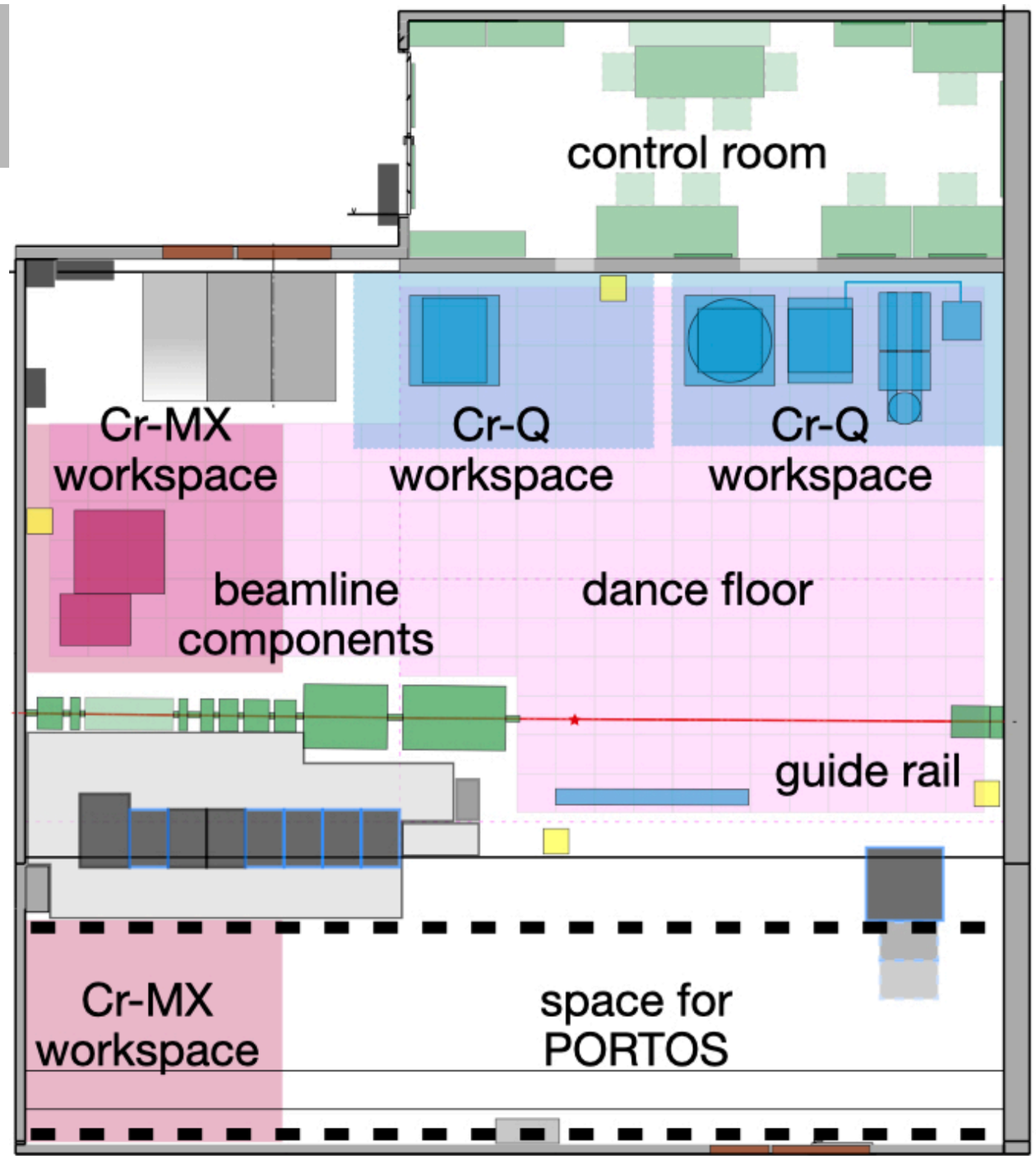


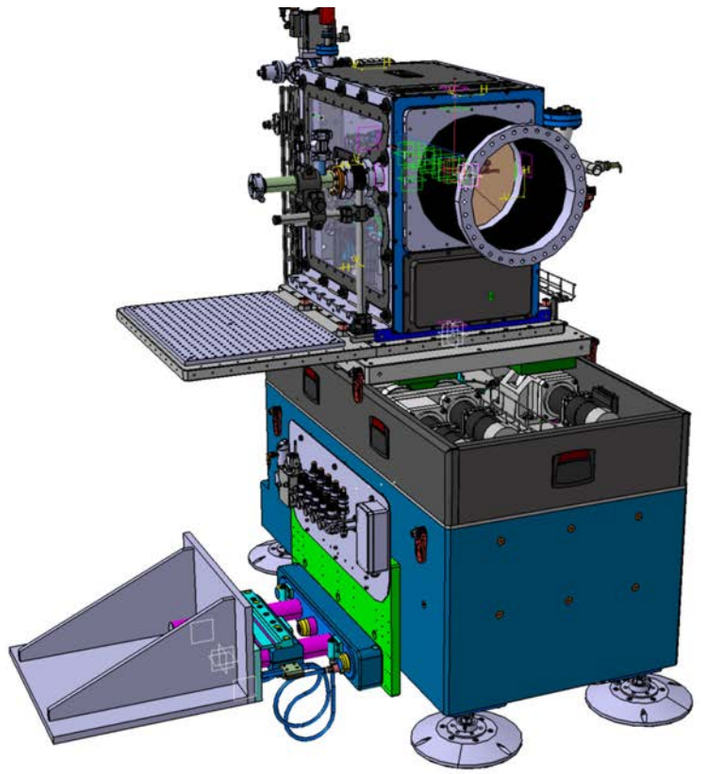


- Alvra-PRIME endstation is very much the home of jetting experiments at SwissFEL and ultra-fast time-resolved measurements.

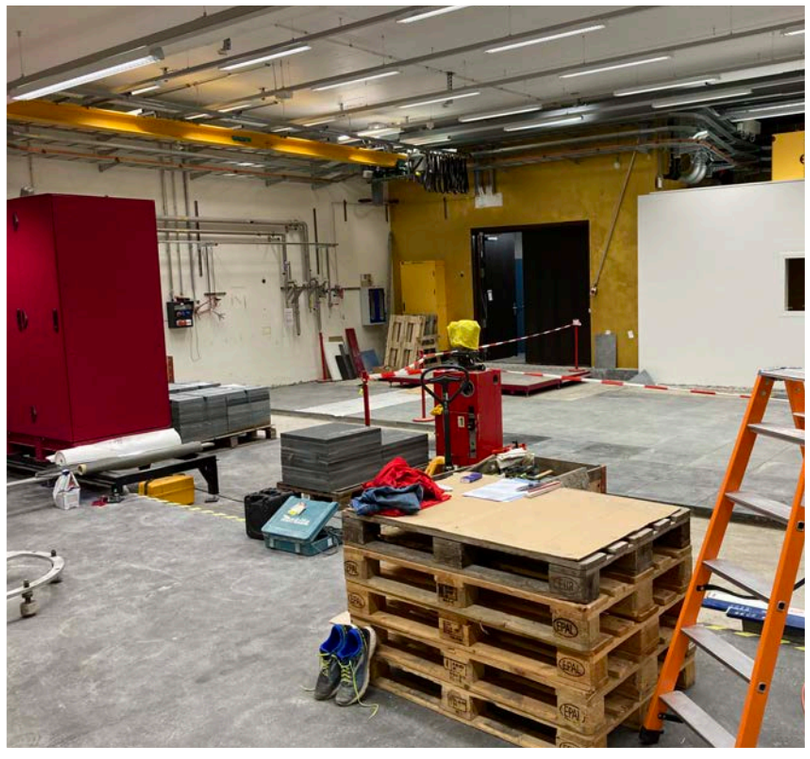
- Cristallina should complement Alvra by offering different sample delivery systems and different experiments.

SwissFEL overview - Cristallina Endstation

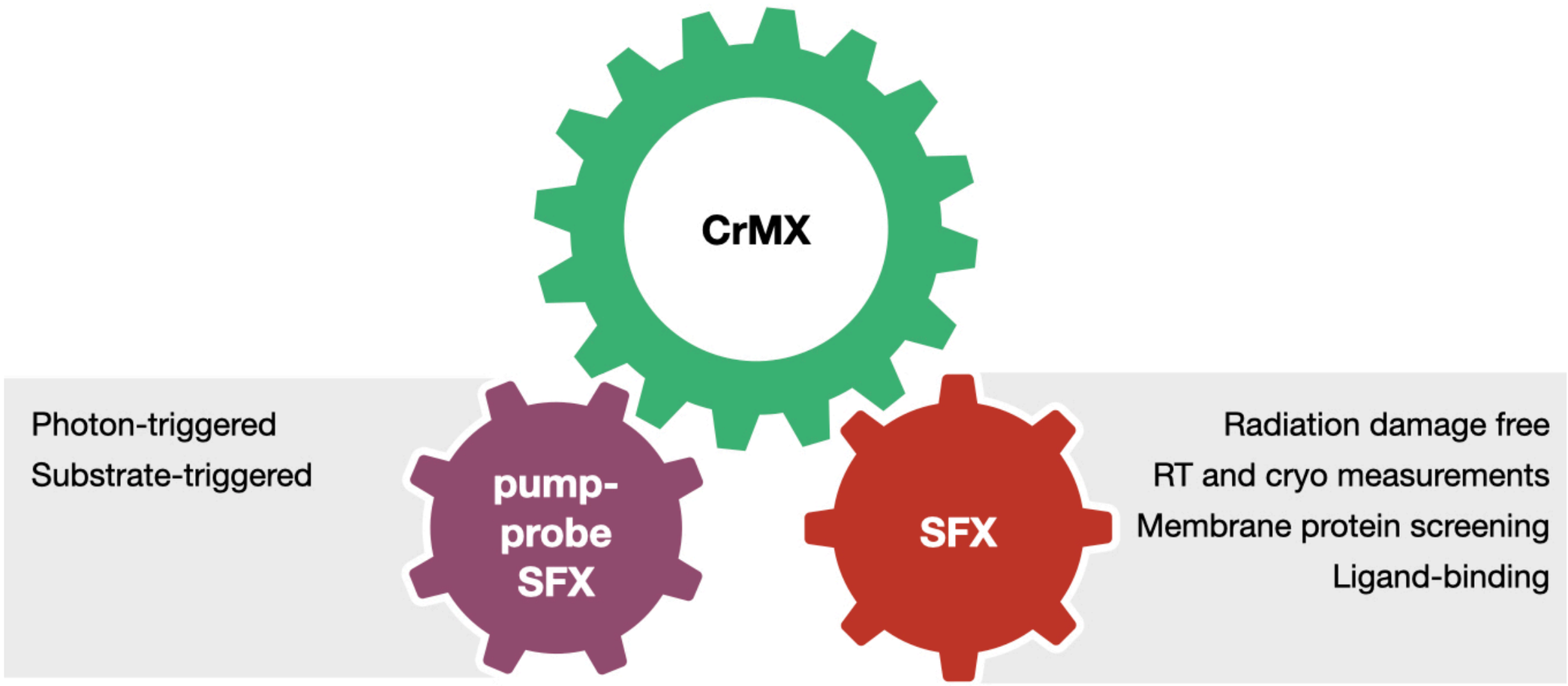




SwissFEL overview - Cristallina Endstation

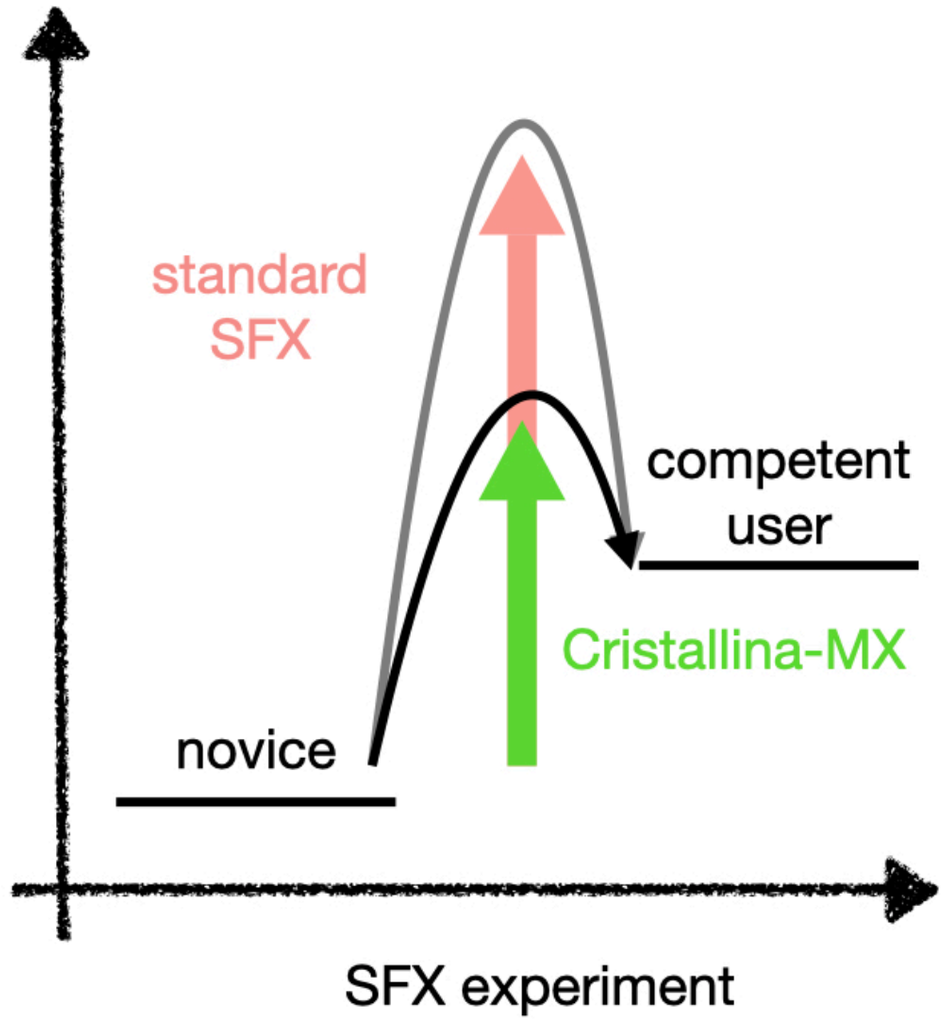


Experimental scope of Cristallina - pump-probe SFX and SFX



- CrMX will aim to do at least 50:50 pump-probe SFX and SFX experiments.
- SFX experiments can be shorter and easier for non-SFX groups.
- SFX can also act as a bridge for new users to gain access and experience at the XFEL.

CrMX mission - increase XFEL access



- The principal goal of the Cristallina-MX project is to reduce the activation barriers to XFEL research and thereby, increase the user pool and breath of proposed projects.

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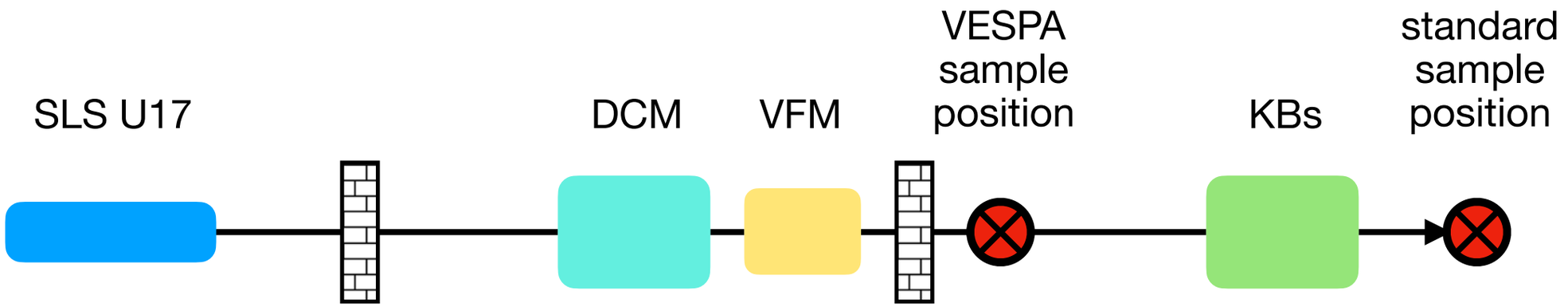
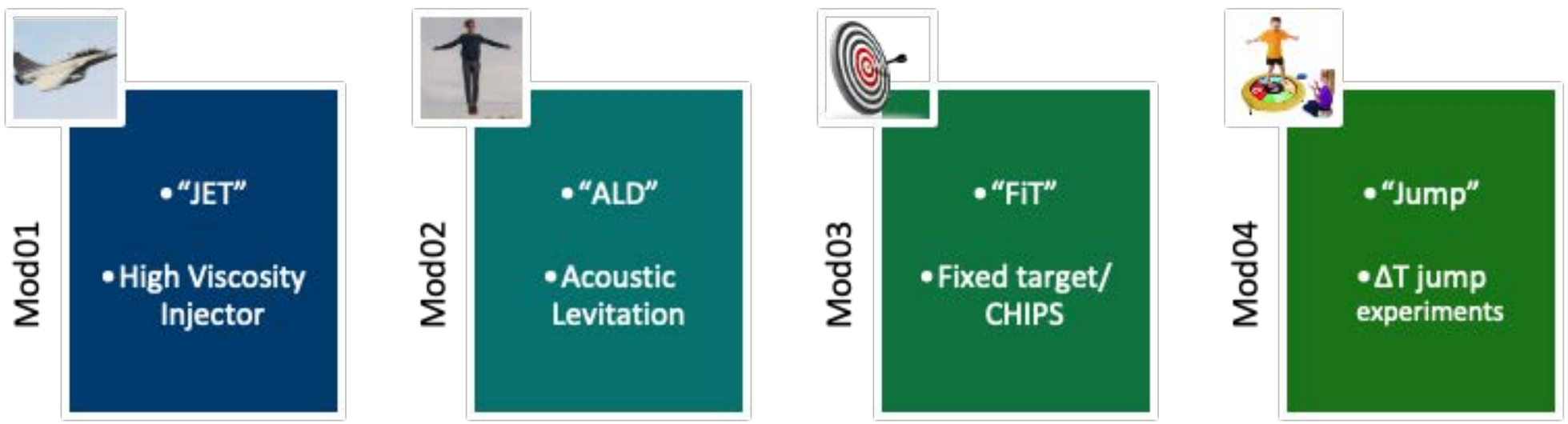
VESPA at PXI - offer complimentary methods to SwissFEL



- Flexible endstation at PXI 2nd source to accommodate different types of serial crystallography experiments and sample delivery systems.

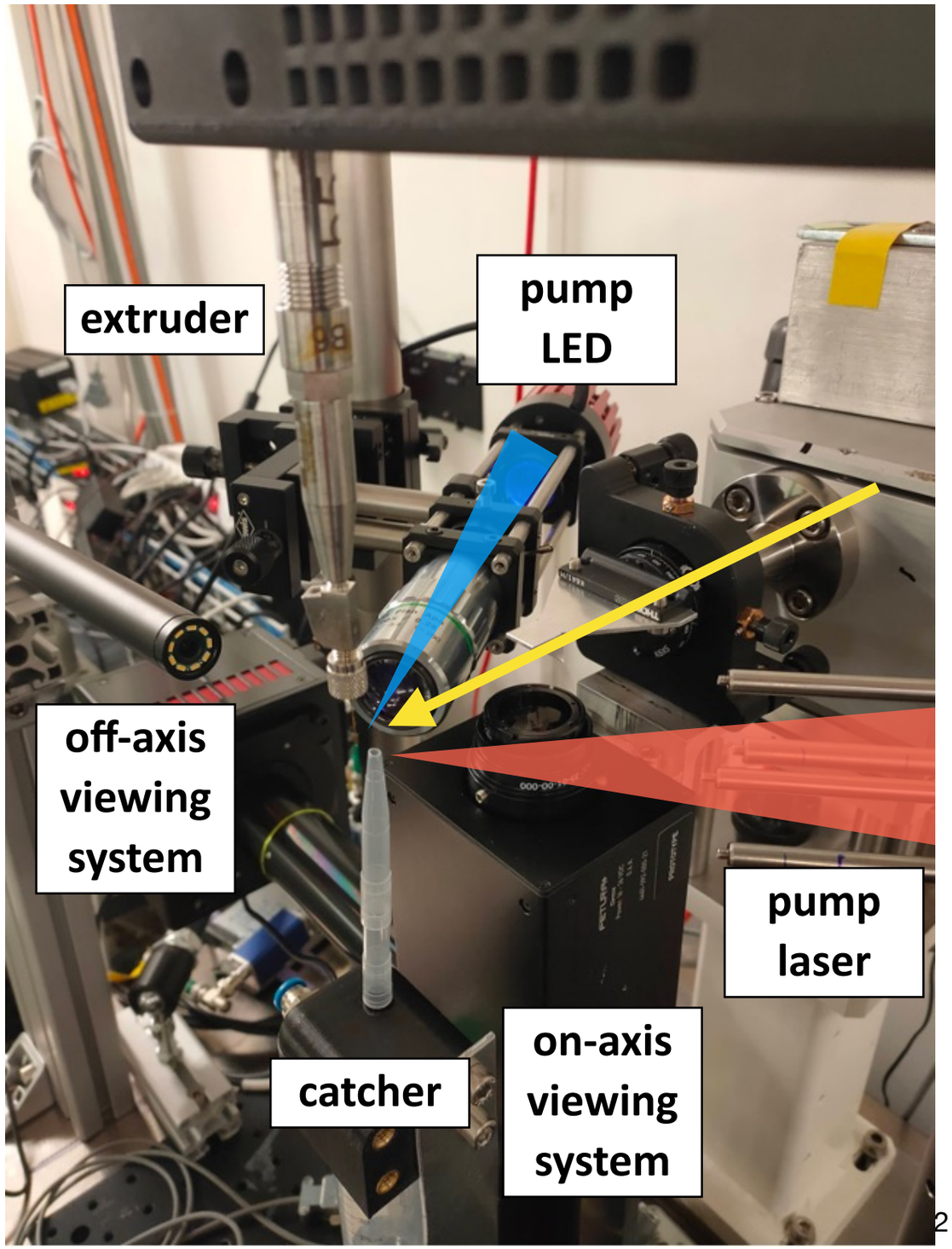


VESPA - "**V**ersatile **E**nd-station for **S**erial **P**rotein crystallography **A**pplications"
- Ezequiel Panepucci

VESPA at PXI - offer complimentary methods to SwissFEL

- MOD1 endstation with the extruder.

- Features:
  - High speed detector (Eiger 1M).
  - Integrated (ns) laser triggering for time-resolved work.
  - Modular setup for different experiments.



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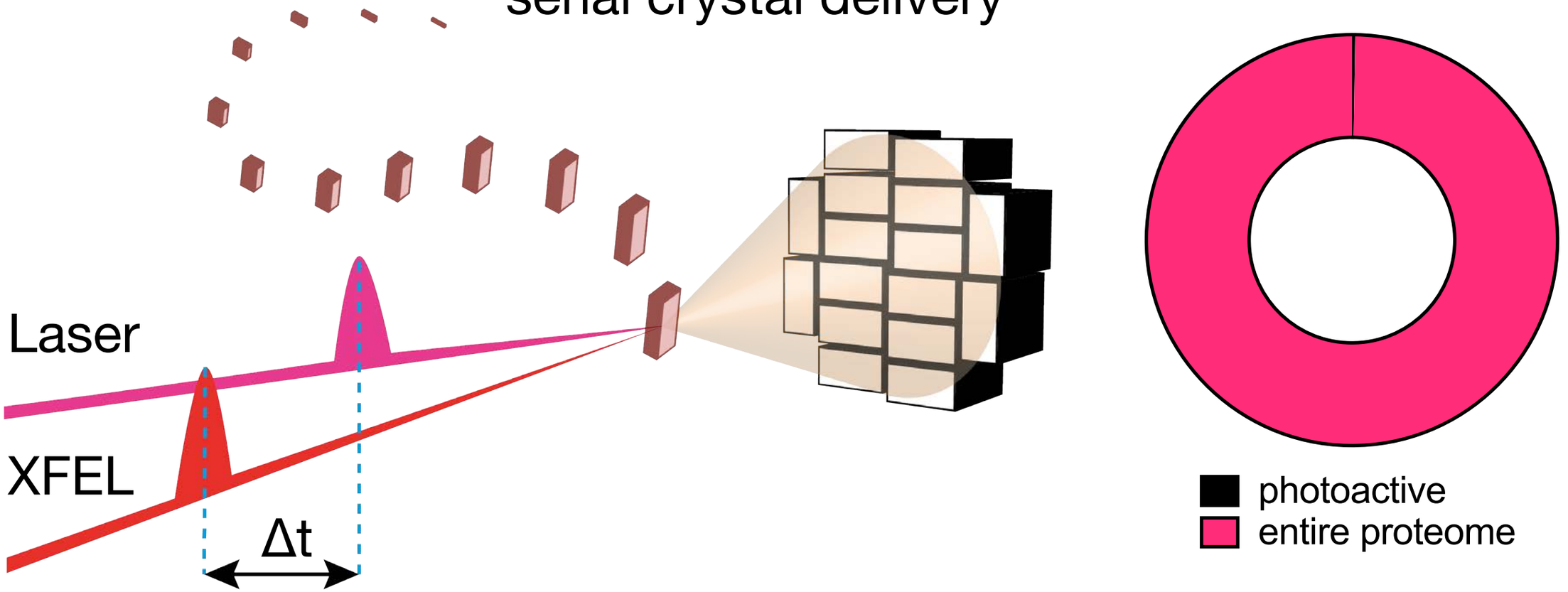
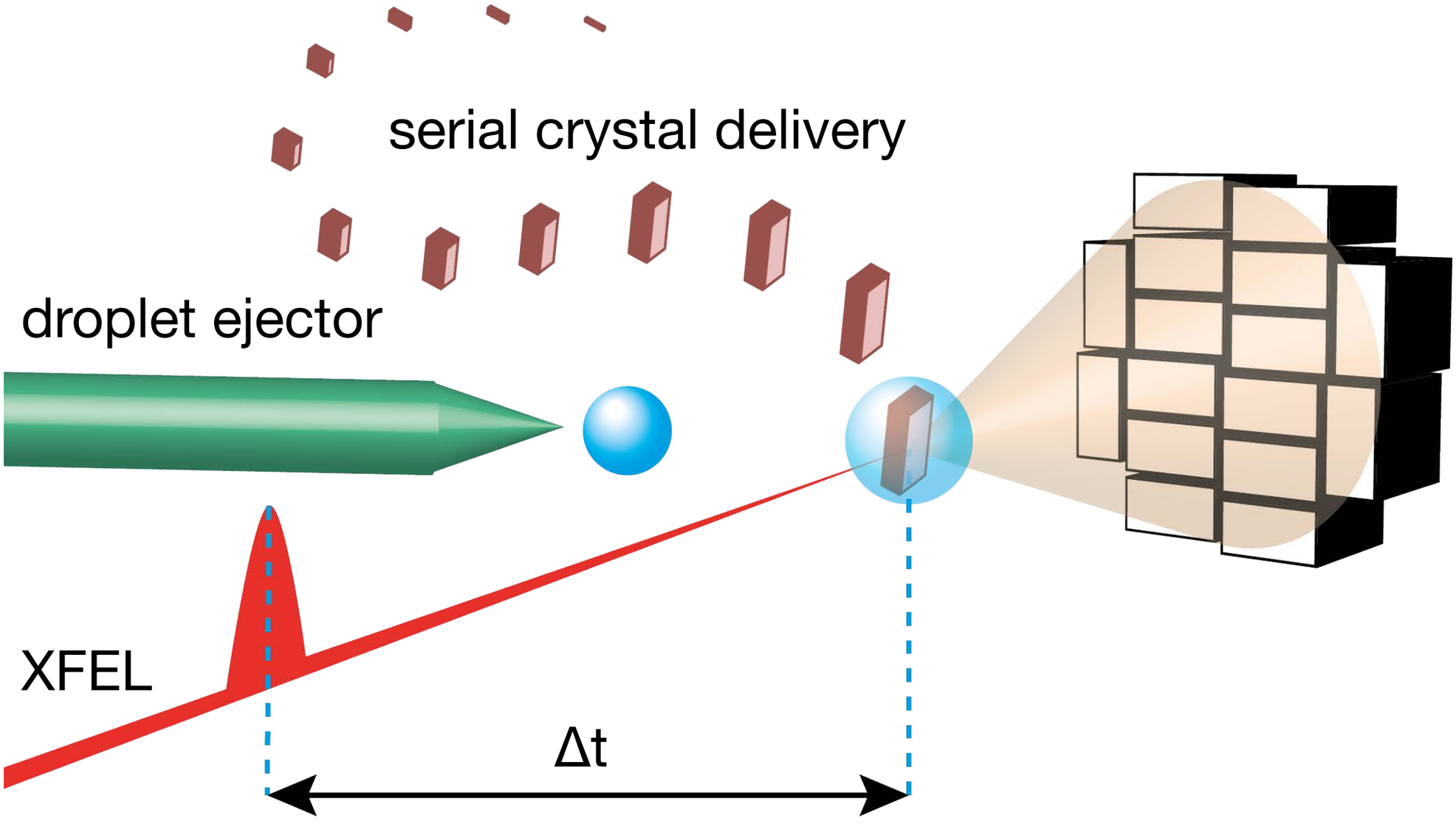
Time-resolved crystallography at SLS and SwissFEL



- Light-triggered, time-resolved crystallography well established at with the extruder at Alvra and PX1.

- However, very few proteins use light as a substrate.

Time-resolved crystallography at SLS and SwissFEL



- We were successful in getting a PSI research grant to establish fixed-target mixing at both VESPA and Cristallina.

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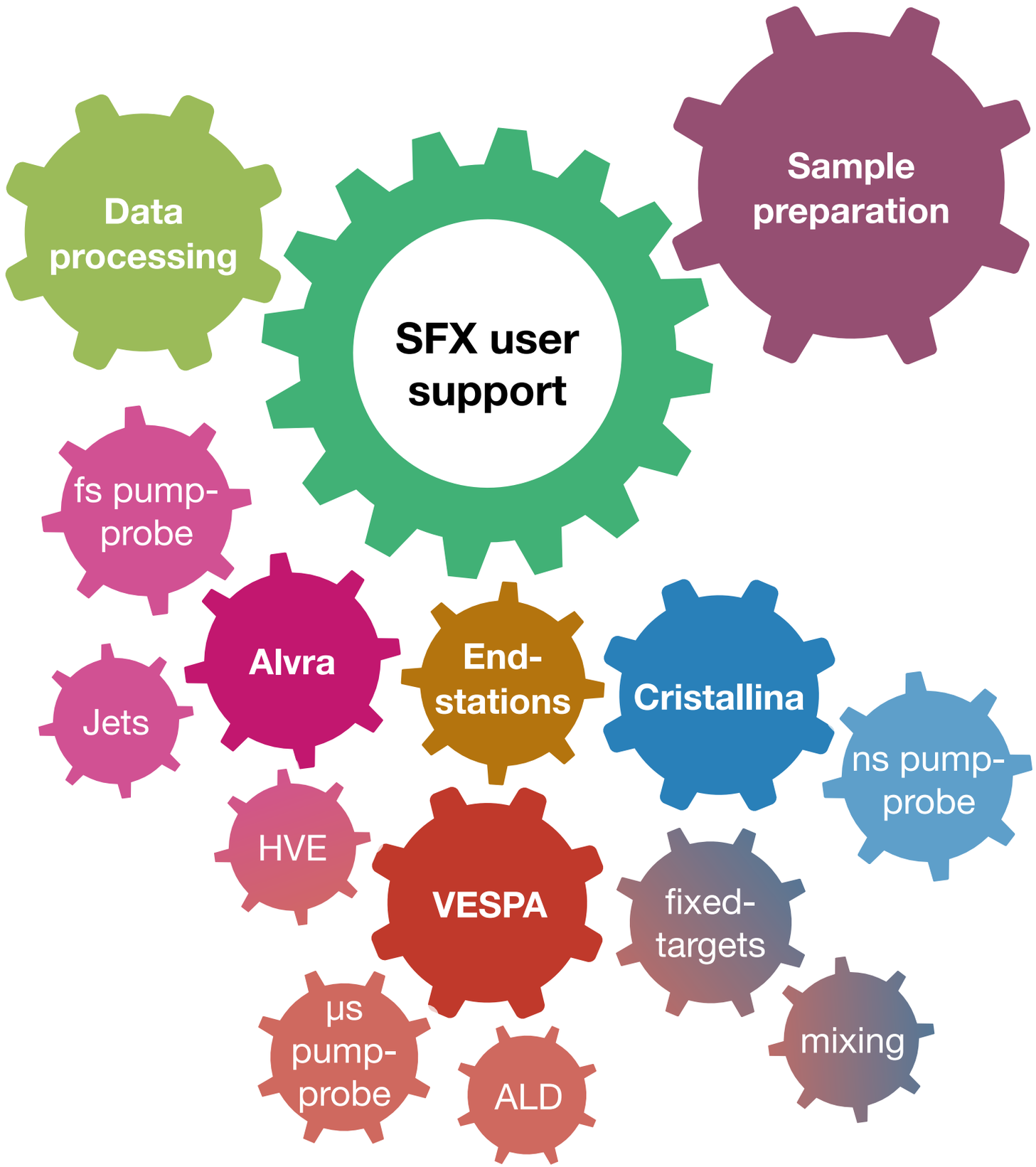
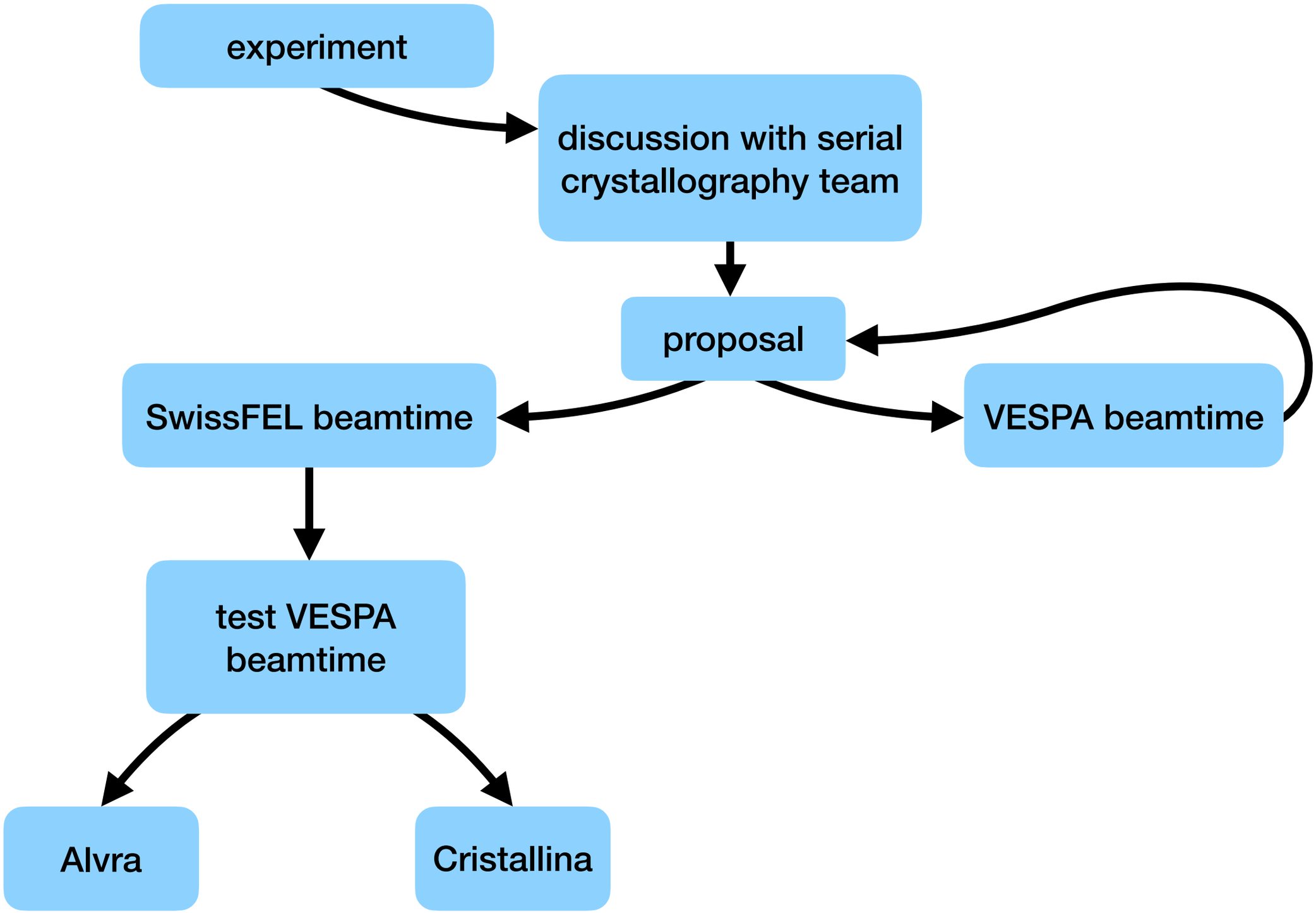
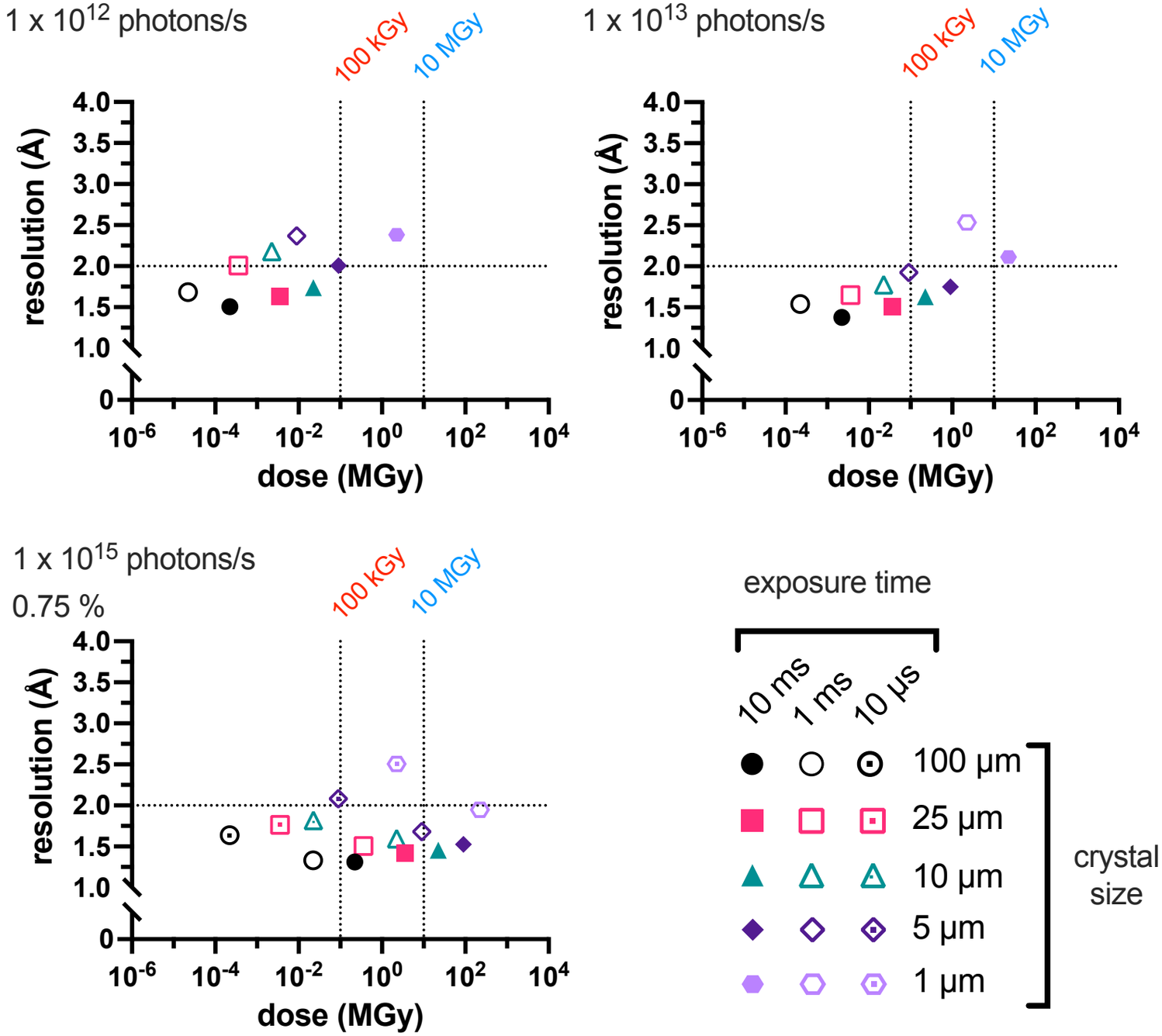
Vision for serial crystallography at PSI



Vision for serial crystallography at PSI



Opportunities and limitations of the SLS 2.0



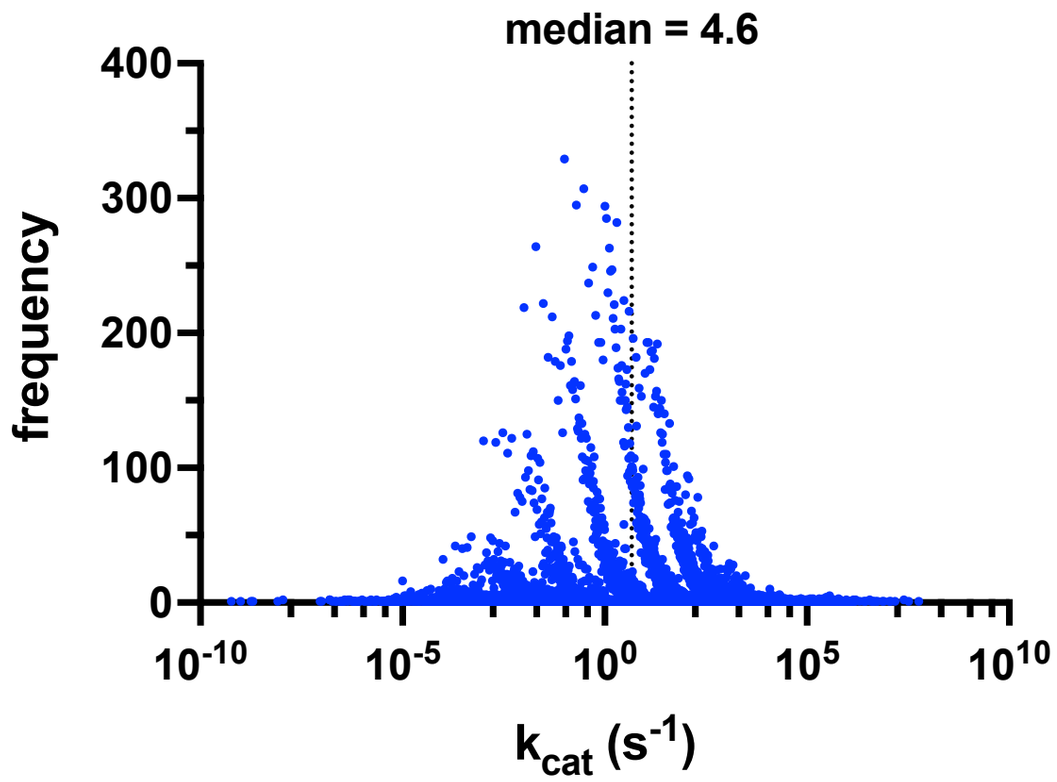
- SLS 2.0 still limited to crystal larger than 5 µm.
- BUT data could be collected in 1/1000 of the time.

https://bl831.als.lbl.gov/~jamesh/simtbx/

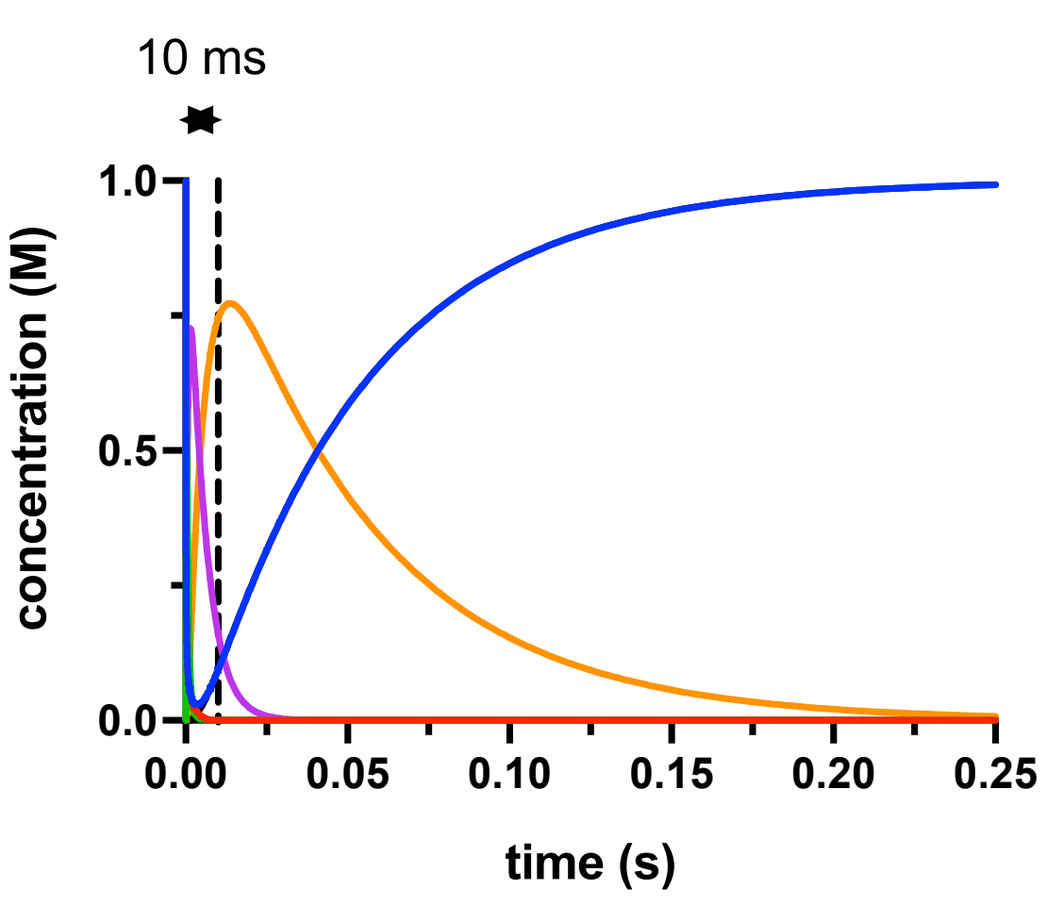
Time-resolved crystallography at the SLS 2.0

- What does a 10 µs data collection time mean for time-resolved crystallography?

$$E + S \Longleftrightarrow ES_1 \longrightarrow ES_2 \longrightarrow ES_3 \longrightarrow P + E$$

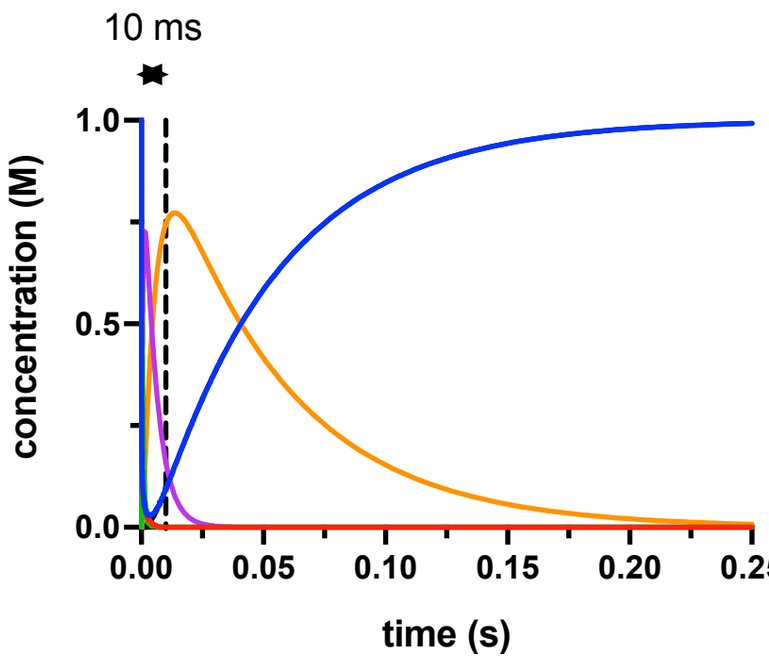


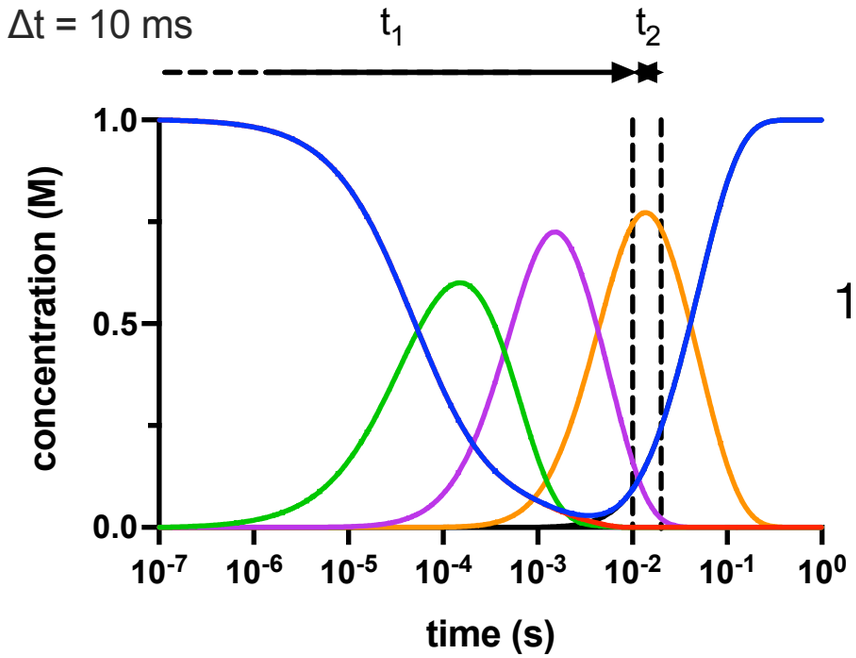
https://www.brenda-enzymes.org/



Time-resolved crystallography at the SLS 2.0

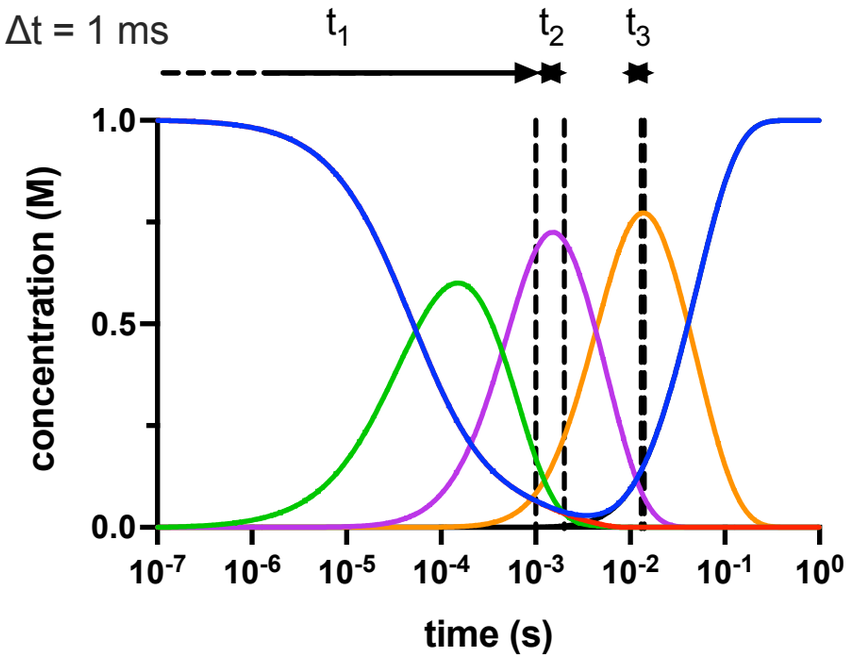
$$E + S \Longleftrightarrow ES_1 \longrightarrow ES_2 \longrightarrow ES_3 \longrightarrow P + E$$

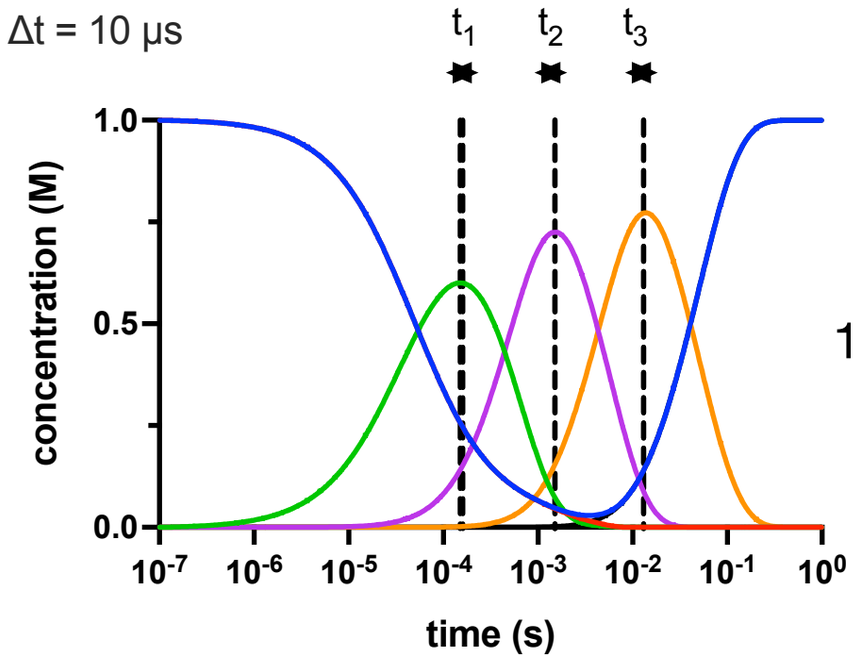




10^{12} photons/s

10^{13} photons/s





10^{15} photons/s

Summary

- There will now be two SFX endstations at SwissFEL:
  - Alvra:
    - Jets
      - fs pump-probe
  - Cristallina:
    - Fixed-tagets
    - ns pump-probe
    - mixing

- VESPA @ PXI able to act as bridge to all thing

- A team is being formed to streamline and assist users to better access and make use of these facilities.

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Celestino Padeste
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Melissa Carrillo

AIK
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Claudio Cirelli
Emma Beale

Pump Laser Group
Yunpei Deng
Philip Johnson

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Simon Gerber
Rübi Kälin

Detector Group
Aldo Mozzanica
Shqipe Hasanaj
Seraphin Vetter

Cristallina Steering Committee