Facility Update

Toshinori Yabuuchi
on behalf of SACLA

SACLA Users' Meeting 2024
Mar. 11-12, 2024@SACLA, Japan

Outline

- Updates after SACLA users' meeting 2023
  - Research highlights
  - Updates of beamlines and experimental capabilities

- Strategic plan to enlarge scientific activities at two hard X-ray (HX) beamlines
  - Current status and recent updates of HX beamline operations
  - Statistics of proposal applications at HX beamlines
  - Plans for enhancing experimental capabilities for efficient use of two HX beamlines

- Summary

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In a year after the last Users' Meeting, a collection of remarkable achievements has been published in high-profile journals

Science

- M. Maestre-Reyna et al., *Visualizing the DNA repair process by a photolyase at atomic resolution*, Science **382**, 1014 (2023).
- K. Katagiri et al., *Transonic dislocation propagation in diamond*, Science **382**, 69 (2023).

nature

- H. Li et al., *Oxygen-evolving photosystem II structures during S1–S2–S3 transitions,* Nature **626**, 670 (2024).
- A. Bhowmick et al., *Structural evidence for intermediates during O_2 formation in photosystem II*, Nature **617**, 629 (2023).
- T. Gruhl et al., *Ultrafast structural changes direct the first molecular events of vision*, Nature **615**, 939 (2023).

nature materials nature chemistry nature physics nature communications

- C. Woodahl et al., *Probing lithium mobility at a solid electrolyte surface*, Nat. Mat. **22**, 848 (2023).
- C. D. M. Hutchison et al., *Optical control of ultrafast structural dynamics in a fluorescent protein*, Nat. Chem. **15**, 1607 (2023).
- A. M. Wolff et al., *Mapping protein dynamics at high spatial resolution with temperature-jump X-ray crystallography*, Nat. Chem. **15**, 1549 (2023).
- K. Takaba et al., *Structural resolution of a small organic molecule by serial X-ray free-electron laser and electron crystallography*, Nat. Chem. **15**, 491 (2023).
- G. A. De La Peña Muñoz et al., *Ultrafast lattice disordering can be accelerated by electronic collisional forces,* Nat. Phys. **19**, 1489 (2023).
- K. Tamasaku et al., *Two-dimensional K_β-K_α fluorescence spectrum by nonlinear resonant inelastic X-ray scattering*, Nat. Commun. **14**, 4262 (2023).

PHYSICAL REVIEW LETTERS PHYSICAL REVIEW RESEARCH

- I. Inoue et al., *Femtosecond Reduction of Atomic Scattering Factors Triggered by Intense X-Ray Pulse*, Phys. Rev. Lett. **131**, 163201 (2023).
- Q. L. Nguyen et al., *Ultrafast X-Ray Scattering Reveals Composite Amplitude Collective Mode in the Weyl Charge Density Wave Material $(TaSe_4)_2I$*, Phys. Rev. Lett. **131**, 076901 (2023).
- D. Kraus et al., *Indirect evidence for elemental hydrogen in laser-compressed hydrocarbons*, Phys. Rev. Res. **5**, L022023 (2023).

“Basic Development Program” has offered the user community to establish new research capabilities in collaboration with the facility

Five projects are ongoing under BDP 2023 at SACLA

- Development of nanoscale SXFEL focusing/imaging systems using Wolter mirrors
  - H. Motoyama (Univ. Tokyo)
- Development of a wide-dynamic-range and high-frame-rate CMOS image sensor for soft X-ray IV
  - J. Miyawaki (QST)
- X-ray experiment in pulsed ultrahigh magnetic field beyond 100 T with a portable single turn coil system “PINK”
  - A. Ikeda (UEC)
- Measurement systems for biomolecular movies using X-ray free electron lasers
  - S. Iwata (Kyoto Univ.)
- Study of Magnetized Solids/Plasmas in the near and above High Energy Density regime
  - B. Albertazzi (LULI – CNRS)

Strong B-field

tr-SFX

Activity Report (Tomorrow morning)

Talks about each project by leading scientists

Breakout Sessions (Tomorrow afternoon)

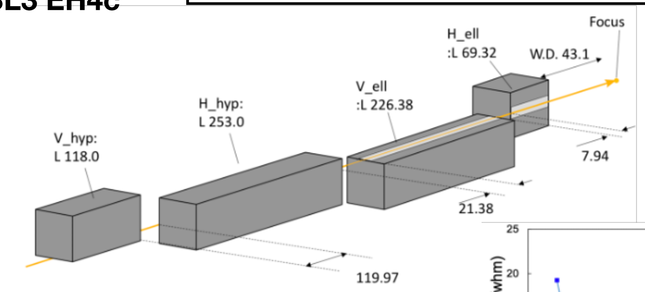
- Experiments using a strong B-field
- TR-SFX with new sample delivery scheme

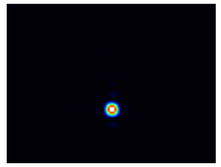
SACLA

SACLA's unique capabilities for producing and utilizing intense XFEL pulses have been further improved

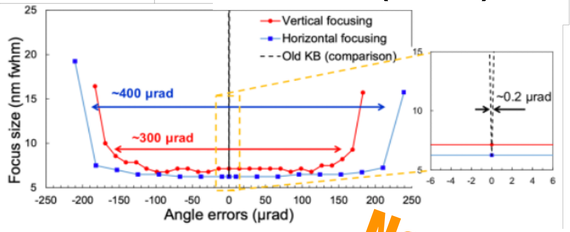
Sub-10 nm Focusing System

BL3 EH4c





6.9x7.0 nm (FWHM)



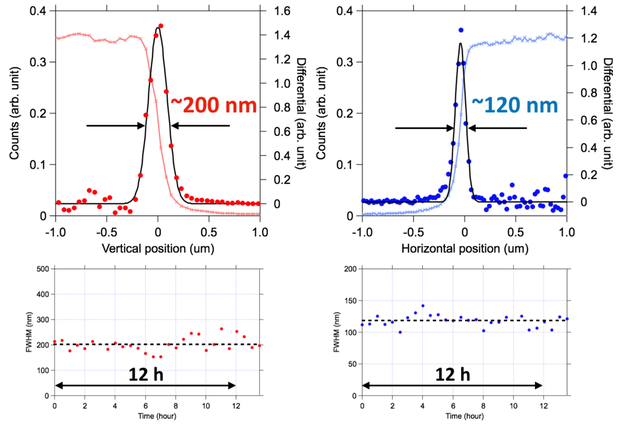
J. Yamada et al., to be published

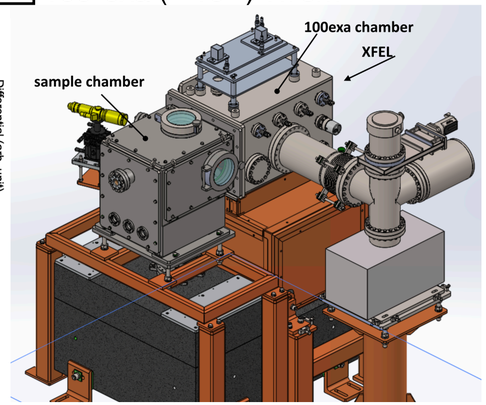
Partially supported by SACLA BDP

100exa

BL3 EH5

100-exa (= 10^{20}) W/cm^2



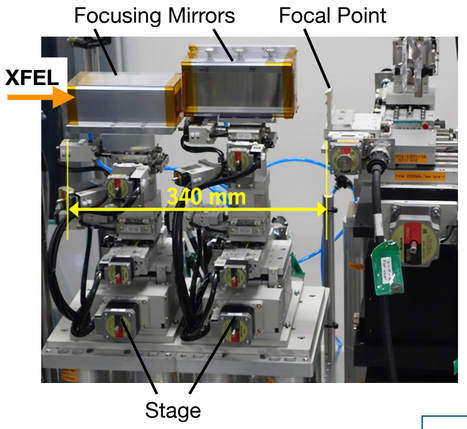


H. Yumoto et al., Appl. Sci. (2020)

Portable Nano-focusing System

New!

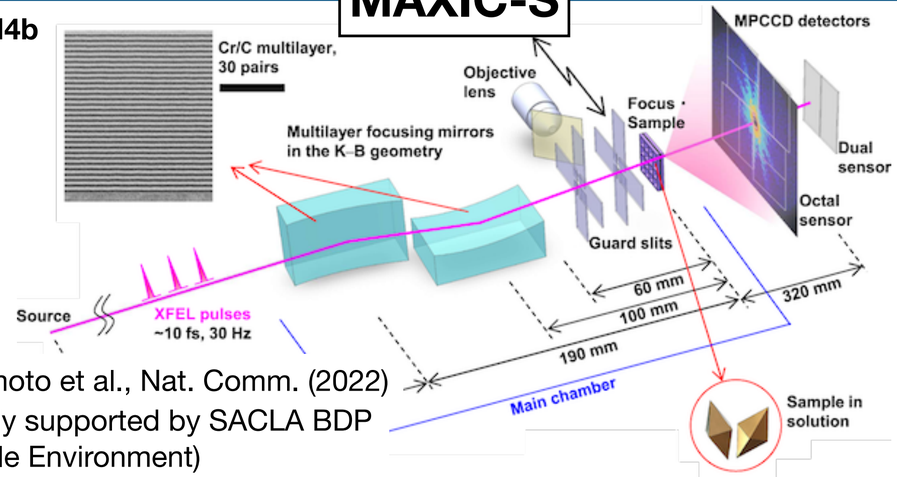
Any EHs



- Focusing of XFELs down to a few 100's nm to achieve ~10^{19} W/cm^2
- Applicable for "pump and probe" experiments with an optical laser
- Works with a large-area detector
- Available from 2024A for use at either BL2 or BL3

MAXIC-S

BL2 EH4b



H. Yumoto et al., Nat. Comm. (2022)

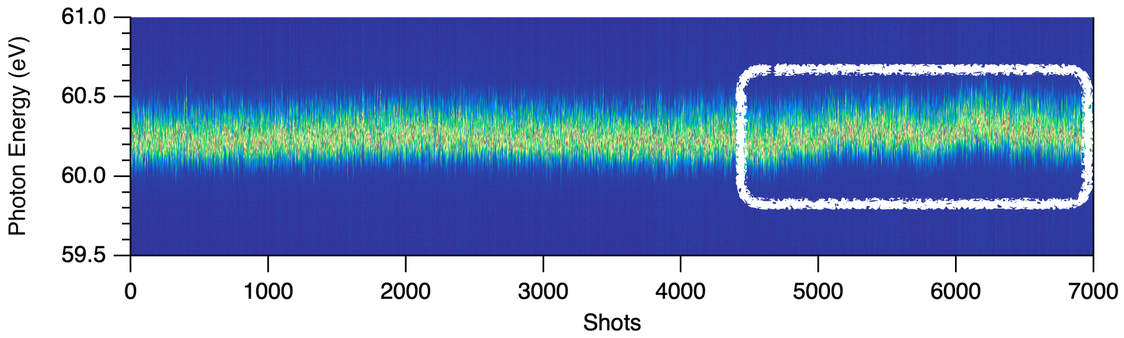
Partially supported by SACLA BDP
(Sample Environment)

Related topics will be presented in the following session.

SACLA

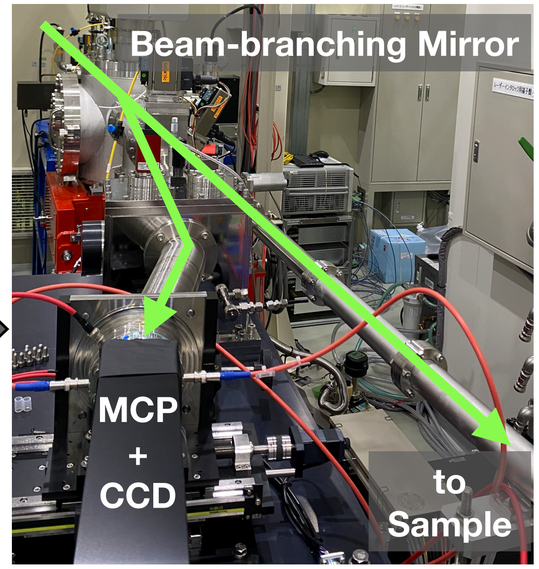
An inline spectrometer is under commissioning at SX-FEL for continuous monitoring of wavelength during user experiments

Example: Trend of photon energies at SX-FEL



- Spectra of SX-FEL sometimes fluctuate during the beamtime.
- Fluctuation of spectra can cause an issue, particularly for spectroscopy or photo-electron spectroscopy.
- Spectra of incoming pulses were able to be monitored only with a “destructive” spectrometer in the beamline.

“Non-destructive” spectrometer



Design of Spectrometer

- Grating:
  - VLS (1200 mm^{-1})
- Detector:
  - MCP Screen + VIS CCD
- Coverage of Photon Energies:
  - from ~20 eV to >150 eV
  - For 3rd/5th order harmonics, higher order diffractions are applicable

A small portion of the beam is deflected by a branching mirror similar to the timing monitor at the beamline.

This inline spectrometer can be used to provide feedback and compensate for drifts of wavelength during user experiments.

SACLA

A large area detector, 20.2 Mpixel CITIUS, will be delivered and integrated to SACLA in FY2024

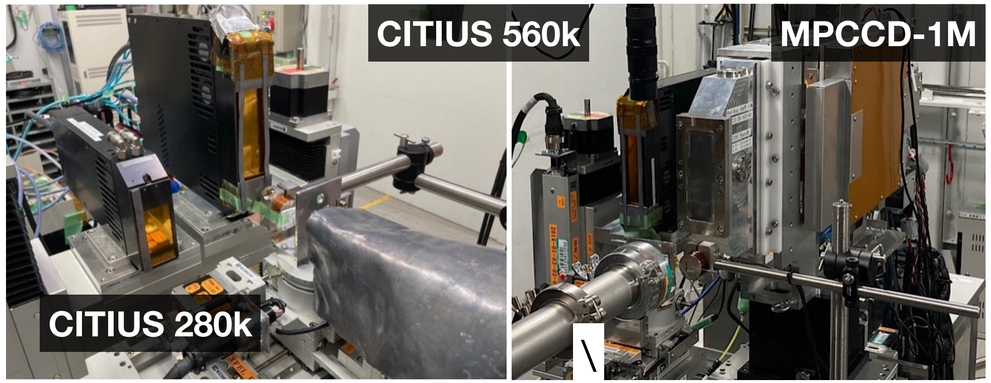
CITIUS 20.2M (comparison with MPCCD)

- Peak signal: 7x
- Noise: 1/7x
- Thickness: 2.1x

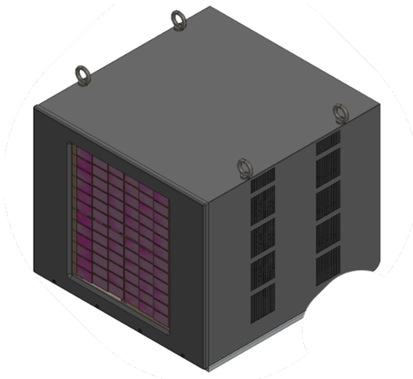
Parameters		Value		Unit
		CITIUS for XFEL (SACLA)	MPCCD (Phase III)	
Sensor	Sensor Material	Silicon	Silicon	
	Thickness	650	300	μm
	Pixel Size	72.6	50	μm
	Pixel Number	0.28	0.5	MPix/Sensor Module
	Peak Signal	17,000	2,400	phs/pix (6 keV)
	Typical Noize	25	250	e-rms
	Frame Rate	60*	60	Hz
	Data Rate	1.6**	0.06	GB/s (Digital Out)
System	Imaging Area	321 x 393	100 x 100	mm^2
	Pixel Number	20.2	4	Mpix
	Data Rate	107*	0.48	GB/s (Digital Out)

*The frame rate of CITIUS is 17.4 kHz (SR variant) and 5 kHz (XFEL variant).
**The data rate of CITIUS is the total raw data rate from the sensor. Each frame data has 16 multi-AD sampled data.

Test and application of CITIUS detector



Development of 20.2M-CITIUS detector



- Completed assembly in Feb. 2024
- Delivery and DAQ integration at SACLA EH3 in Apr. (plan)
- Feasibility test in early summer (plan)

Two posters are about CITIUS. Invited talk is also partially relevant to this new detector.

SACLA

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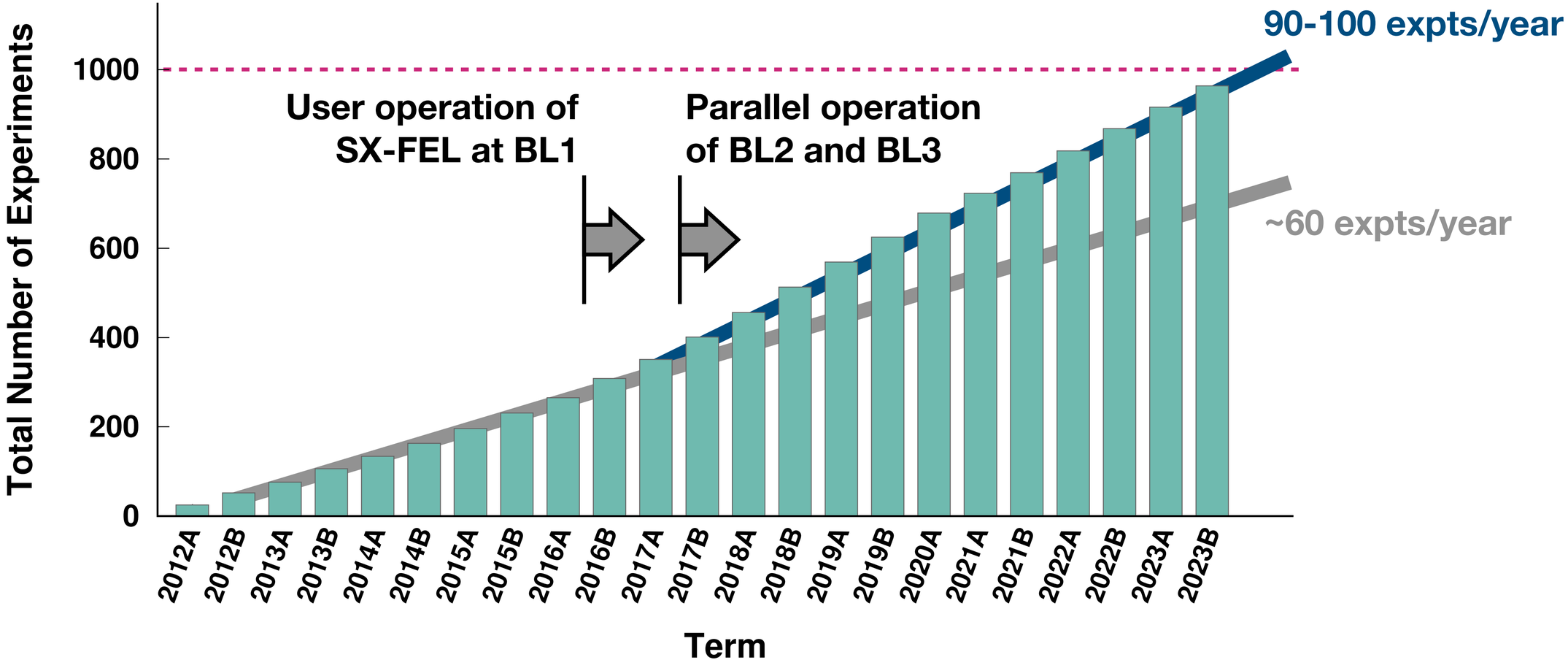
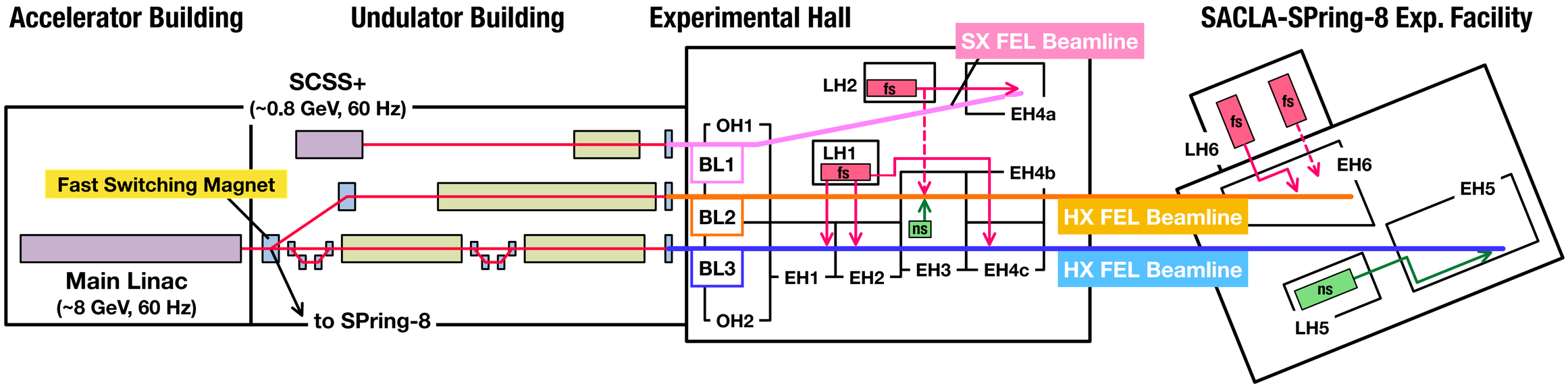
The 1000th user experiment is expected to be conducted before next summer since we started user operation in March 2012



“Parallel operation” enhanced the number of experiments to be conducted at SACLA.

SACLA

“Parallel operation” of two HX-FEL beamlines is an essence to sustain and improve the performance of research activities



- The fast switching magnet delivers the electron bunches to both HX FEL beamlines, BL2 and BL3, in a pulse-by-pulse manner equally.
- Two user experiments can be carried out simultaneously using 30 Hz rep-rated XFELs when the accelerator is operated at 60 Hz.
- Moreover, the electron beam is now injected also into SPring-8.

How can we improve the parallel operation scheme to enlarge research outcomes further?

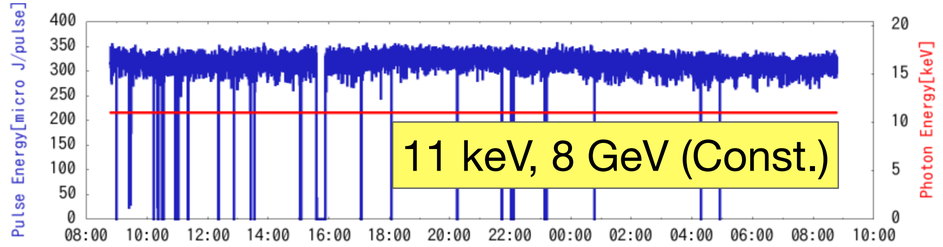
SACLA

Tuning capabilities of beam parameters in a pulse-by-pulse manner make independent optimization feasible for two HX beamlines

- “Parallel operation” has been challenging sometimes when the photon energies have a large difference between BL2 and BL3.
- Pulsed quadrupole magnets have been fully installed in the summer of 2023.
- Beam parameters, such as beam energy and envelope, can now be optimized in a pulse-by-pulse manner.

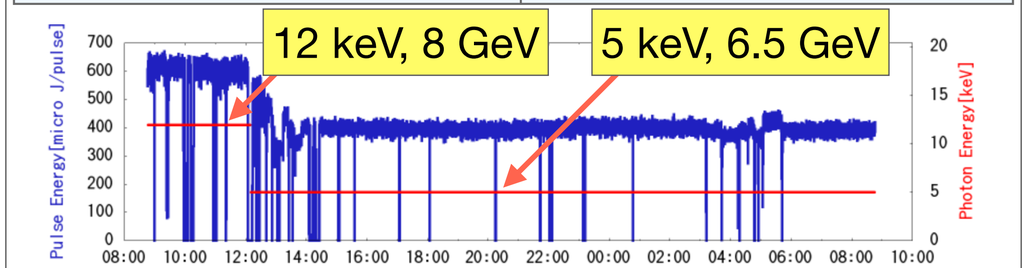
BL2

2023/10/18	SACLA Operation Status	08:47:20
Operation Mode		
BL2 UserOperation		
Hutch in Use		
BL2 EH3,4b		
Pulse Energy	Photon Energy / Wavelength	
297.2 micro J/pulse	11.0 keV / 0.112 nm	
Repetition Rate	Intensity Fluctuation in 30 shots (STD)	
30 Hz	18.5 %	



BL3

2023/10/18	SACLA Operation Status	08:46:00
Operation Mode		
BL3 UserOperation		
Hutch in Use		
BL3 EH2		
Pulse Energy	Photon Energy / Wavelength	
419.6 micro J/pulse	5.0 keV / 0.249 nm	
Repetition Rate	Intensity Fluctuation in 30 shots (STD)	
30 Hz	16.4 %	



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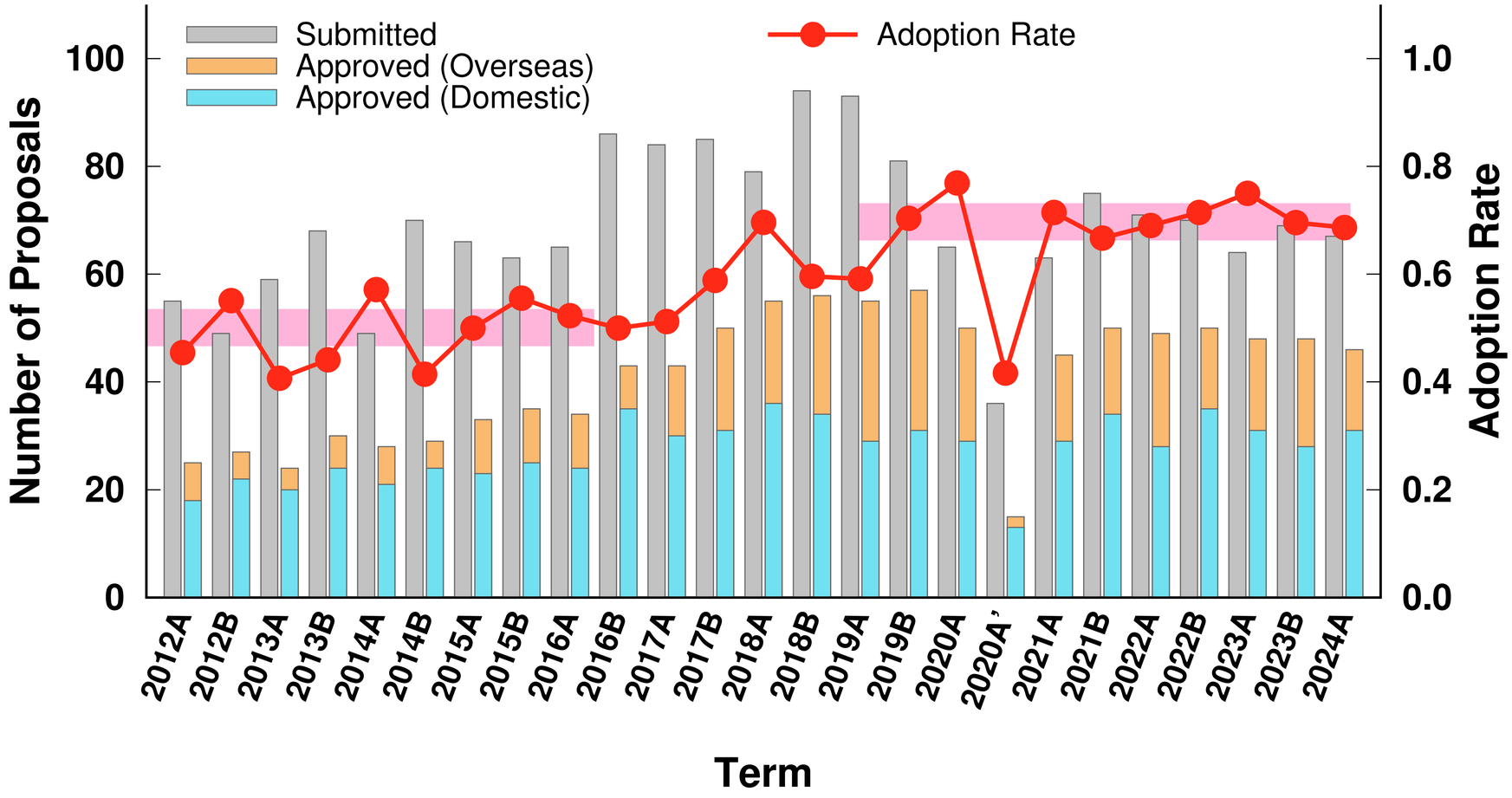
Extension of user time helps to increase the adoption rate overall, however, getting beamtime at BL3 remains highly competitive



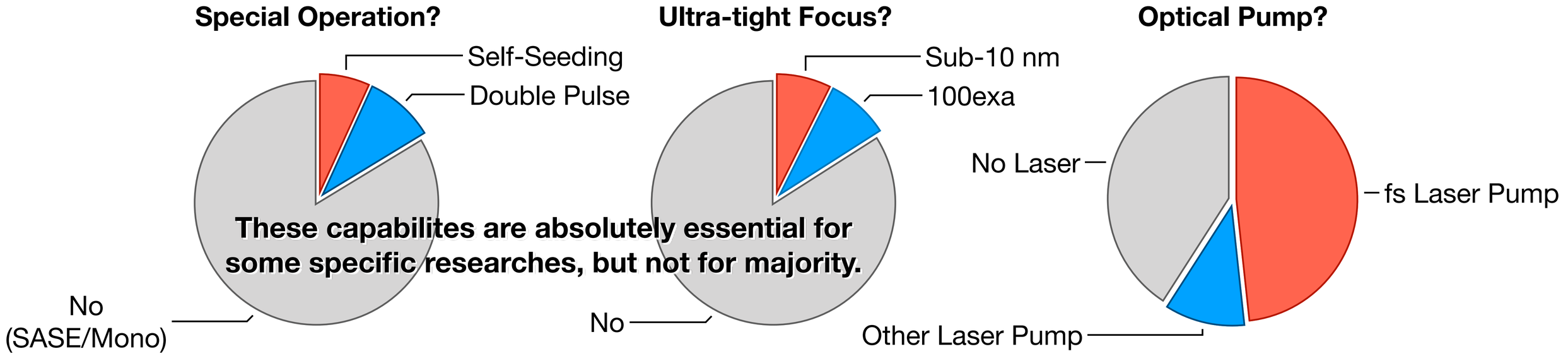
The demands for BL2 and BL3 have been largely imbalanced and caused a highly competitive situation at BL3 compared to BL2.

SACLA

Underlying reasons why users tend to submit proposals to BL3

Potential reasons (Major capabilities available at BL3 but not BL2)

1. Special operation modes of XFEL (i.e. self-seeding, two-color&double-pulse, etc)
2. Capabilities of ultra-tight focusing (i.e. sub-10 nm focus, 100exa system)
3. Ultra-fast pump capabilities using femtosecond optical laser



Shown breakdown is based on the approved proposals for BL3 in FY2022 and FY2023.

➡ **Ultra-fast pump capabilities with fs-laser to be implemented to EH3 BL2.**

SACLA

Delivery of fs-laser pulses to EH3 BL2 is in progress and will be commissioned mostly during this spring shutdown period

FY2023 (Apr. 2023 – Apr. 2024) | FY2024 (Apr. 2024 – Apr. 2025) | FY2025 (Apr. 2025 – Apr. 2026) | FY2026

Preparation

Phase I

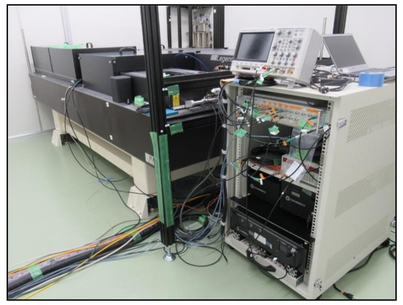
Phase II

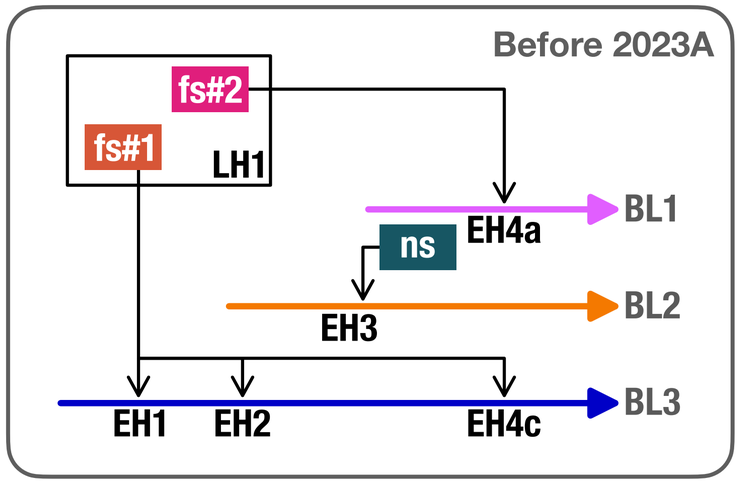
Today

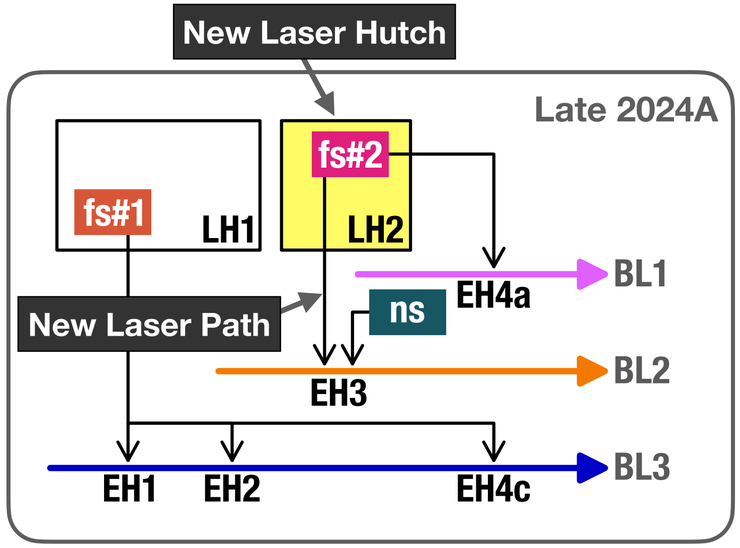
Construction of New Laser Hutch (LH2)

2023B Start LH2 Operation for User Expts. at BL1

Transport of Laser Pulse to EH3 and Commissioning of OPA System in EH3



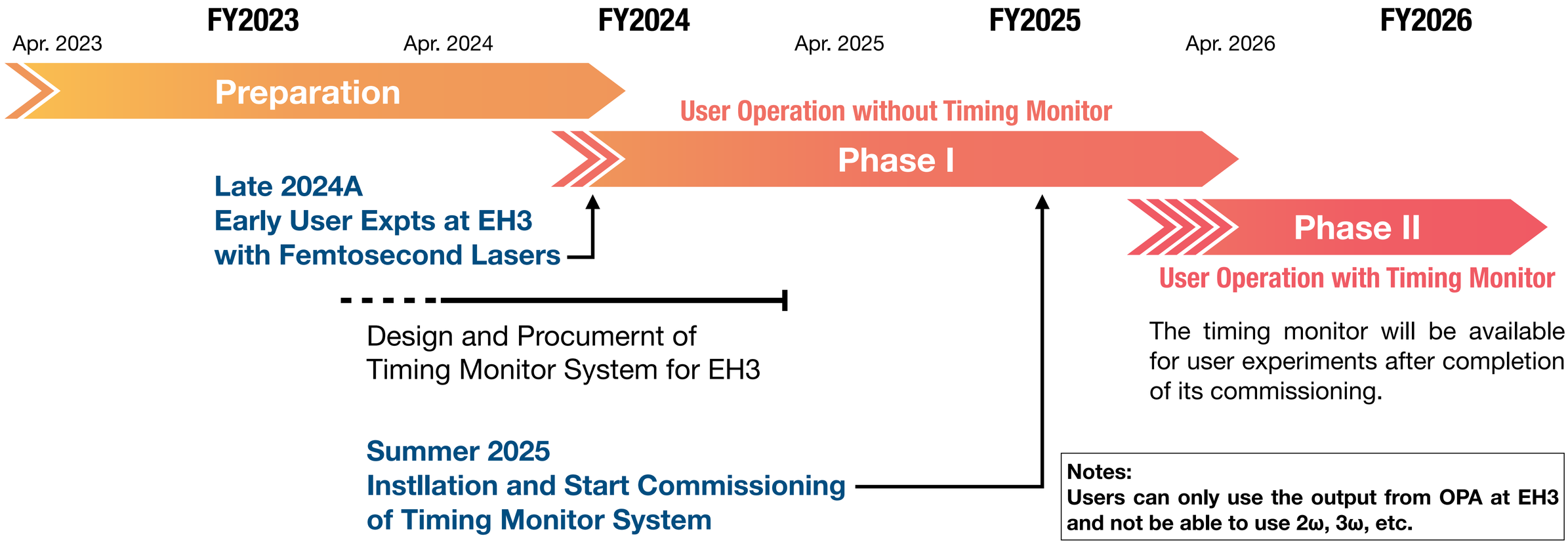




Details of synchronized laser systems are given in a poster.

SACLA

Early user experiments using fs-laser at EH3 will begin in 2024A followed by the installation of a timing monitor system in FY2025



The new laser platform at EH3 will expand the opportunities for conducting ultra-fast pump-probe experiments, contributing to an increase in research outcomes.

SACLA

Summary

- The continuous success of stable facility operation enables remarkable outcomes in high-profile publications.
- Unique capabilities have been established and improved through close collaborations between the user community and the facility.
- Further optimization of the “parallel operation” scheme is ongoing to improve the XFEL parameters and to add more flexible capabilities in the HX beamlines for enlarging the facility's productivity.

We always appreciate your thoughtful input to improve SACLA activities.

If you have technical questions to design your future experiments or would like to learn the up-to-date capabilities of our facility, please contact us.

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