LCLS Run 23 Users Town Hall

January 30th 2024

Agenda

Time (PST)	Topic	Presenter
Plenary Session - Join via Zoom >>		
9:00 am	Current LCLS Status & Plans	**Mike Dunne** Director, LCLS
9:23 am	User Executive Committee Update	**Nicholas Hartley** LCLS UEC Vice Chair
9:27 am	Accelerator Plans for Run 23	**Axel Brachmann / Tim Maxwell** Accelerator Dept. Head
9:40 am	New instrument Update (introduce breakouts)	**James Cryan & Georgi Dakovski** TMO/ChemRIXS Instrument Leads
9:50 am	Hard X-ray instruments brief overview (introduce breakouts)	**Sebastien Boutet** Experimental Operations Director
9:55 am	Data systems	**Jana Thayer** Data Systems Dept. Head
Breakout Sessions/Office Hours by Instrument		
10:10 am - 11:00am	Session 1	
	•TMO Join via Zoom >>	James Cryan
	•MEC Join via Zoom >>	Eric Galtier
	•MFX Join via Zoom >>	Leland Gee
	•qRIXS Join via Zoom >>	Georgi Dakovski
	•XCS Join via Zoom >>	Matthieu Chollet
	•ChemRIXS Join via Zoom >>	Kristjan Kunnus
	•CXI Join via Zoom >>	Meng Liang
	•XPP Join via Zoom >>	Takahiro Sato
	•TXI Join via Zoom >>	Andy Aquila

Current LCLS Status & Plans

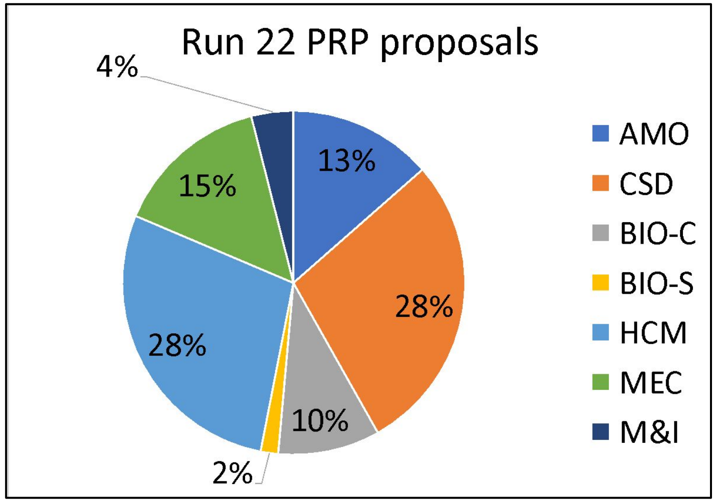
Mike Dunne

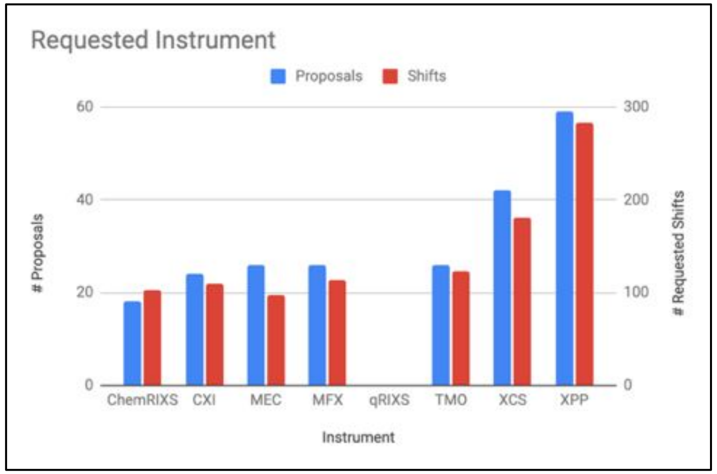
LCLS Director

January 30th 2024

LCLS user program status

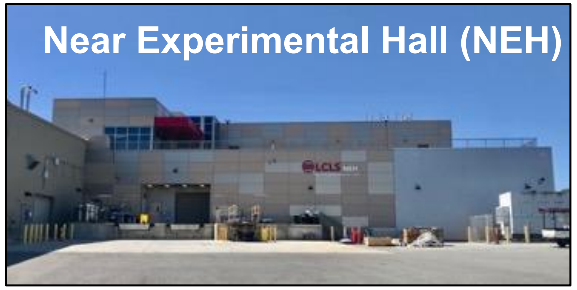
- **LCLS facility status** was greatly impacted by SLAC-wide incidents during 2023
  - Serious electrical accident at SLAC in December 2022
  - Site-wide power outage due to storms in March 2023
  - Run 21 restart delayed from January to July 2023
- **Run 22** (Jan – July 2024)
  - 177 proposals (back to historical high levels)
  - Increase in chemistry (CSD) and materials science (HCM)
  - Acceptance rate 23%, with 50 PRP experiments fielded
- **LCLS-II Project and SCRF operations**
  - Completed! (September 2023)
  - Slower-than expected initial commissioning
  - Focus on beam emittance, diagnostics to deliver useful beam
  - Instruments commissioning prior to “Early Science”

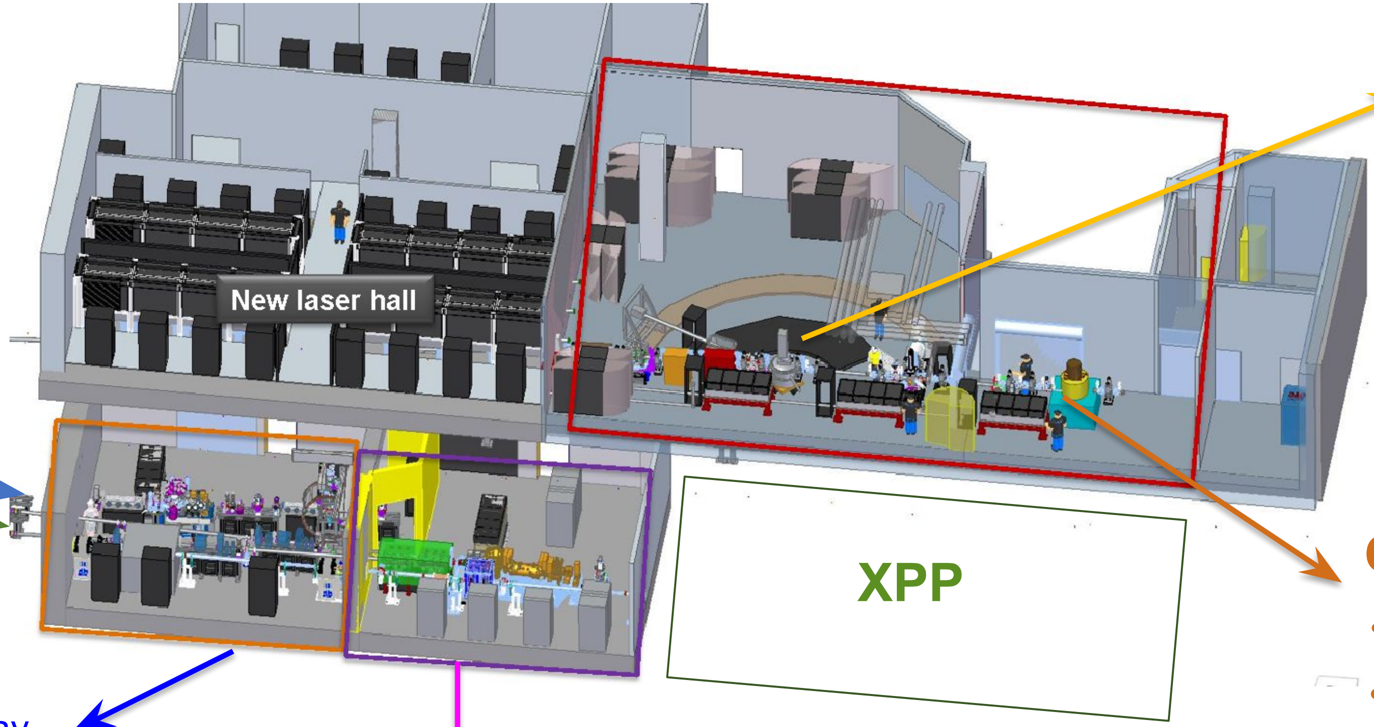




We will work to keep you better informed on our progress with the new SCRF beam

The LCLS-II instrument suite comprises 4 new instruments with 6 interaction points and 11 new endstations





qRIXS

- Mono 250 – 1600 eV
- **qRIXS** endstation
- **XPFS** endstation

ChemRIXS

- Mono 250 – 1600 eV
- **ChemRIXS** endstation
- **SurfSpec** endstation
- **k-Microscope** endstation

TMO

- High flux soft X-ray
- 250 – 2000 eV
- **MBES, MRCO** endstations
- **DREAM** endstation

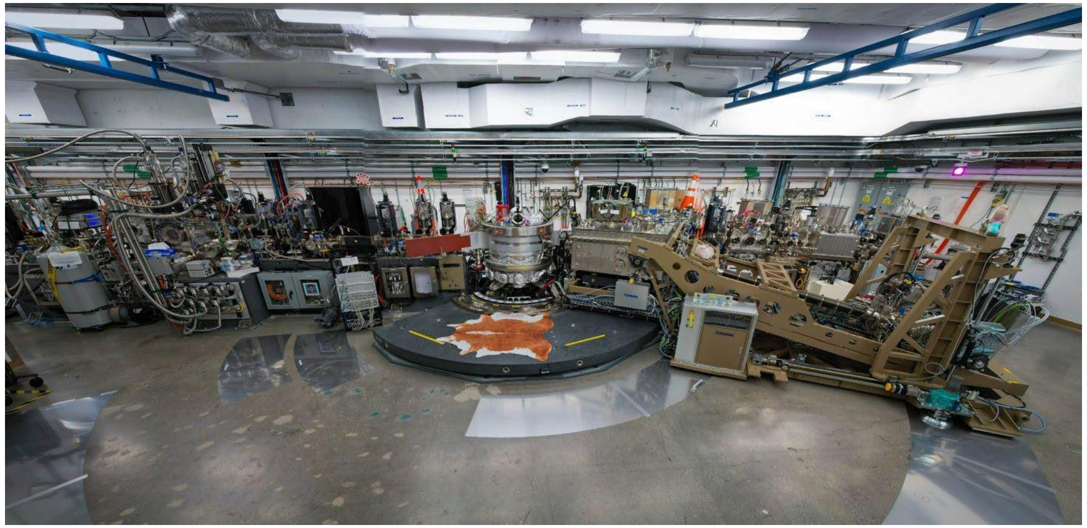
TXI

- Tender Spectroscopy endstation
- Forward scatter, nano-imaging endstation
- **Dual XFEL**, nonlinear science endstation

Phased introduction of these new endstations,
alongside the ramping of LCLS-II performance and ongoing delivery of LCLS Operations

SCRF instrument commissioning, Early Science, and PRP access for Runs 22/23/24

LCLS-II commissioning has started, using a resource- and priority- informed approach to bringing the soft X-ray endstations online:



TMO: MBES, followed by DREAM and MRCO

RIX: ChemRIXS, followed by qRIXS and user-supplied endstations (surface science endstation and k-mic)

TXI: Tender-x-ray spectroscopy, then x-ray scattering (e.g., SPI), then x-ray-pump/x-ray probe (2-beam)

Order of events:

1. **Beam Commissioning** to deliver a suitably capable and stable beam
2. **Phased Instrument Commissioning** to validate experimental capabilities
3. **Early-science** to demonstrate the science potential of LCLS-II, with broad community representation
4. **PRP experiments** follow early-science

The timeline will depend on the pace of commissioning

The next upgrade is already underway: LCLS-II-HE (High Energy)

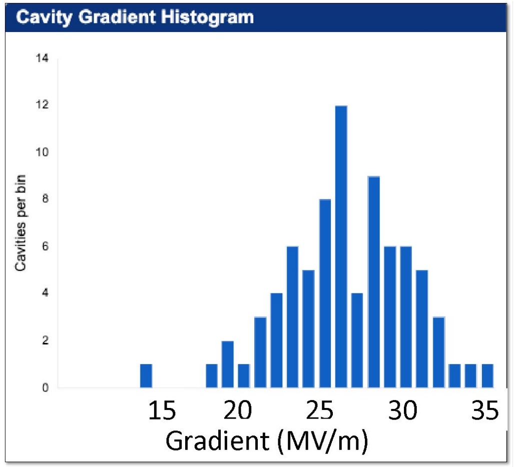
Extend the SC linac from 4 to 8 GeV, to feed a new hard X-ray instrument suite (5-13 keV)

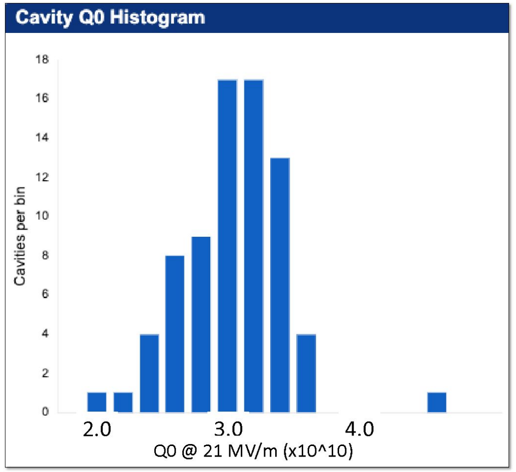
First HE cryomodule arrives at SLAC

4 (of 24) cryomodules delivered to SLAC

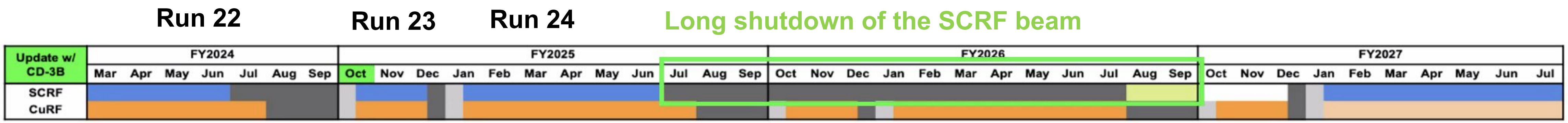
- Average Q0: 3.0×10^{10}
- Average Gradient: 24.5 MV/m (LCLS-II was 16)

74 (of 193) 9-cell cavities qualified





Timeline for initial use of the SCRF beam



Two shutdowns of the SCRF beam for installation of LCLS-II-HE equipment :

- July 2024 – Aug 2024: summer shutdown
- July 2025 – Sep 2026: long shutdown (note: the Cu linac will continue to operate)

This leaves <u>14 operating months</u> for the initial use of the LCLS-II SCRF beam prior to the long shutdown for HE

Making best use the available SCRF beamtime in Runs 22, 23, 24 …

- Demonstrate the capabilities of LCLS-II in delivering high-impact science
- Show capabilities in multiple science areas and with initial flagship instruments (TMO, ChemRIXS, qRIXS)
- Honor our commitments with regard to user-supplied endstations / existing programs
- Defer experiments that can make good use of Cu-Linac during the long shutdown

User Executive Committee Update

Nicholas Hartley
LCLS UEC Vice Chair

January 30th 2024

LCLS User Executive Committee

The UEC is here to represent you!

We meet monthly with LCLS Management to communicates the needs and desires of users regarding:

- LCLS operating policies
- use of LCLS
- user support
- other issues of concern to users

Current Members & Minutes: https://lcls.slac.stanford.edu/lclsuo

Please feel free to contact the LCLS UEC members with any suggestions or questions!

lcls-uec@slac.stanford.edu

User Meeting: Call for workshops

2024 LCLS/SSRL Users' Meeting: 23-27 September (tentative)

We are seeking suggestions for full- or half-day workshops

Deadline: March 31st

E-mail suggestions to LCLS UEC (lcls-uec@slac.stanford.edu) or User Office (lcls-user-office@slac.stanford.edu)

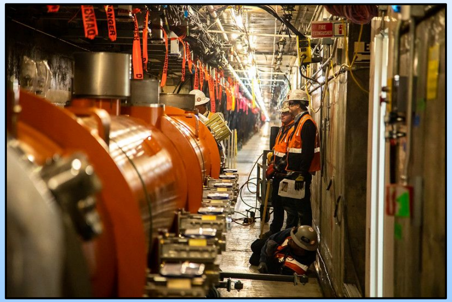
LCLS Run 23 Users Town Hall
Accelerator Update

Axel Brachmann, Tim Maxwell, Yuantao Ding

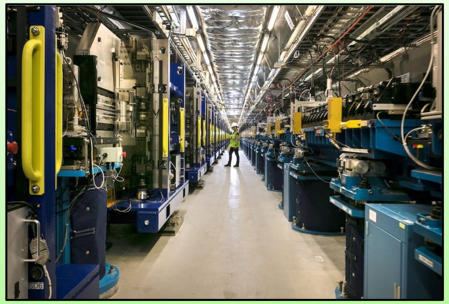
January 30th 2024

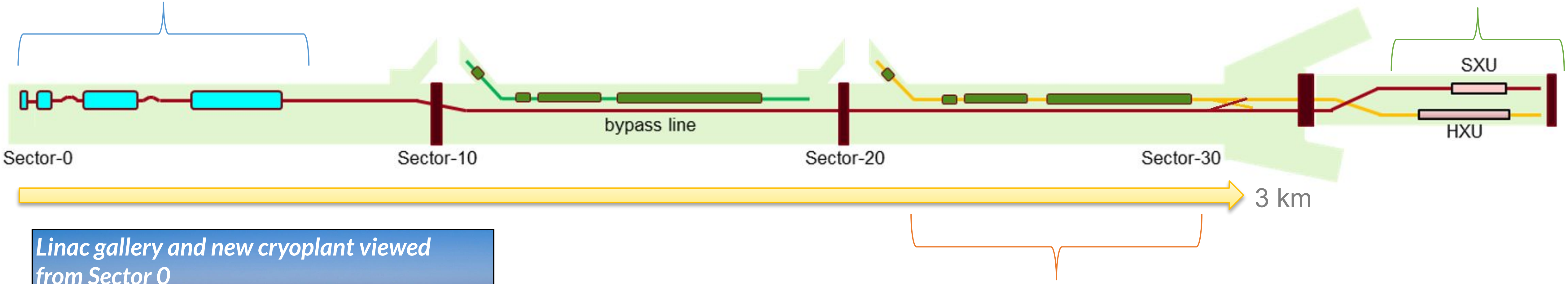
LCLS NC/SC Linac FEL Complex

Superconducting Linac
4 GeV, High
rep-rate, CW RF



Soft and Hard X-ray Variable Gap Undulators (VGUs)

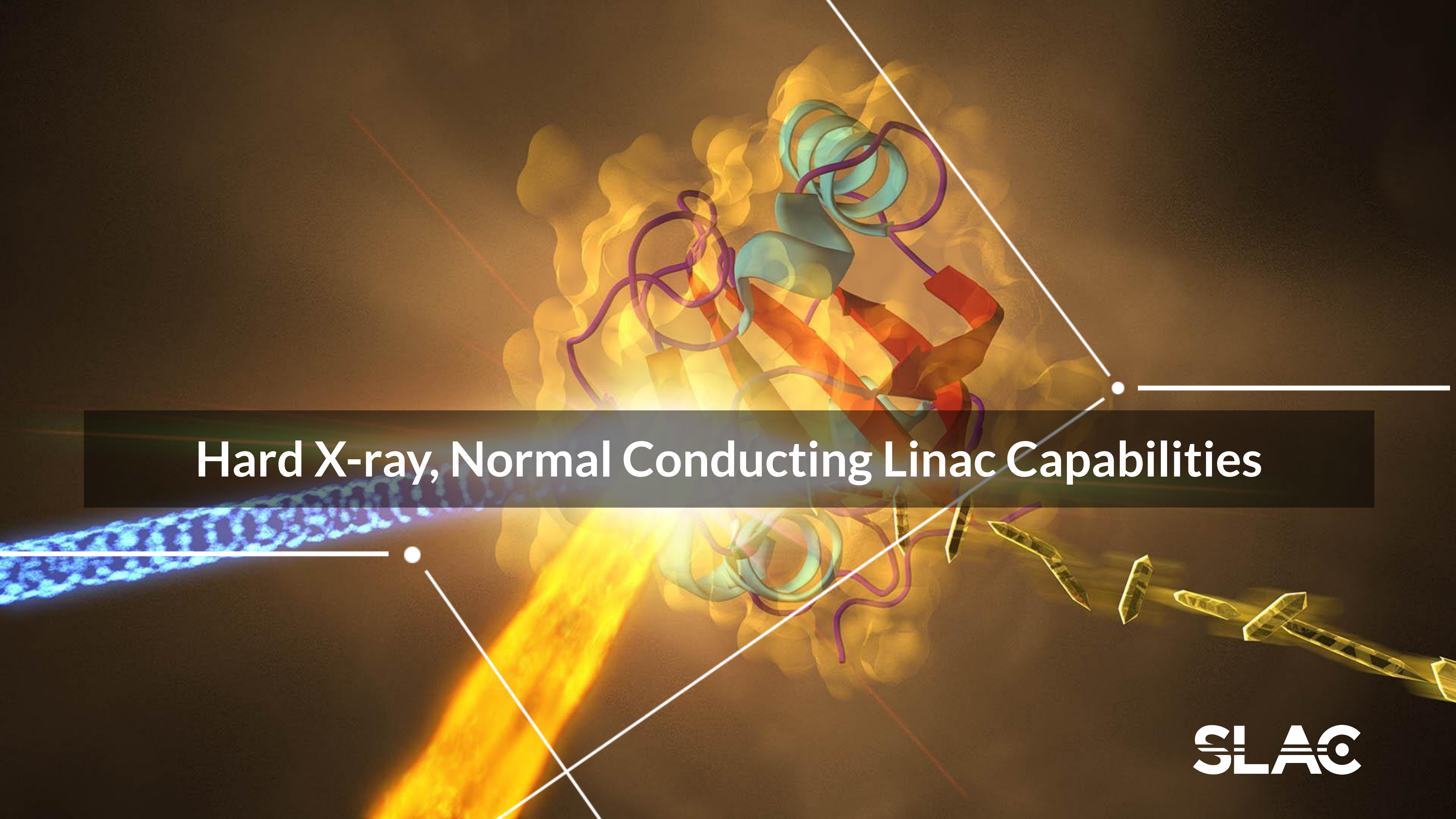





Linac gallery and new cryoplant viewed from Sector 0

Normal Conducting Linac
3.5-17 GeV,
120 Hz Pulsed RF

Hard X-ray, Normal Conducting Linac Capabilities



HXR single-pulse SASE w/ NC Linac

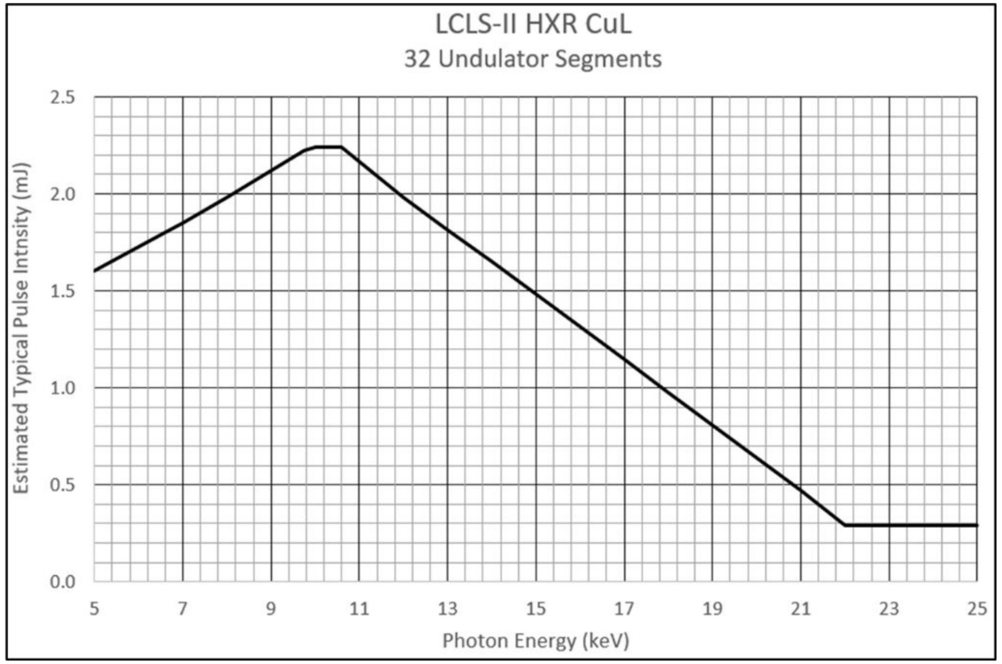
Beam Parameters	Symbol	Cu-HXU x-rays		Unit
		□ω_{max}	□ω_{min}	
Photon Energy	$\hbar\omega$	**25000**	**1000**	**eV**
Fundamental wavelength	λ_r	0.5	12.4	Å
Final linac e- energy	γmc^2	16.5	3.5	GeV
FEL 3-D gain length	L_G	4	1	m
Peak power	P	20	80	GW
Pulse duration range (FWHM)		10 – 50		fs
Nominal pulse duration (FWHM)	$\Delta\tau_f$	**~30**		**fs**
Max Pulse Energy*	U	**0.6**	**2**	**mJ**
Photons per pulse*	$N\gamma$	0.15	14	10^{12}
Peak brightness*	$B_{pk,\,SASE}$	7800	425	10^{30} §
Average brightness (120Hz)*	$\langle B\rangle$	280	16	10^{20} §
SASE bandwidth (FWHM)	$\Delta\omega/\omega$	30	2	eV
Photon source size (rms)	σ_s	8	20	µm
Photon far field divergence (FWHM)	$\Theta_{FWHM,x,\infty}$	1	12	µrad
Max. Beam Rate	φ_{FEL}	**120**		**Hz**
Avg. x-ray beam power	P_x	0.07	0.24	W
Linear Polarization (100%)	$\langle P\rangle$	Vertical		

*Assuming nominal duration and undulator strength

§Brightness units are photons/sec/mm^2/mrad^2/0.1%-BW

High photon energy (to 25 keV) and pulse energy (0.5-2mJ)

Varies w/ duration, energy, beamline transmission, etc.



SLAC

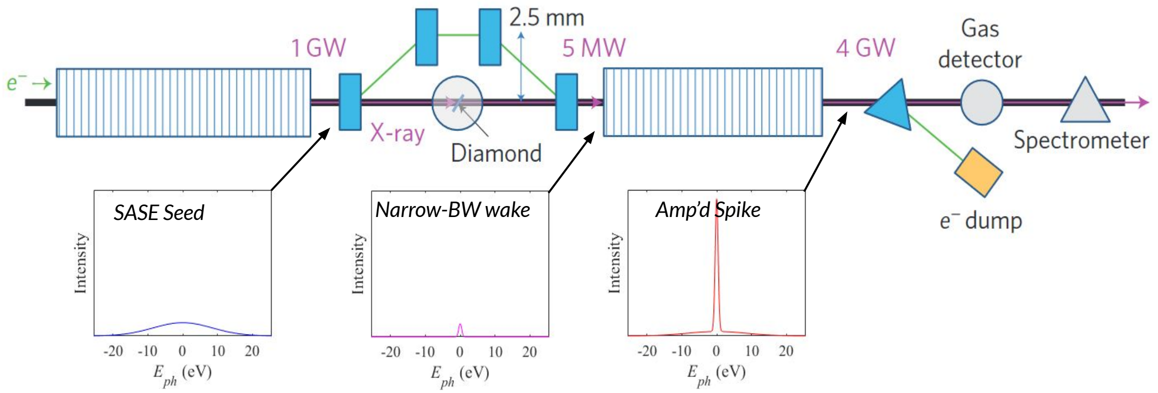
https://lcls.slac.stanford.edu/machine/parameters

Hard X-ray Self-Seeding (HXRSS)

Spectral brightness enhancement for narrow bandwidth experiments

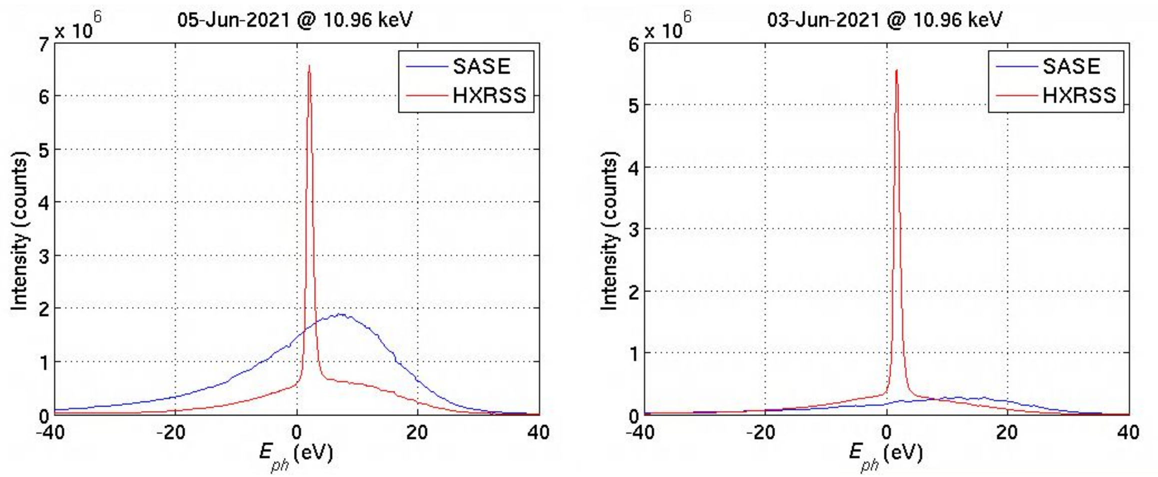
- Updated for LCLS-II *vertically* polarized HXU (90° rotation of crystal optics)
- 3-6x spectral brightness at sample vs. SASE

Photon energy	4.5 – 11 keV
Bandwidth (FWHM)	**0.35 – 1.5 eV**
Max pulse energy	0.2 – 0.5 mJ
Duration	30 fs



Initial SASE passes diamond wake monochromator, narrow BW amplified in 2nd half of undulator

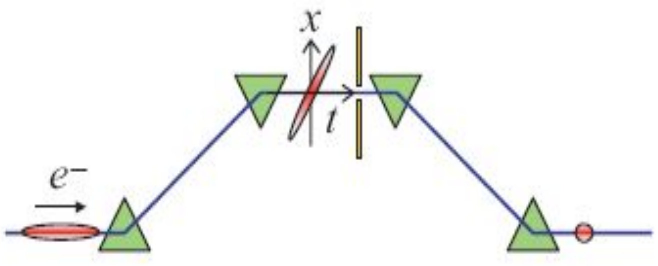
Full SASE vs. HXRSS average spectra at 11 keV



Short Pulses

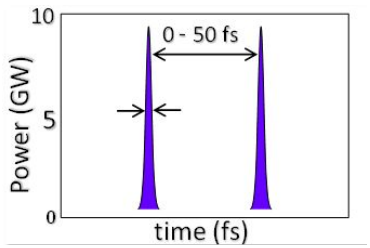
- **~5-10 fs HXR pulses readily achievable** with corresponding reduction in pulse energy (change of charge, use of "slotted foil")

- Methods are available for **< 1 fs HXR pulses**, approaching single SASE spike limit



Slotted foil inserted in beam to spoil lasing in time

Make short single or double pulses



Technique	Min Pulse Duration	Energy/Pulse	single-spike rate
Slotted foil / optics / taper	400 as	5 uJ (76% fluct.)	65%
Non-linear bunch compression	200 as	10 uJ	45%

Discuss special requirements with your LCLS POC

Advanced Multi-Pulse/Color Modes

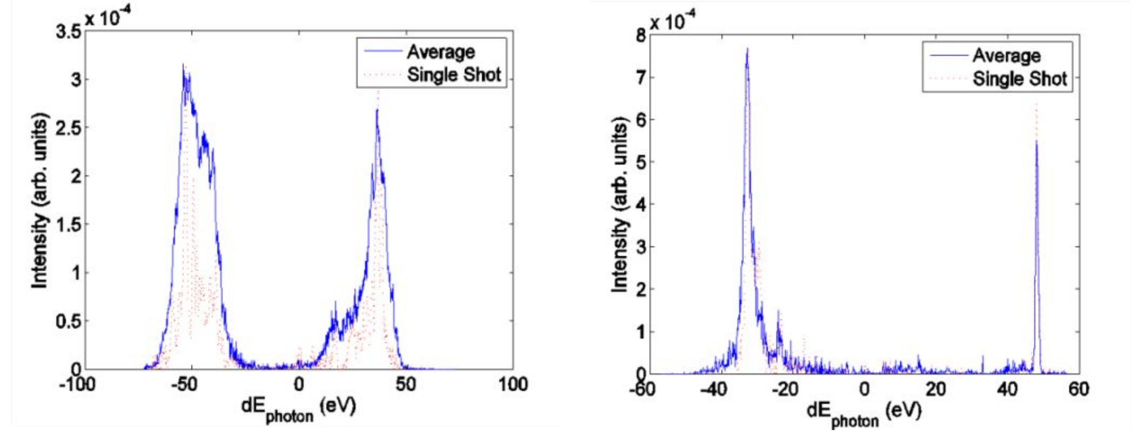
Multiple accelerator-based means for x-ray pump, x-ray probe on variety of time scales

One electron bunch:

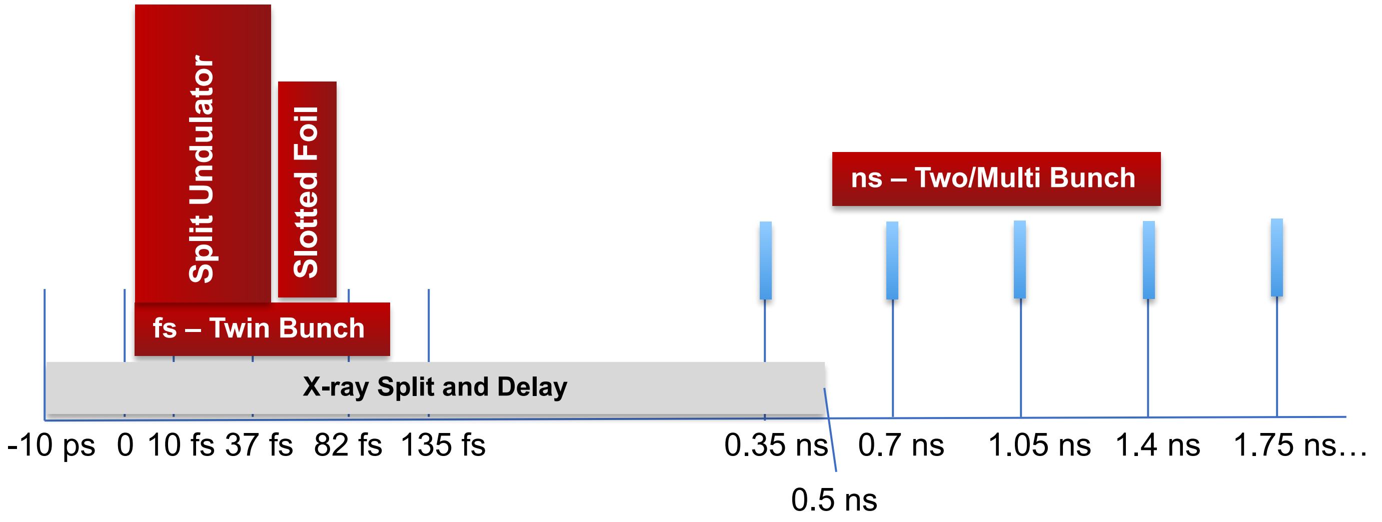
- Double slotted foil

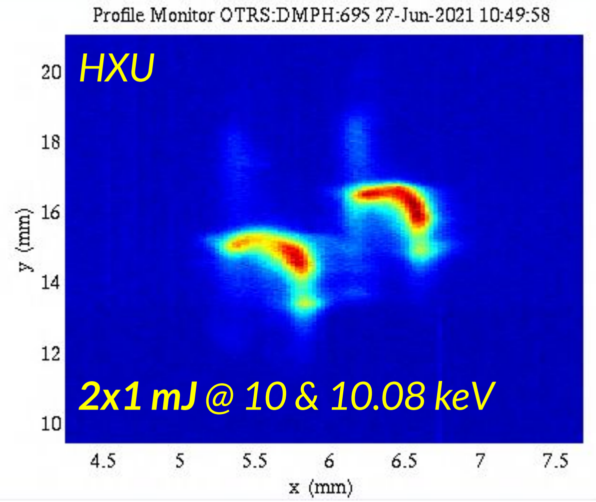
Two electron bunches:

- fs spacing: Injector laser pulse splitting ("twin bunches")
- ns spacing: Multiple laser pulses at cathode ("two/multi bunches")



Two-bunch XTCAV Images (ns spacing)





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Advanced Multi-Pulse/Color Modes

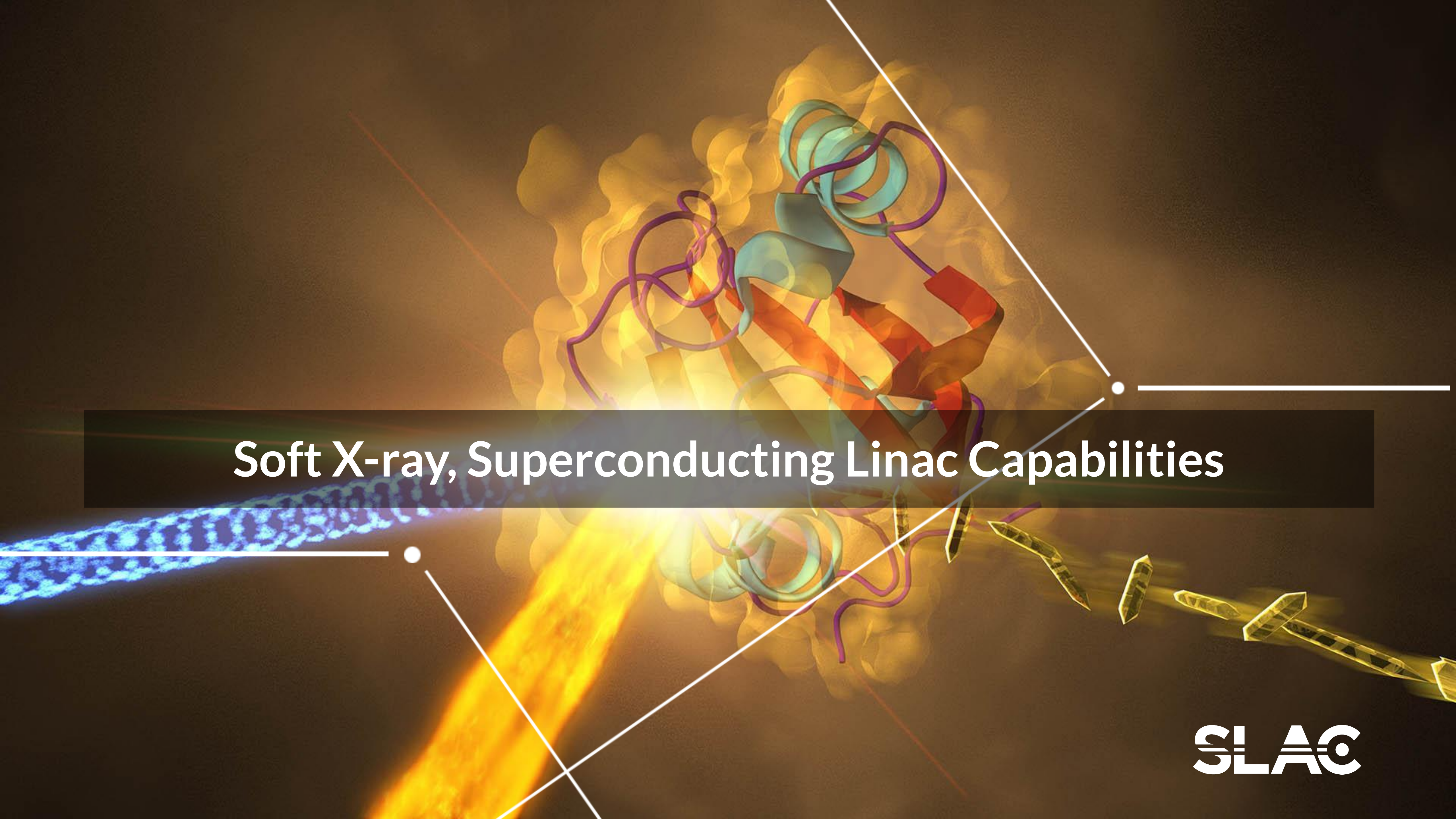
Multiple accelerator-based means for x-ray pump, x-ray probe on variety of time scales

Technique	Pulse Separation	Pulse Duration	Energy Separation	Max Energy/Pulse
Split Undulator SASE	0 - 30 fs	15 fs	Up to factor 1.2 ratio in photon energies	40 uJ (25 fs pulse duration)
Double Slotted Foil	7-20 fs	~ 10 fs	+/-1.5%	100-200 uJ
Twin Bunches				
Two SASE Pulses	0 - 125 fs	~ 10 fs	0.2-2%	0.3 mJ (20 fs duration)
With slotted foil (shorter pulses)	+/- 50 fs	~5-10 fs	~2%	40 uJ
Two-(multiple) bunch				
Two bucket	350 ps increments, up to 120 ns	20 fs	~ 1%	0.5-1 mJ (30 fs duration SASE)
Multi bucket (4 or 8 bunches)	Two trains of 4 pulses. 700 ps between each pulse in the same train.	20 fs	~ 1%	To be tested

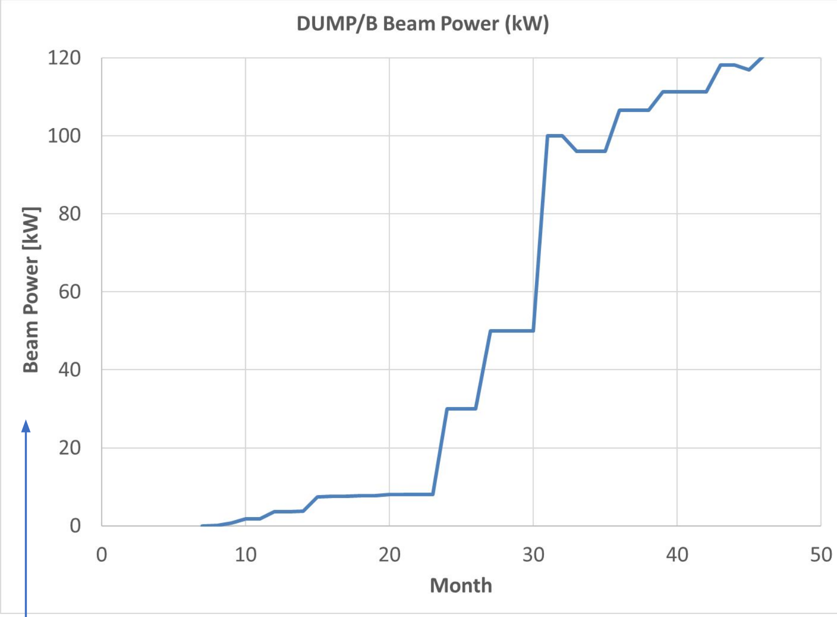
Discuss special requirements with your LCLS POC

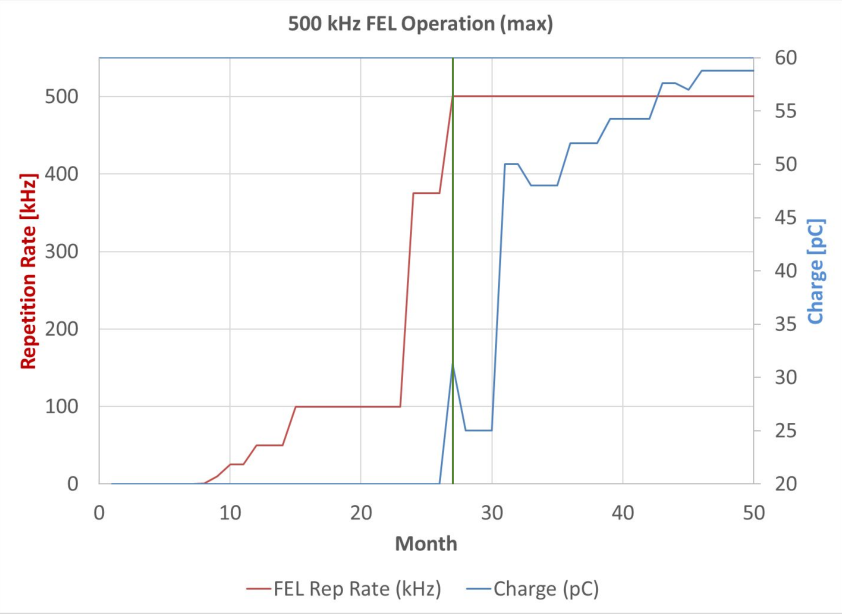
SLAC

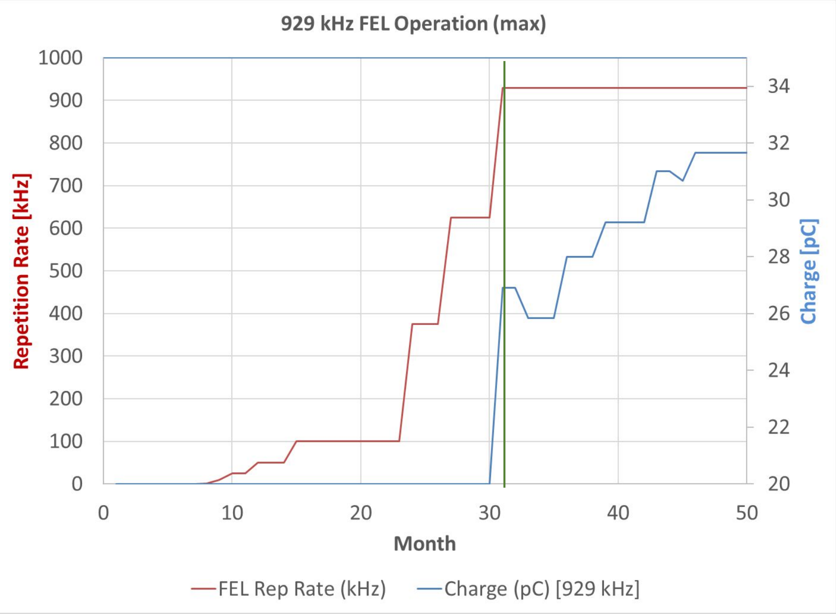
Soft X-ray, Superconducting Linac Capabilities



SC Linac Rate Ramp-Up







- Beam Power related to [Repetition Rate * Charge], limited to 120 kW max at final beam dumps
- Beam losses & undulator irradiation are major potential issues/hazards
- Facility has 2 year plan for beam/radiation monitoring with a gradual increase of power
- Goal is to ramp up to 33 kHz in Run 22, ~ 10 kW of beam power

Run 23 General Parameters: 4 GeV , *33 kHz*, 50 pC

SXR single-pulse SASE w/ SC Linac

Beam Parameters	Symbol	SC-SXU x-rays			Unit
		$h\omega_{max}$	$h\omega_{nominal}$	$h\omega_{min}$	
Photon Energy	$h\omega$	**1300**	**800**	**200**	**eV**
Fundamental wavelength	λ_r	9.5	15.5	62.0	Å
Final linac e- energy	γmc^2	3.5-4.0			GeV
FEL 3-D gain length	L_G	TBD			m
Peak power	P	3	2.5 - 7	8	GW
Pulse duration range (FWHM)		20 – 40			fs
Nominal pulse duration (FWHM)	$\Delta\tau_f$	**20**			**fs**
Max Pulse Energy*	U	**0.06**	**0.05 - 0.14**	**0.16**	**mJ**
Photons per pulse*	$N\gamma$	0.28	0.4 - 1.1	5.0	10^{12}
Peak brightness*	$B_{pk, SASE}$	20	8.6 - 24	1.7	10^{30} §
Average brightness* **(@33 kHz)**	$\langle B \rangle$	137	57 – 161	12	10^{20} §
SASE bandwidth (FWHM)	$\Delta\omega/\omega$	4	3	3	eV
Photon source size (rms)	σ_s	TBD			µm
Far field divergence (FWHM)	$\Theta_{FWHM,x,\infty}$	TBD			µrad
Max. Beam Rate	φ_{FEL}	1,000 – 40,000 **			Hz
Avg. x-ray beam power **(@33kHz)**	P_x	2.0	1.7-4.6	5.3	W
Linear Polarization (100%)	$\langle P \rangle$	**Horizontal**			

*Assuming nominal duration and undulator strength

§Brightness units are photons/sec/mm²/mrad²/0.1%-BW

**** Highest rate will depend on accelerator protection and beamline acceptance**

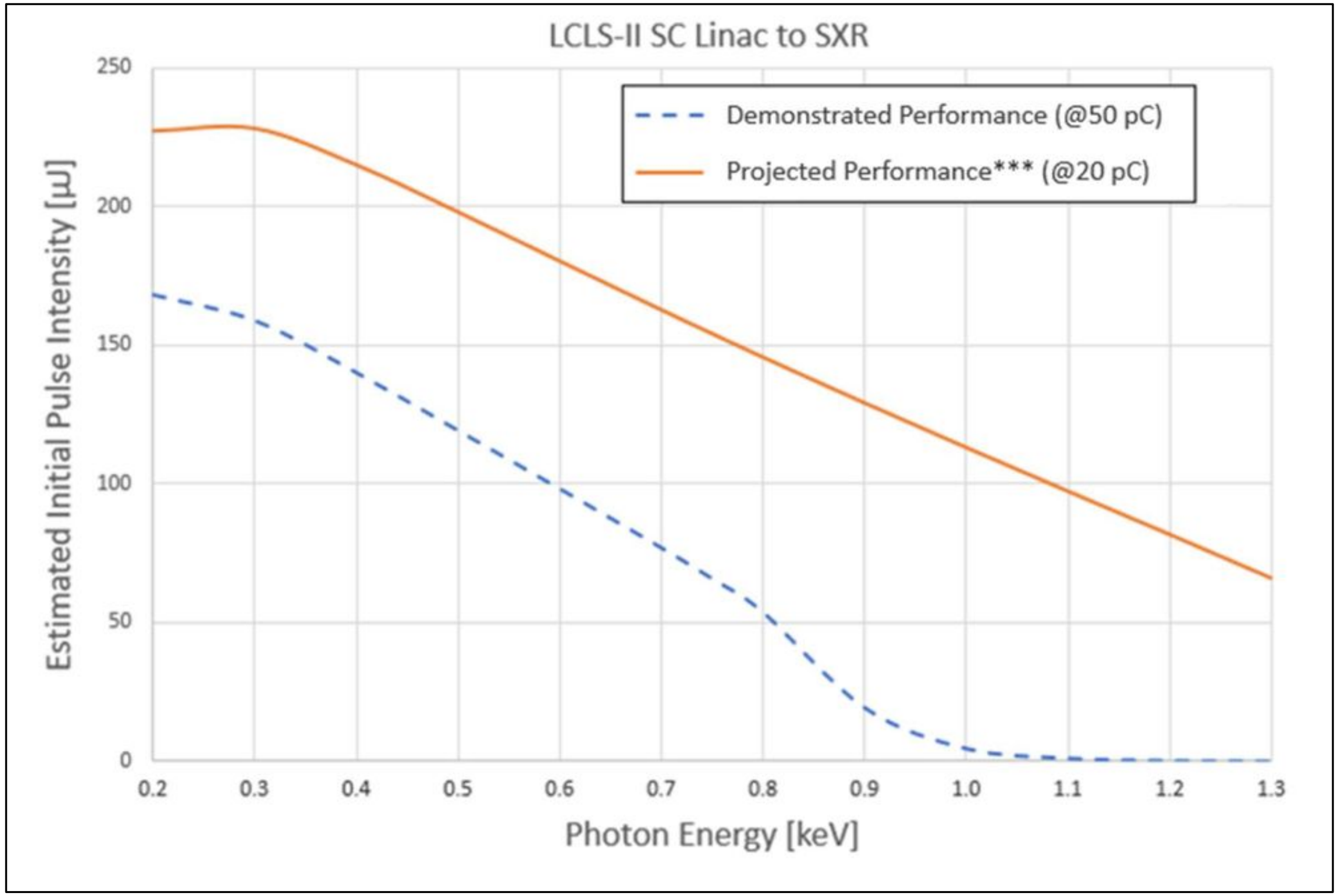
Pulse energies of >100 µJ in <40 fs

https://lcls.slac.stanford.edu/machine/parameters

SLAC

SC Linac Beam Quality Ramp Up

- FEL performance to improve in Run 22



*** Projected SC linac parameters depend on optimization of initial demonstrated performance

Shorter Pulses

- Laser heater shaping (few fs pulses) and XLEAP (sub-fs pulses) demonstrated with NC Linac
- Capability to be extended to SC linac as performance improves

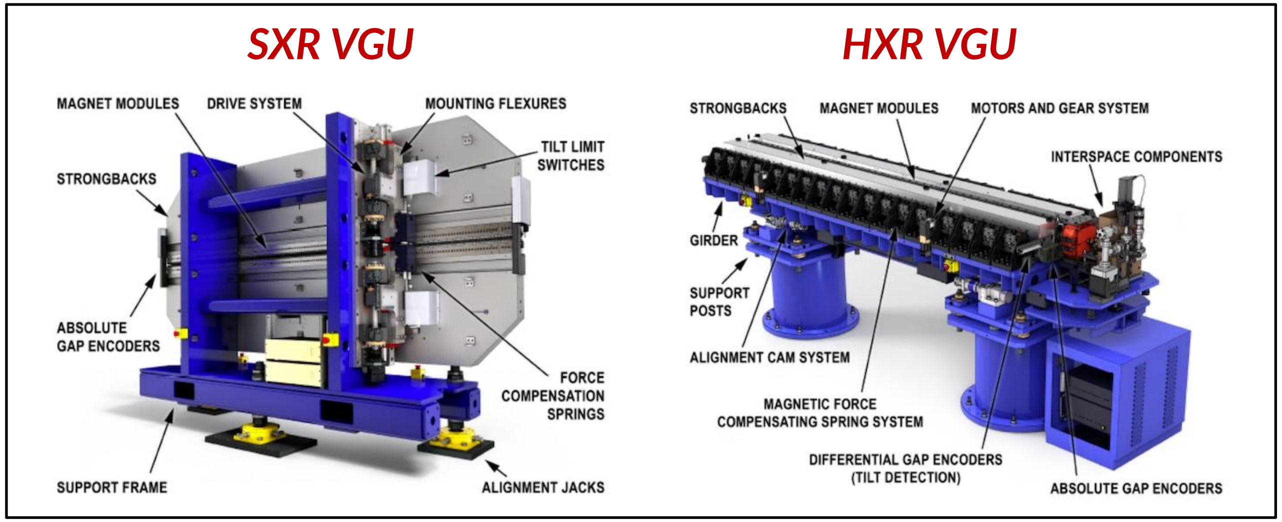
Technique	Min Pulse Duration	Linac (Max Rate)	Energy range	Energy/Pulse	Single Spike rate
Laser Heater Shaping	< 8 fs	**SC (1 kHz+)**	**SXR**	10-20 uJ	TBD
XLEAP	TBD	**SC (1 kHz+)**	**SXR**	TBD	TBD

fs and sub-fs pulses to be demonstrated w/ SC linac during Run 22

Photon Energy Scanning

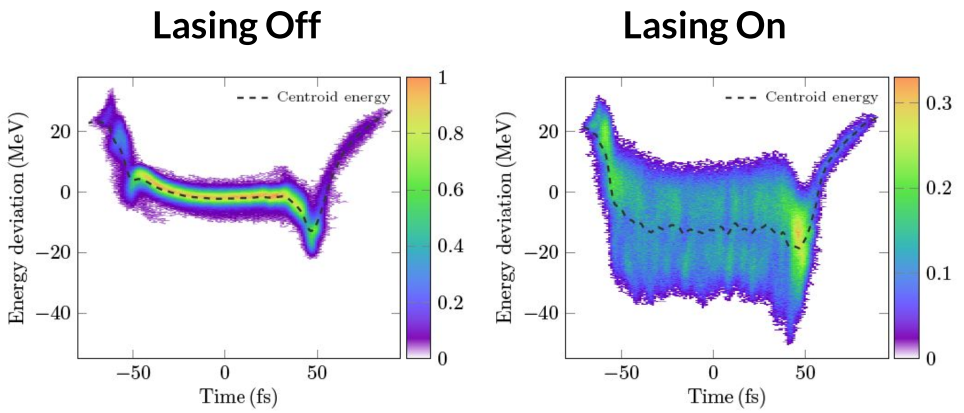
Linac+Und	Mode	Energy delta	Speed/step	Notes
NC + HXR	Und Gap (coarse)	20%	seconds	Range is performance limited
	Vernier (fine)	1-2%	milliseconds	
SC + SXR	Und Gap (coarse)	50-100%	seconds	Range is performance limited
	Vernier (fine)	1-2%	milliseconds	TBD Run 22

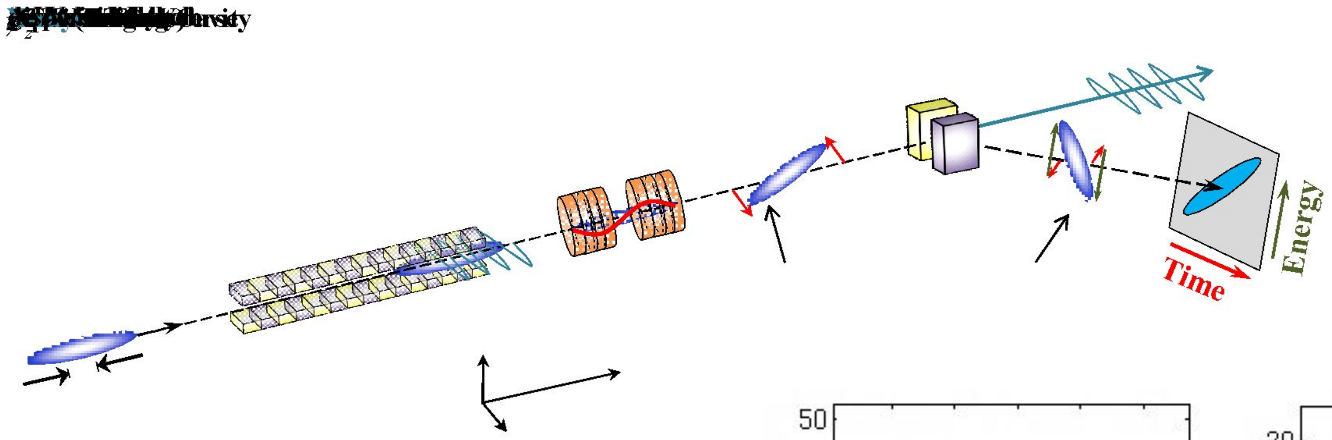
User control of photon energy scans ready and available via new variable gap undulators



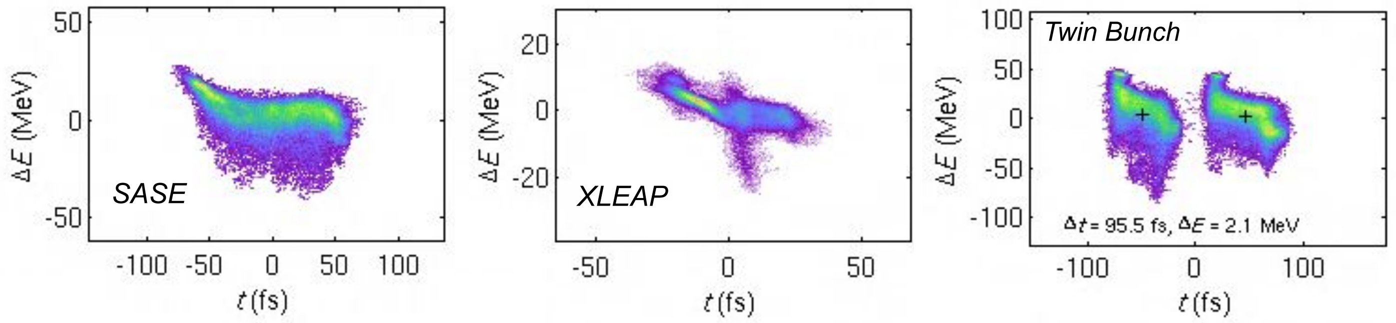
XTCAV: Femtosecond "streak camera" for e- beam

- 120 Hz images of e- beam time-energy distribution
- Observe energy loss due to FEL, **calculate x-ray temporal profile shot-by-shot w/ fs resolution**
- Available for recording/analysis at beamlines in coordination with ACR





XTCAV available for both undulators *and* linacs in Run 23 (120 Hz max)



SC Linac Summary

Will deliver for Early Science to the SXU for Run 22

- **Rate:** Up to 33 kHz delivery over Run 23
- **Intensity/quality:** Ramp intensity/ph. energy in Run 22
- Special capabilities for Run 23:
  - **Photon energy scans** ready
  - **Short pulses** (fs to sub-fs) –to be commissioned (Risk)
  - **SXRSS** – still under redevelopment (N/A)

Communication with the Accelerator Team

- Weekly 'User Meeting' with the ACR team:

  Wednesday before your experiment starts, share experiment background and summarize key FEL parameters: photon energy, pulse energy, pulse length, other special conditions/requests important for FEL source requirements. (~10 min presentation each)

- LCLS POC is the conduit for communication with the Accelerator teams

Thank you and Good Luck

TMO in Run 23

LCLS Run 22 Users Town Hall

January 30th 2024

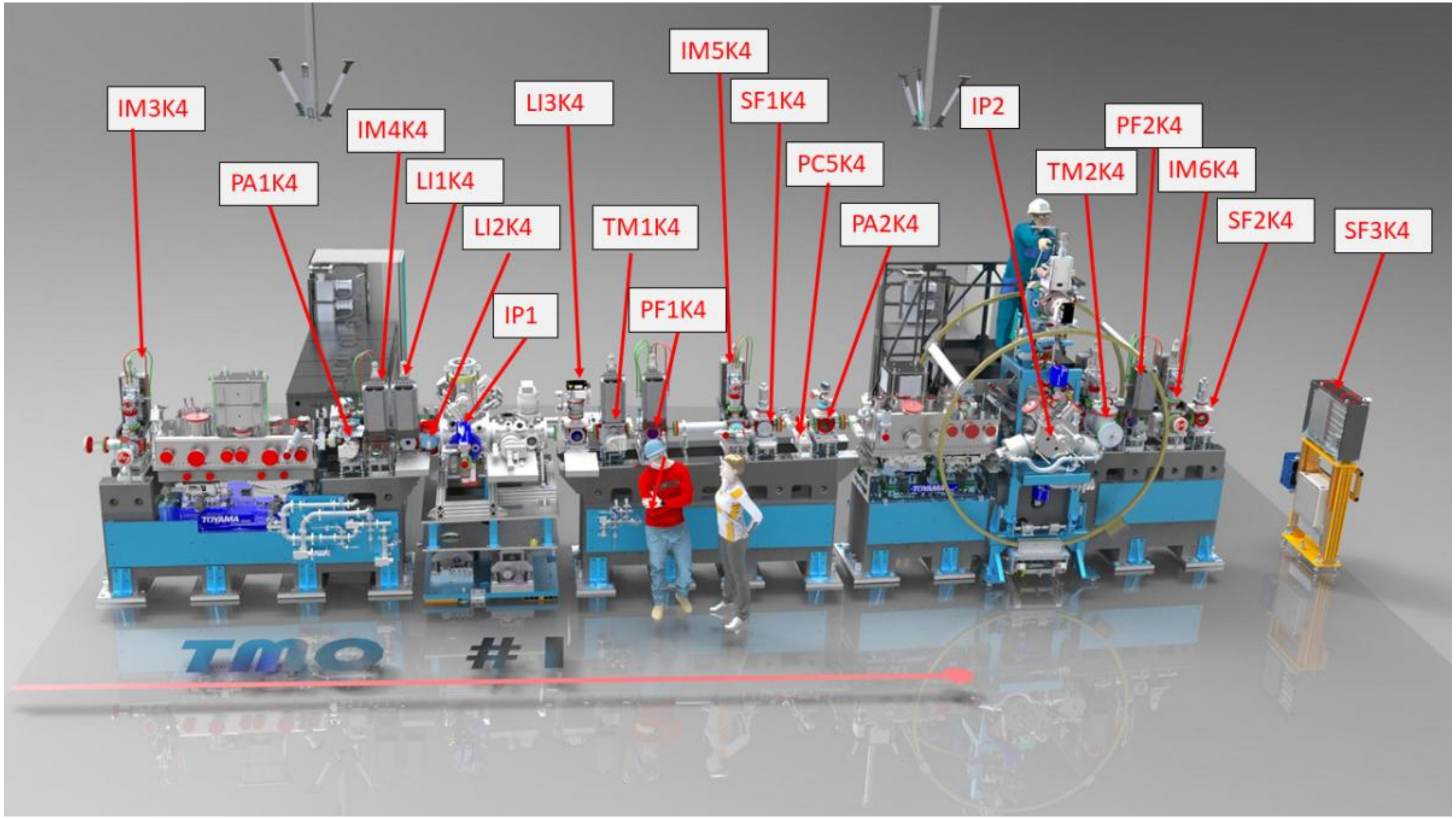
James Cryan

TMO Instrument Lead

AMOS Department Head

TMO Beamline for Run 23

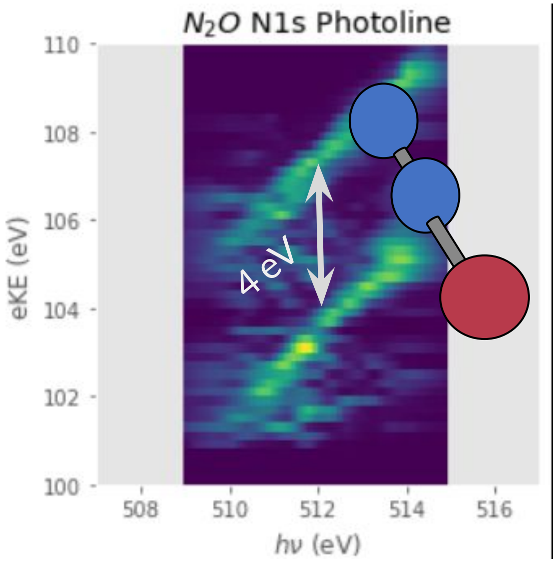
- For Run 23, TMO will offer two endstations: MBES and MRCO at IP1
- Commissioning of IP2 will continue in Run 23.
- DREAM should be available for User science in Run 24

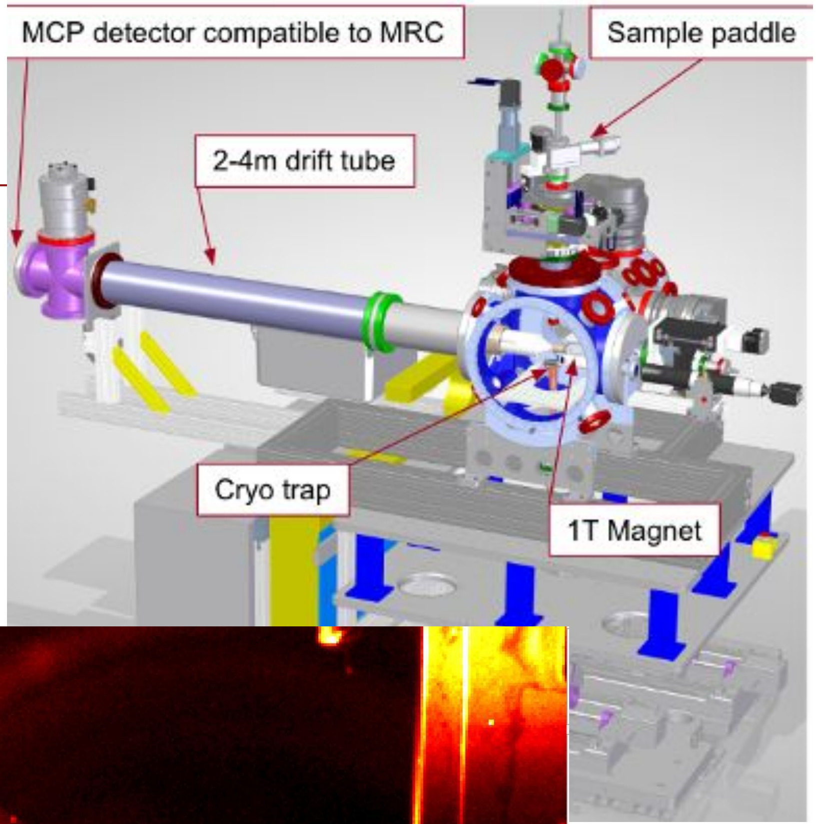


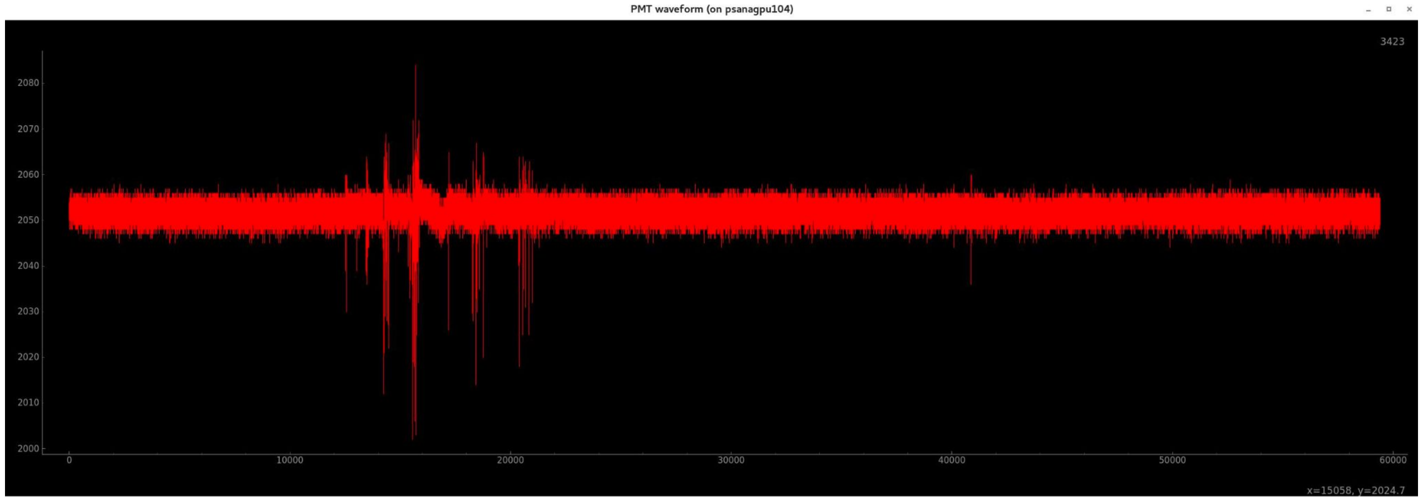
TMO Standard Configuration

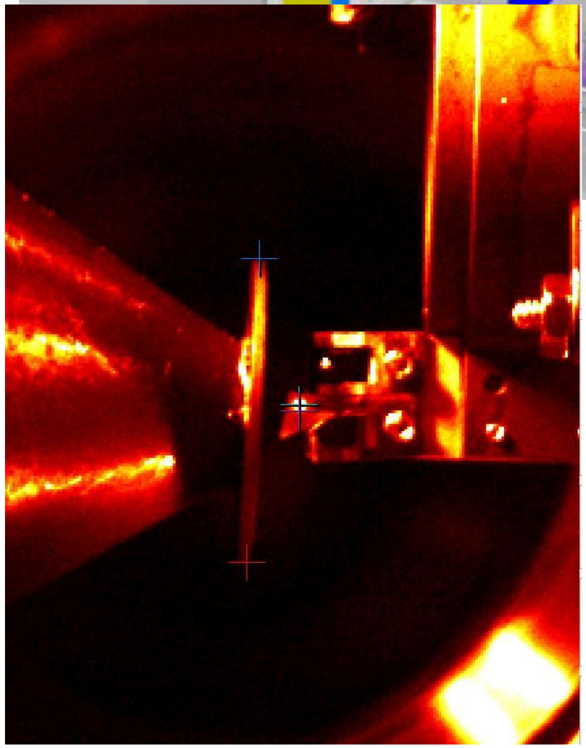
Magnetic Bottle Electron Time-of-Flight Spectrometer (MBES)

- 2m flight tube with retardation section, >50% collection efficiency
  - Retardation up to 400 eV
- Gas targets:
  - Either heated gas needle or
  - In-vacuum oven
- Ion extraction plate and coincident Ion ToF capability







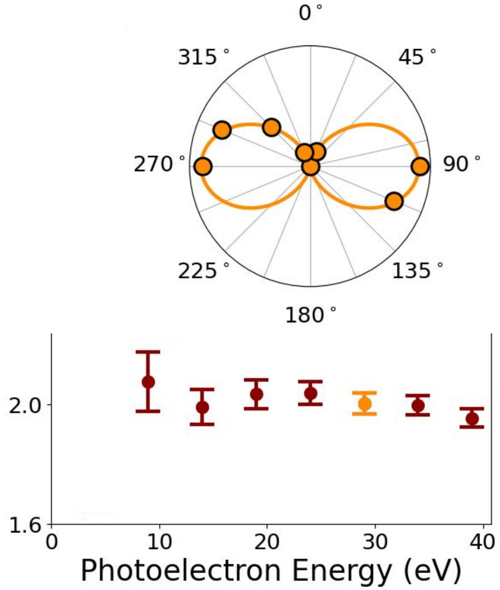


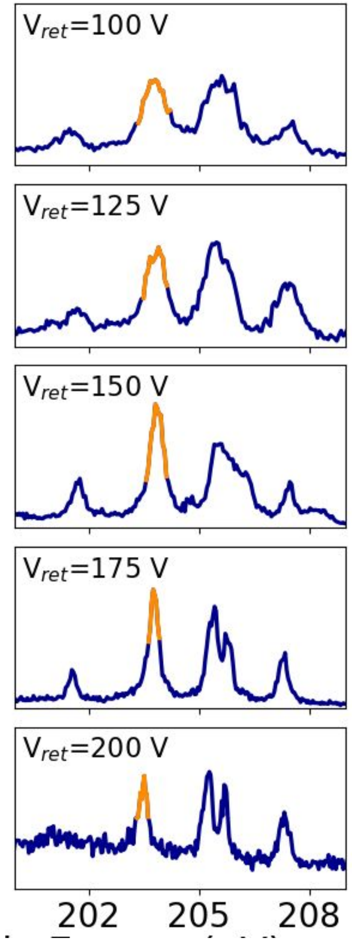
SLAC

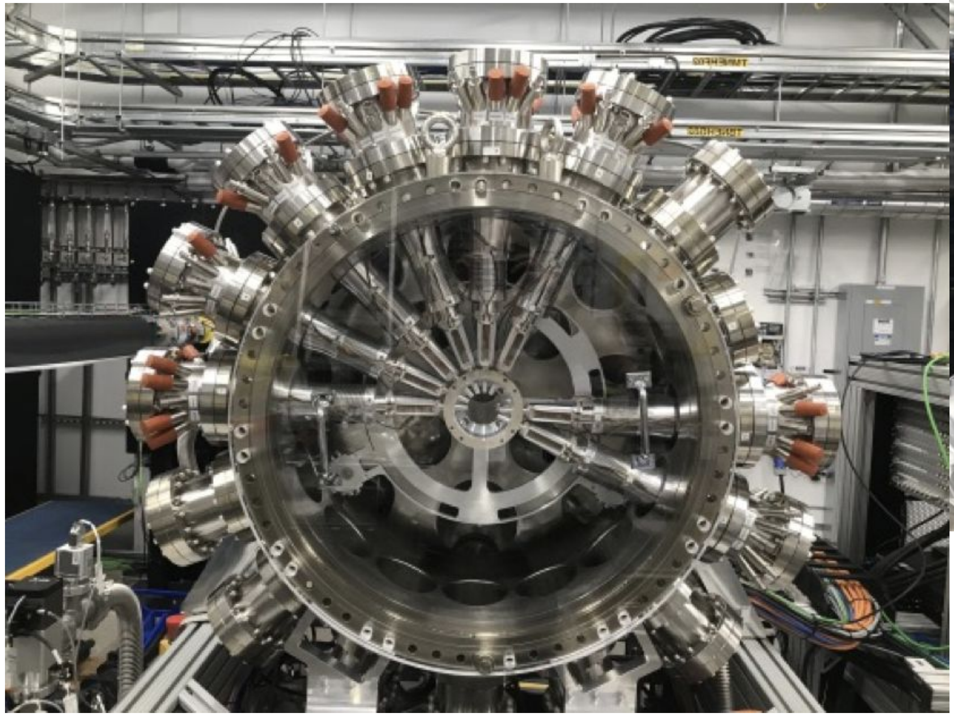
TMO Standard Configuration

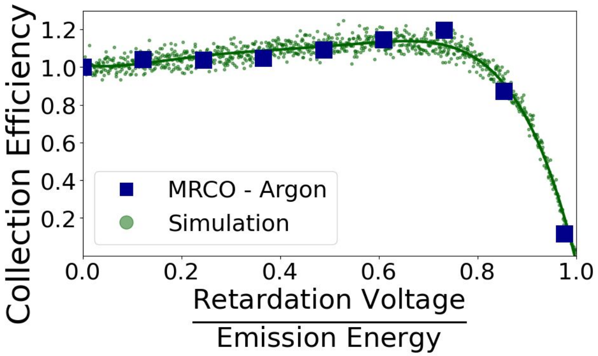
Angle-resolving Time-of-Flight Spectrometer (MRCO)

- Array of ToF spectrometers:
  - 8 guaranteed, 16 planned
  - 1% Total collection efficiency
- Retardation upto 2000 V
- Heated needle for sample delivery

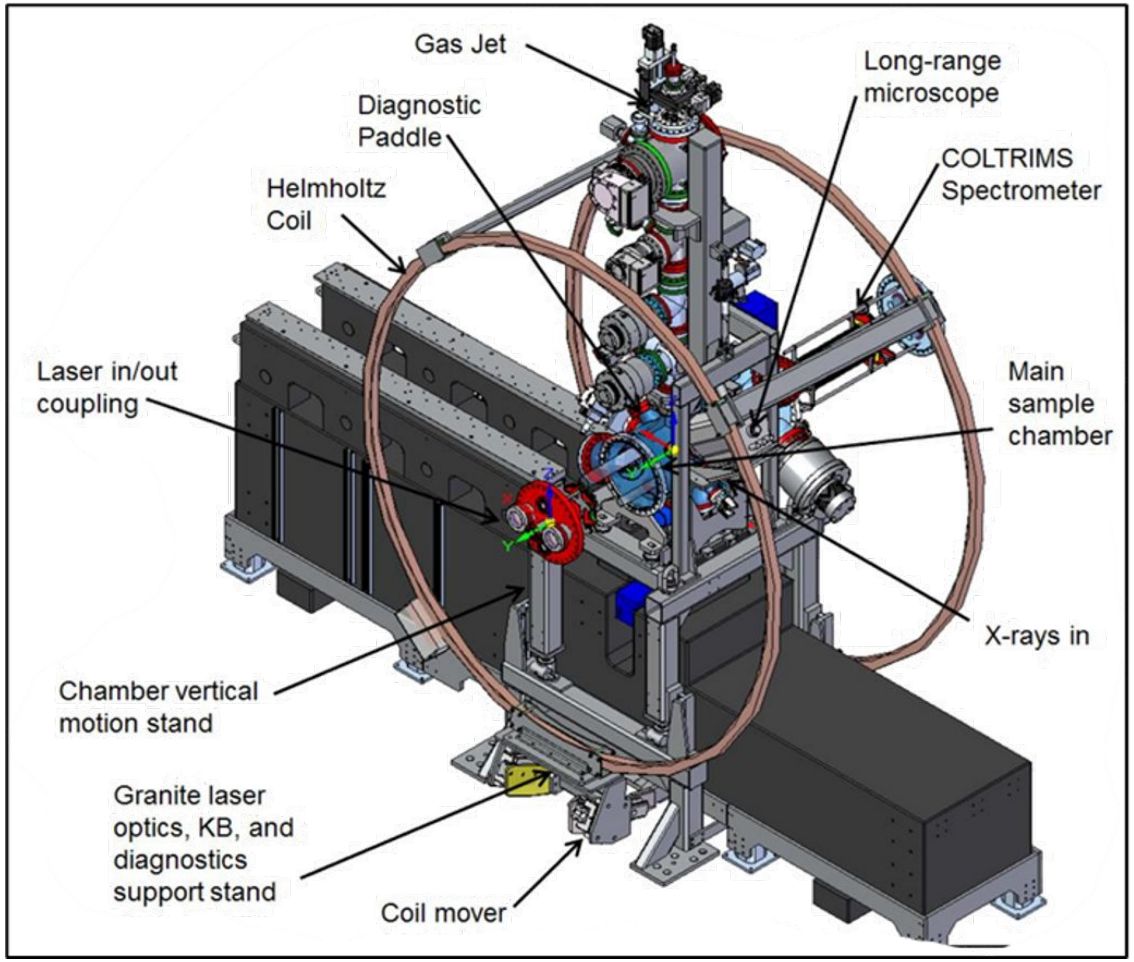








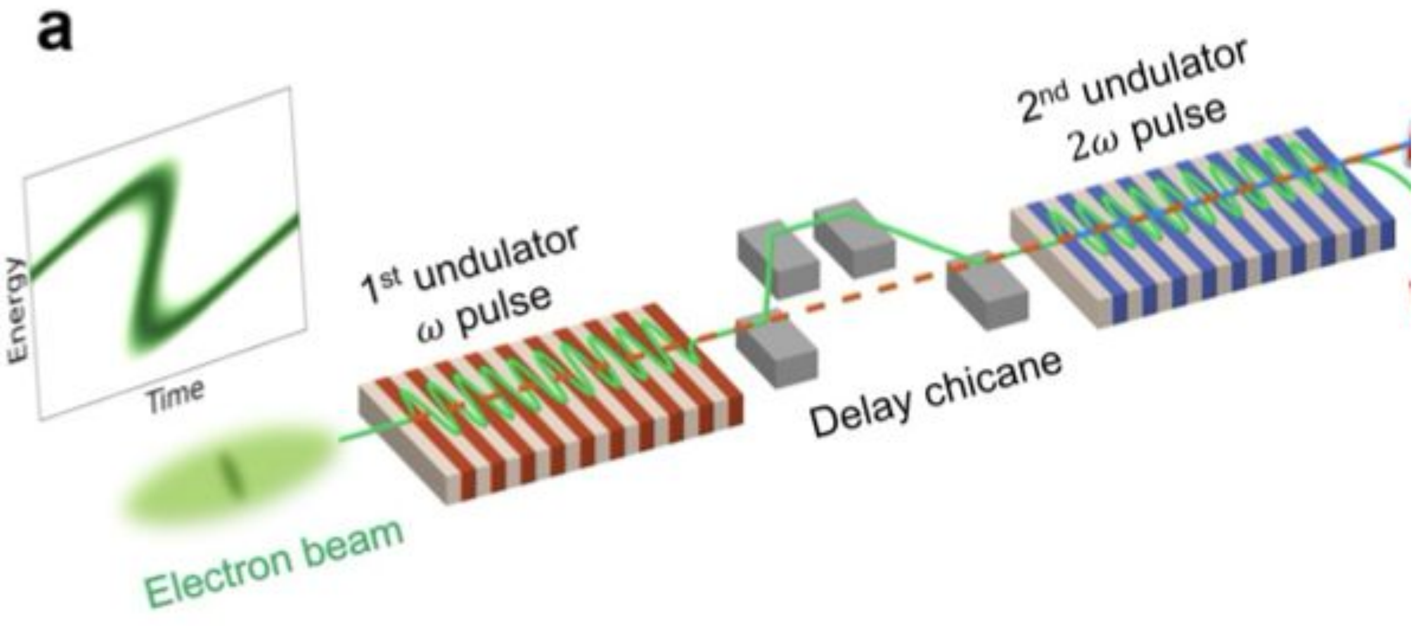
Dynamic REAction Microscope (DREAM)



Status

- Planned Laser-based commissioning
  - Assembly is ongoing:
  - We hope to finish in mid-February
  - Then we will start commissioning with the OPCPA laser system.
- Time allocated in Run 22 and 23 for X-ray commissioning
- Early Science:
  - We will plan for Early Science in Run 23.
  - We have several proposals from the community.
  - We plan to have a workshop once construction is complete.

Attosecond Pulses @ TMO



- Recommissioning Attosecond pulses in Run 22.
- Expect two-color (atto/atto) for Run 23 (baseline > 1 kHz rep. rate)

chemRIXS in Run 23

LCLS Run 23 Users Town Hall

January 30th 2024

Kristjan Kunnus, DJ Hoffman, Douglas Garratt
and Georgi Dakovski

chemRIXS Run 23 call

Liquid standard configuration:

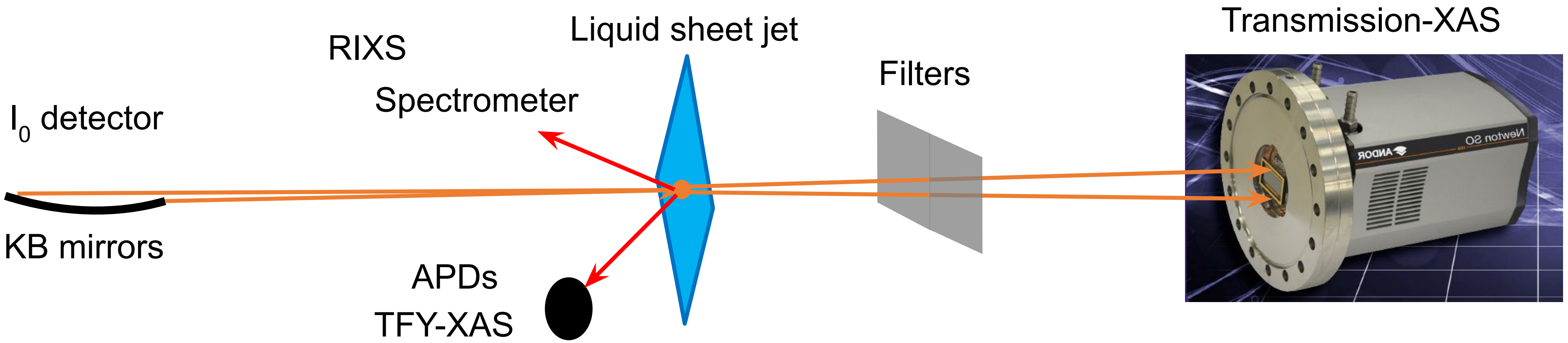
Liquid samples, sheet jets

- Time-resolved XAS with monochromatic beam (scanning)
  - Transmission experiments (sheet jets)
  - Total Fluorescence Yield (TFY) mode
  - Partial Fluorescence Yield (PFY) mode
- Time-resolved RIXS/XES

- Please contact beamline scientist for non-standard configurations

  - Zero-order operation at high rep-rate (e.g. attosecond XLEAP experiments), note: no in-line spectrometer available in run 23
  - Solid samples

chemRIXS Liquid Standard Configuration



SCRF operation
- Repetition rate up to 33 kHz
- Pulse energy up to 100 uJ

RIX beamline
- I_0 at the IP >10^{14} photons/s
- Photon energy range 250 – 1000 eV and up to 1600 eV
- Mono resolving power 2000
- Spot size 10 – 1000 um (variable)
- I_0 detector 5% shot-by-shot noise

OPCPA laser system
- Repetition rate 33 kHz
- 800, 400 and 266 nm
- Vis-OPA 480 – 900 nm

Transmission XAS
- Direct detection with downstream X-ray CCD
- 2048x512 Andor CCD read-out 1 Hz (Image), 120 Hz (FVB)

TFY-XAS
- APDs mounted close to the jet
- Shot-by-shot readout

RIXS/XES/PFY-XAS
- VLS spectrometer mounted at 45 deg backscattering
- 2048x512 Andor CCD read-out 1 Hz (Image), 120 Hz (FVB)
- Resolving power ~2000
- Detection efficiency $4{\cdot}10^{-8}$ (FVB), $1.6{\cdot}10^{-7}$ (Image)

Sample Delivery

Liquid sheet jets for Transmission XAS

- Thin gas accelerated sheets (Nat. Commun. 9, 1353)
  - Thickness 0.1 - 1 μm
  - Flow rates 250 μl/min
  - Optimal for bulk liquids measurements
- Converging nozzles (Phys. Rev. Fluids 3, 114202)
  - Thickness 0.2 - 2 μm
  - Flow rates 2 - 4 ml/min
  - Optimal for solutes

Cylindrical jets for FY-XAS and XES

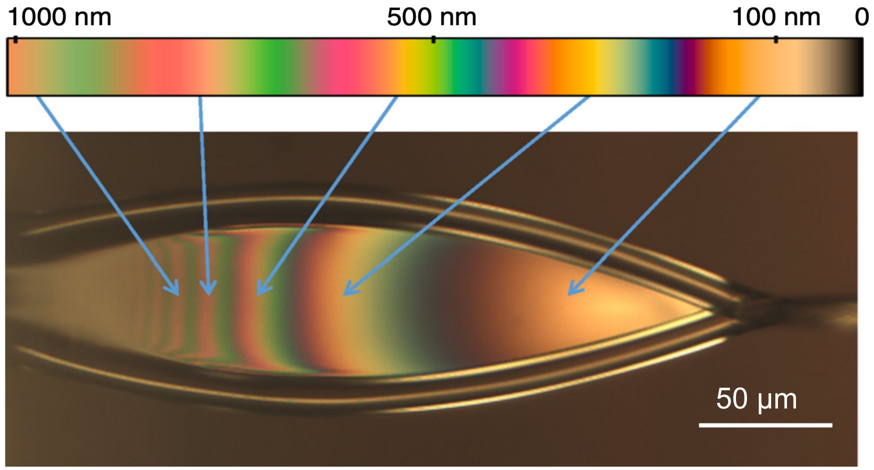
- Gas Dynamic Virtual Nozzle (GDVN)
  - Diameter 1 - 10 μm
  - Flow rates ~20 μl/min
- Rayleigh jet
  - Diameter >20 μm
  - Flow rates ~1 ml/min

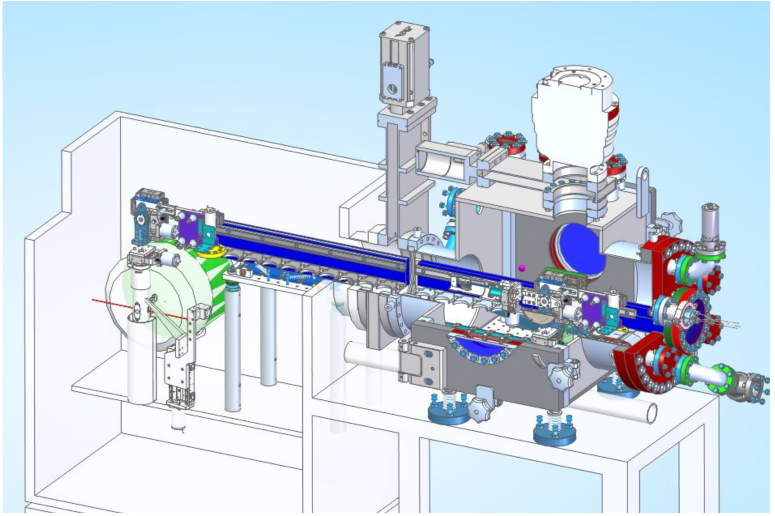
Sample recirculation

- Min. sample volume requirement 50-100 ml

Load-lock systems

- Enables fast nozzle exchange

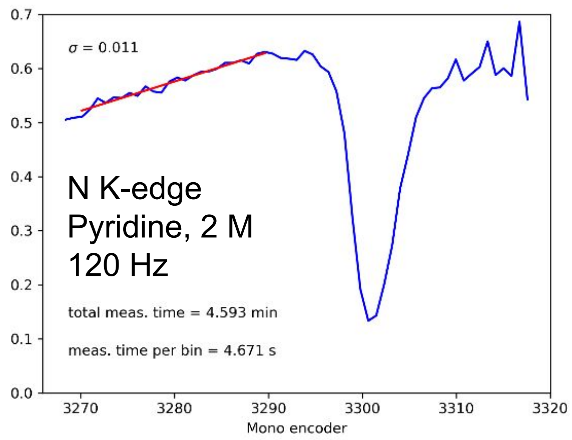


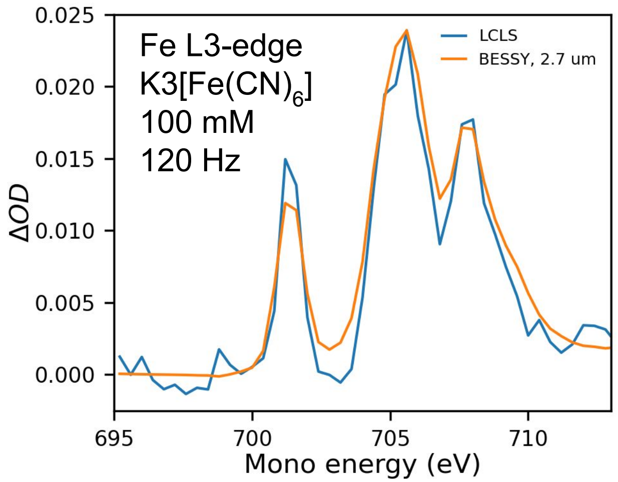


SLAC

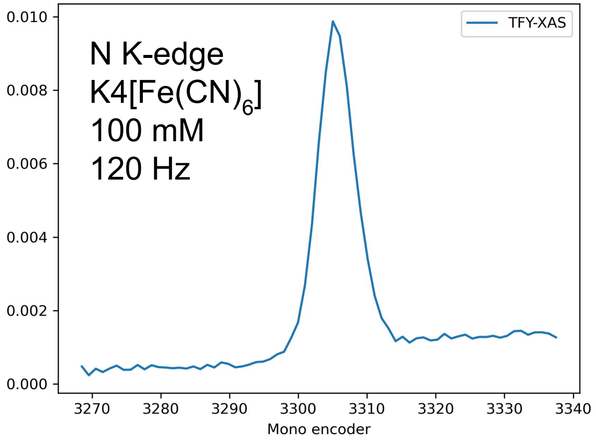
Performance Expectations

Transmission-XAS





TFY-XAS



Noise ~1% (10 mOD) at 120 Hz **-> <0.1% (1 mOD) at 33 kHz**

x10 SNR improvement at 33 kHz

RIXS

33 kHz
$I_0 = 10^{14}$ photons/s
VLS throughput = 10^{-7}
Fl. Yield = 0.005

Concentration (mM)	μ_{solute}/μ_{total}	Total count rate (1/s)	Tr-RIXS?
1000	1/2	10^4	Yes
100	1/20	10^3	Possible
10	1/200	10^2	Hard

chemRIXS Run 23 Key Parameters

X-ray

Repetition rate (Hz)	Up to 33 kHz
Energy Range (eV)	250 - 1600 eV
Pulse Duration (fs)	20 fs (nominal, SASE)
Energy per pulse at the IP (monochromatic)	>100 nJ (250 - 1000 eV) >10 nJ (1000 - 1300 eV) >1 nJ (1300 - 1600 eV)
Beamline Resolving Power	>2000
Spot Size, FWHM (range)	10 - 1000 (um) diameter
Polarization	Linear, Horizontal

Laser

Repetition rate (Hz)	Synchronized up to 33 kHz				
Wavelength (fs)	800	400	266	480 - 600	600 - 900
Pulse Duration (fs)	20	30	35	<50	<50
Energy per pulse (μJ) (on target)	500	50	5	>15	>5
Spot Size, FWHM (800 nm)	50 to 100 μm				
Polarization	Variable: linear, circular				
Angle	~0.5 deg angle with x-ray beam				
Arrival Time Monitor	< 20 fs accuracy in x-ray/laser arrival time tagging should be available. Overall temporal resolution will be dependent on machine and instrument configuration.				

Please contact us for any questions.

G. Dakovski
dakovski@slac.stanford.edu
K. Kunnus
kristjan@slac.stanford.edu

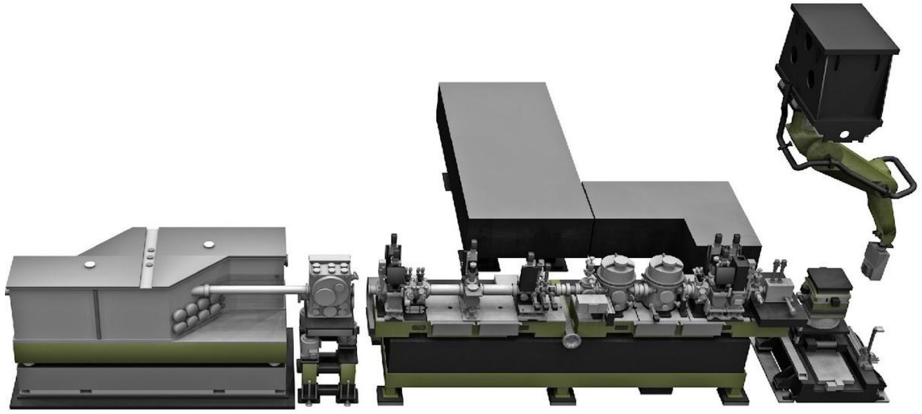
Hard X-ray Instruments in Run 23

LCLS Run 23 Town Hall

January 30th 2024

Sebastien Boutet for all LCLS Hard X-ray Instrument Team Members

XPP



Standard Capability Offering in Run 23

- **trWAXS** up to at 20keV+, vacuum environment supporting fixed target rapid replacement.
- **trXRD** in both ambient (cryojet) and vacuum environment with broad pump wavelength coverage (UV-THz).
- **Compact Split&Delay for X-ray pump probe**
- **trXANES/EXAFS**: will be largely offered at **XCS**.

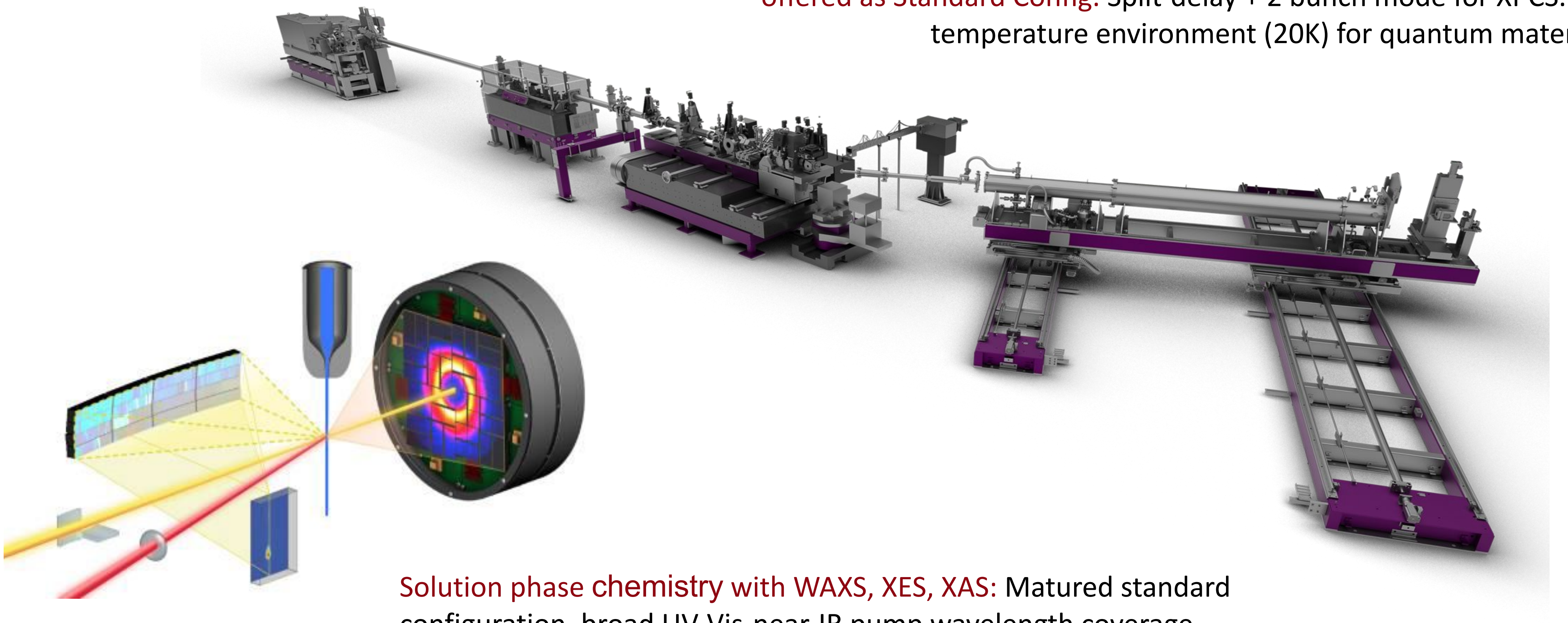
New capabilities

- **Hard x-ray polarization control** established to switch on a near pulse-to-pulse bases between circular left/right and linear polarizations
- **High resolution monochromator** (50-100meV) supporting trRIXS/IXS.
- **Sub-micron focusing**
- **Compact Split&Delay for X-ray pump probe and XPCS**
- **10m tables space offering secondary interaction point for flexible in air setup.**

Instrument Lead: Takahiro Sato

XCS

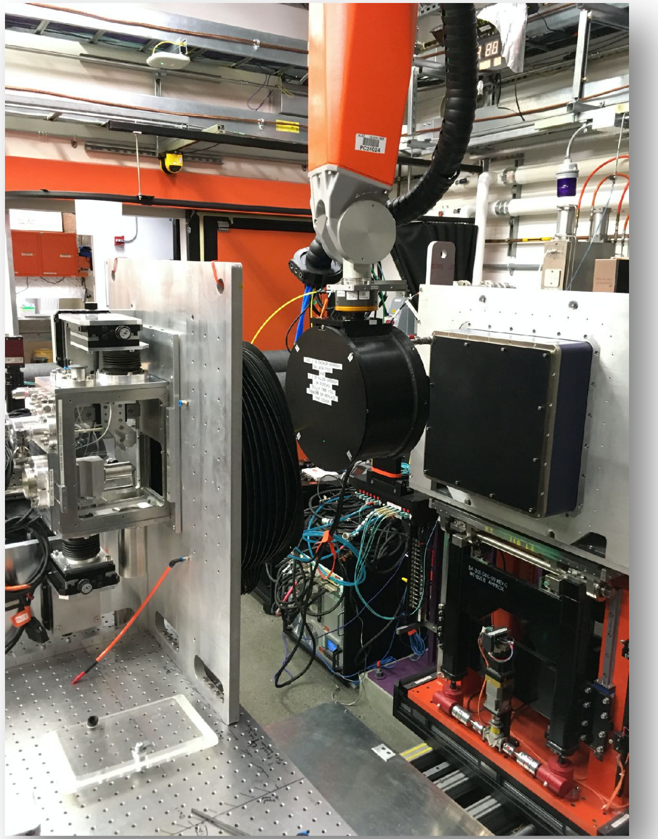
Time-resolved coherent diffraction and small angle coherent scattering offered as Standard Config. Split-delay + 2 bunch mode for XPCS. Low temperature environment (20K) for quantum materials.



Solution phase chemistry with WAXS, XES, XAS: Matured standard configuration, broad UV-Vis-near-IR pump wavelength coverage. Enhanced suite of multi-crystal spectrometers.

Instrument Lead: Matthieu Chollet

MFX



Key Capabilities: Femtosecond Crystallography and time-resolved forward scattering (WAXS/SAXS).

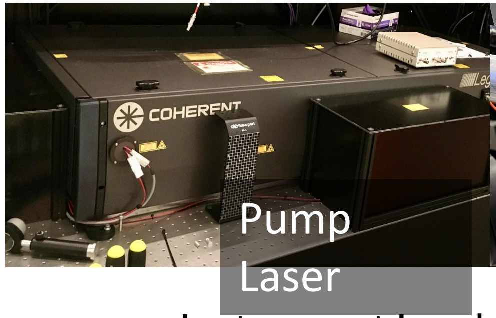
Newer Capabilities

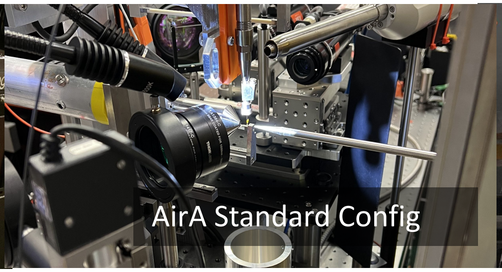
Femtosecond Pump Laser: Collinear incoupling geometry with wavelength coverage from UV to near IR.

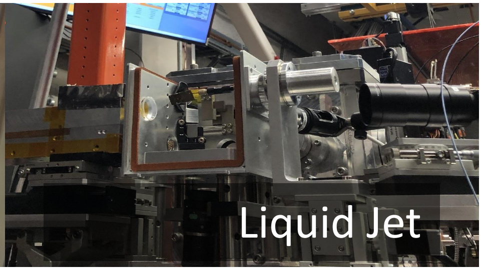
AirA Stanford Configuration: In-air environment (not He enclosure) with multiple sample delivery modes. Compatible with collinear optical pump.

Liquid Jet Endstation: Helium environment horizontal jet sample delivery compatible with emission spectroscopy and forward scattering. Dedicated mutli crystal spectrometer.

Droplet on Demand: Semi-automated droplet delivery system with low sample consumption

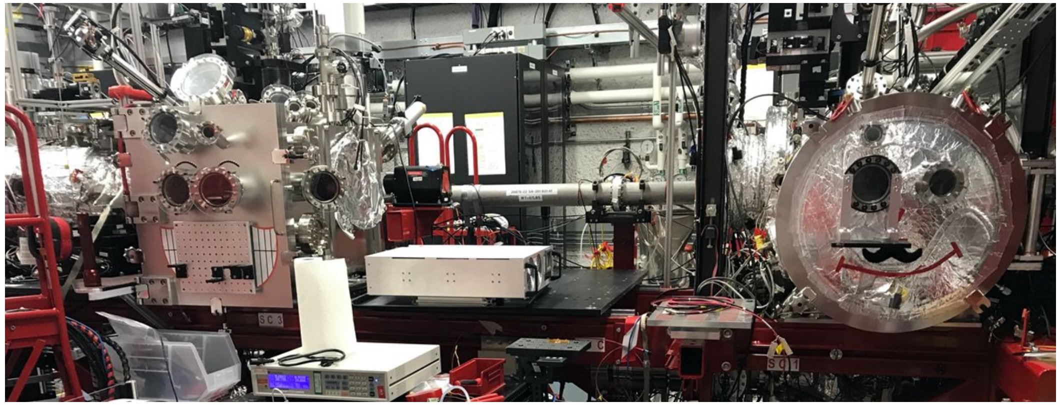


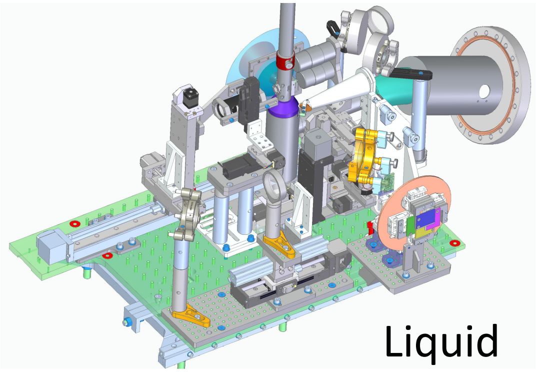




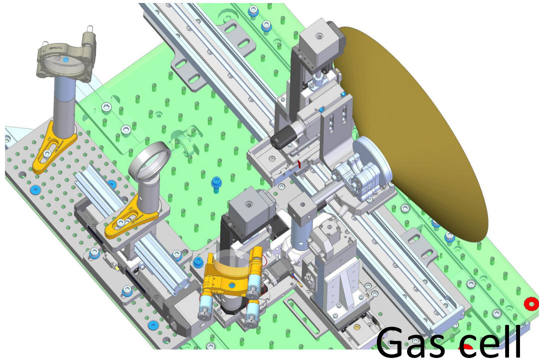
Instrument Lead: Leland Gee

CXI





Liquid jet



Gas cell

Serial Femtosecond Crystallography: variety of sample injection options from jets (GDVN, hi-viscosity, MESH, mixing) to fixed target. Higher photon energy available for potentially higher resolution.

Gas Phase Photochemistry: In vacuum gas cell, short-pulse UV pump (<50fs), multisample gas exchange manifold.

Nanofocus for high field physics and nonlinear x-ray science: 100nm KB system allows reaching power density of 10^{20} W/cm^{2}. Improved nanofocus monitoring with wavefront sensor.

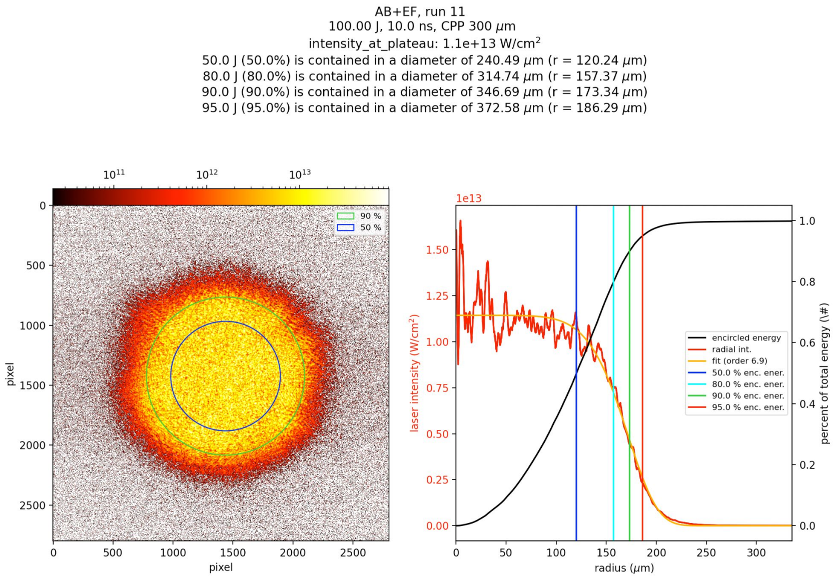
Instrument Lead: Meng Liang

MEC

Discuss with the staff to evaluate the use of these capabilities for your experiment!

100J for Long Pulse Laser

- Delivery of up to 100J in 10 ns on target with the LPL system
- Peak power of 10 GW for any temporal configuration
- Pulse shaping (e.g. flat top, ramp)
- CPP: 150, 300 and 600 μm

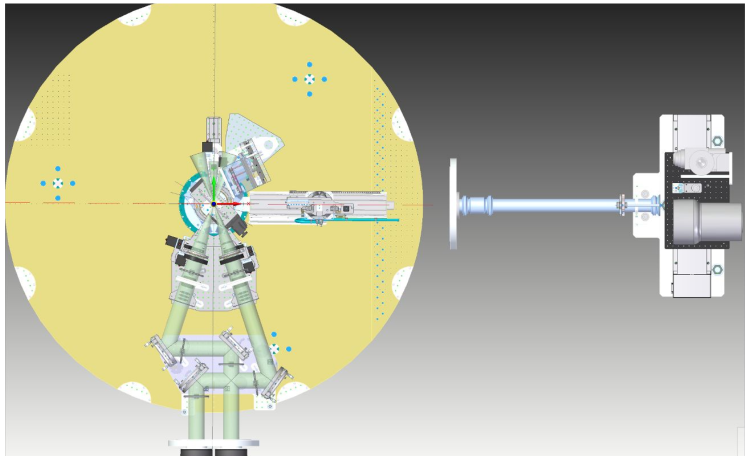


New submission avenues

- Regular PRP proposal
  - up to 50% towards Inertial Fusion Energy
  - about 50% standard configuration
- Data Set Collection
  - 1-2 shifts to complete previous X-rays beamtimes necessary for publishing
  - reviewed by PRP
- Rapid Access
  - VISAR only shots
  - can be submitted at any time during the year
  - reviewed by the MEC team

Std configurations

1. X-Ray Diffraction configuration with long pulse laser in colinear geometry (vs the FEL)
2. X-Ray Imaging geometry with Long Pulse Laser perpendicular to the FEL, X-Ray Diffraction with 3 ePix10k



Instrument Lead: Eric Galtier

TXI

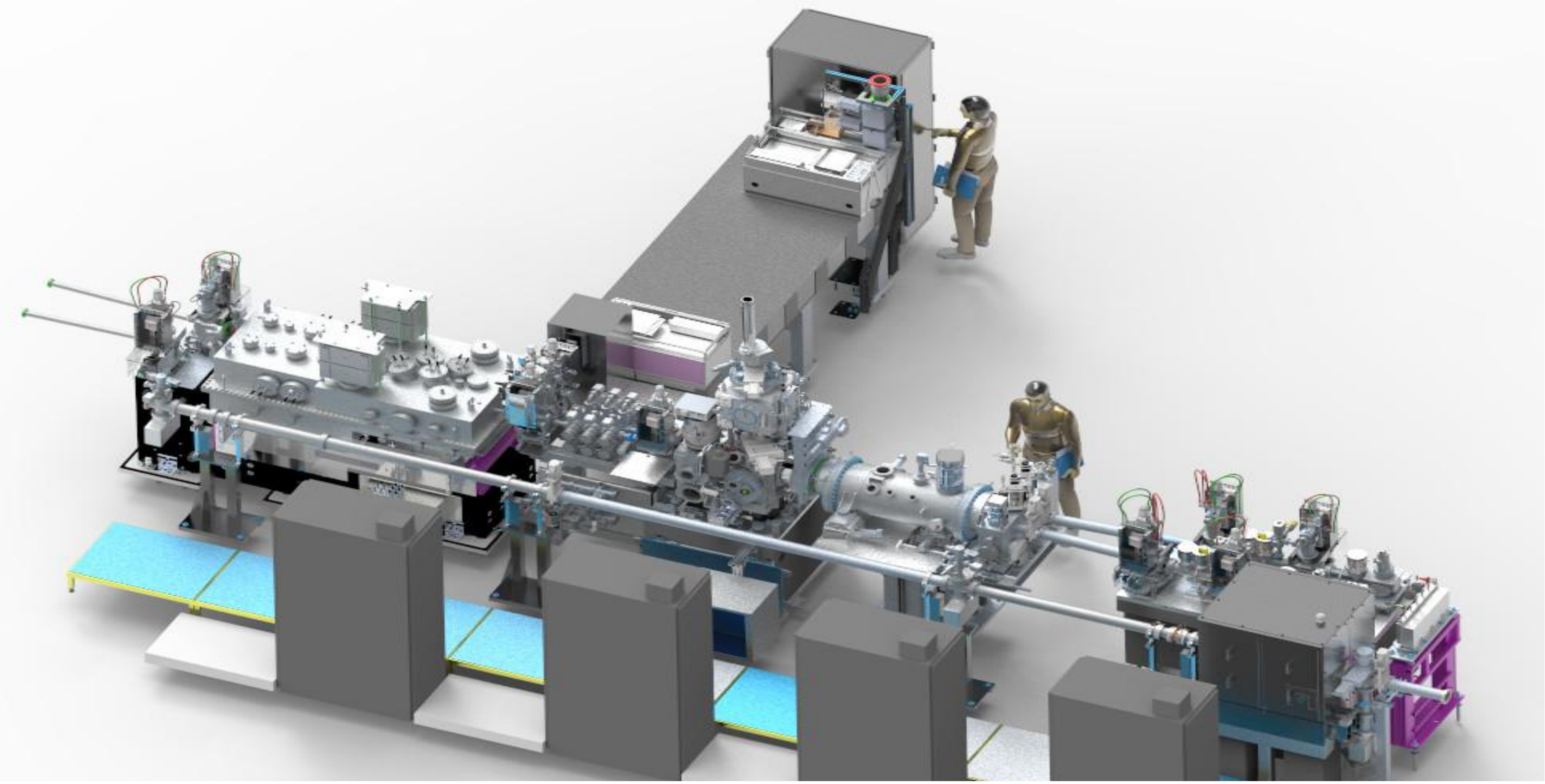
Run 23 | Run 24

~Oct 2024 — ~Jan 2025 — ~Mar 2023

Commissioning → ES TES → PRP TES

TXI commissioning: We will commission the Tender Spectroscopy Endstation during run 23, with Early Science panned for run 24.

Visit the breakout sessions/office hours for more details.



Instrument Lead: Andy Aquila

Data Systems

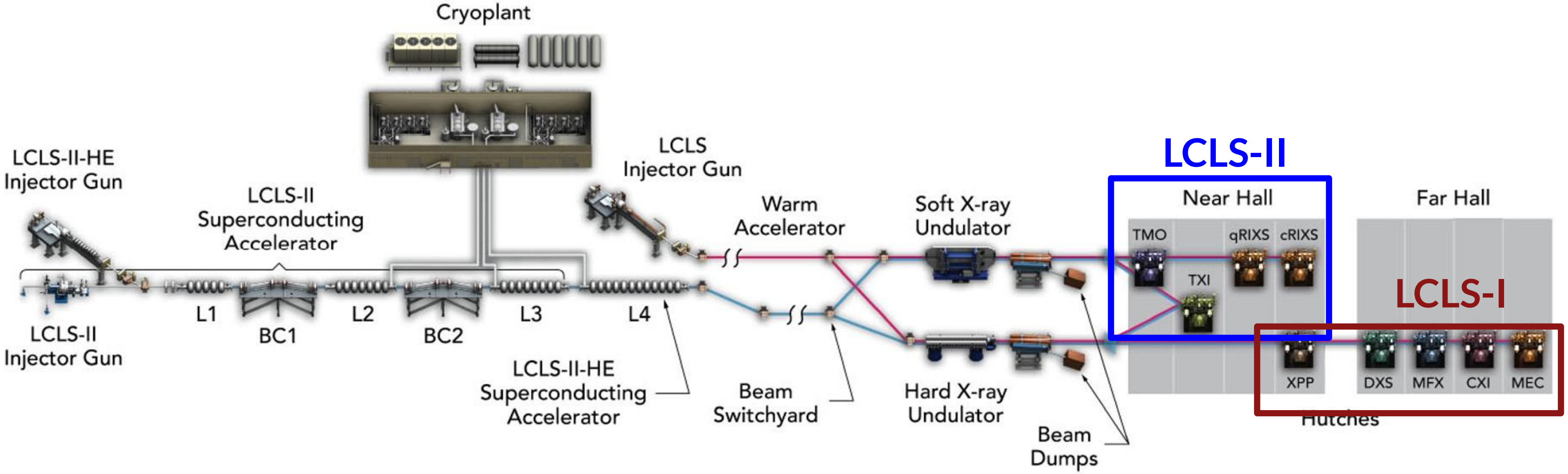
Jana Thayer for the LCLS Data Systems Team

LCLS Data Systems: Zhantao Chen, Richard Claus, Daniel Damiani, Mikhail Dubrovin, Christopher Ford, Wilko Kroeger, Xiang Li, Valerio Mariani, Stefano Marchesini, Riccardo Melchiorri, Christopher O'Grady, Ariana Peck, Frederic Poitevin, Murali Shankar, Monarin Uervirojnangkoorn, Cong Wang, Matthew Weaver, Chun Hong Yoon

January 30th 2024

Reminder: LCLS-I and LCLS-II Use Different Data Systems

LCLS-I and LCLS-II have different DAQ, psana analysis framework, and AMI



LCLS-I is used for hard x-ray instruments **XPP, XCS, MFX, CXI, and MEC** - limited to 120 Hz and ~10 GB/s

LCLS-I psana analysis framework (psana) documentation: https://confluence.slac.stanford.edu/display/PSDM/LCLS+Data+Analysis

LCLS-II is used for the new soft x-ray instruments in **TMO and RIX and soon TXI** - up to 1 MHz and ~TB/s

LCLS-II psana analysis framework (psana2), documentation:

https://confluence.slac.stanford.edu/display/LCLSIIData/LCLS-II+Data+Acquisition+and+Analysis

Data management system, eLog, and Automated Run Processing are common to all instruments.

SLAC Shared Science Data Facility (S3DF)

S3DF is the replacement for the aging psana and FFB processing farms

- S3DF is a common shared computing infrastructure optimized for data analytics characterized by large, massive throughput and high concurrency storage systems.
- S3DF will enable critical, data-heavy computing workflows for LCLS, UED, CryoEM, SSRL, Rubin, ML, HEP, FES
- S3DF storage and computing will scale with LCLS' growing needs
- For more information:
    - S3DF description: https://s3df.slac.stanford.edu/public/doc/#/
    - LCLS getting started on S3DF: https://confluence.slac.stanford.edu/display/PCDS/Running+at+S3DF

How is S3DF Different From psana?

Changes to expect when migrating from psana to S3DF

- In Run 23, all new experiments will be stored and analyzed in S3DF.
- We are in the process of migrating ***all*** users/experiments, including old experiments, to use S3DF
- By August 2024, all legacy systems will be retired.
- Changes from psana to S3DF:
  - Home directory (backed up) is now be in weka (/sdf/home/<first letter of username>/<username>)
  - Shared software packages and tools are in /sdf/group/lcls/ds
    - /sdf/group/lcls/ds/ana psana1/psana2 releases, detector calibration, etc.
    - /sdf/group/lcls/ds/tools smalldata-tools, cctbx, crystfel, om, …
    - /sdf/group/lcls/ds/dm data-management releases and tools
  - LCLS experimental data is accessible on the interactive and batch nodes (but not the login nodes)
    - Offline storage: /sdf/data/lcls/ds/<instr>/<expt>/<expt-folders>
    - FFB storage /sdf/data/lcls/drpsrcf/ffb/<instr>/<expt>/<expt-folders>
  - S3DF batch compute uses Slurm batch processing and requires a Slurm account to submit a job in order to track resource usage per experiment. The slurm account is lcls:<experiment-name>
    - Contact your POC if you require a reservation with a certain number of nodes.
    - We are investigating on-shift/off-shift priority mechanisms; keep an eye on confluence as our policies and recommendations may be in flux as we learn which techniques provide users with the best performance.

Try out Automated Run Processing (ARP)

Automated Run Processing (ARP) capabilities are available via eLog →Workflow → Definitions

- The Automatic Run Processor (ARP) is a web service that allows for automatic workflows and for the easier submission of batch jobs via a web interface: see eLog →Workflow → Definitions
- A script that submits the batch job is all that is needed for this system to work.
- ARP will automatically launch the configured workflow and return status and results to eLog.
- Examples and documentation: https://confluence.slac.stanford.edu/pages/viewpage.action?pageId=219269619
- Working on some standardized workflows for complex analysis tasks.
- For more information on using this resource, reach out to Silke Nelson (snelson@slac.stanford.edu)

Info eLog Samples Run Tables File Manager Shifts Feedback Workflow Summaries Collaborators Switch jana Home Zoom ?

Definitions
Control

Logbook for xcslx2619

Name	Executable	Parameters	Location	Trigger	As user
DataQualityPlots	/cds/data/drpsrcf/xcs/xcslx2619/scratch/smalldata_tools/arp_scripts/submit_plots.sh	--postStats --queue ffbl2q --directory /cds/data/drpsrcf/xcs/xcslx2619/scratch/hdf5/smalldata	SRCF_FFB	RUN_PARAM_IS_VALUE SmallData_ffb == done	snelson
PedestalPlots	/reg/g/psdm/sw/tools/smalldata_tools/pedplot/arp_scripts/submit_plots.sh	--queue psfehprioq --pedestals	SLAC	RUN_PARAM_IS_VALUE pedestal == done	snelson
cube	/cds/data/drpsrcf/xcs/xcslx2619/scratch/smalldata_tools/arp_scripts/cubeRun.sh	--cores 60 --postRuntable --queue ffbh2q	SRCF_FFB	MANUAL	yanwen
smd	/cds/data/drpsrcf/xcs/xcslx2619/scratch/smalldata_tools/arp_scripts/submit_smd.sh	--queue ffbh2q --norecorder --postRuntable --cores 60 --wait --epicsAll	SRCF_FFB	START_OF_RUN	yanwen

S3DF Quick Reference

S3DF Quick Reference: https://s3df.slac.stanford.edu/public/doc/#/

SSH	s3dflogin.slac.stanford.edu
NoMachine	s3dfnx.slac.stanford.edu
OnDemand	https://s3df.slac.stanford.edu/ondemand
Globus Endpoint	slac#s3df
Help (slack channel)	slac.slack.com#comp-sdf
Help (email)	s3df-help@slac.stanford.edu
Banking & Accounting	https://s3df.slac.stanford.edu/coact
S3DF Dashboard & Monitoring	https://s3df.slac.stanford.edu/monitoring

Agenda

Time (PST)	Topic	Presenter
Plenary Session - Join via Zoom >>		
9:00 am	Current LCLS Status & Plans	**Mike Dunne** Director, LCLS
9:23 am	User Executive Committee Update	**Nicholas Hartley** LCLS UEC Vice Chair
9:27 am	Accelerator Plans for Run 23	**Axel Brachmann / Tim Maxwell** Accelerator Dept. Head
9:40 am	New instrument Update (introduce breakouts)	**James Cryan & Georgi Dakovski** TMO/ChemRIXS Isntrument Leads
9:50 am	Hard X-ray instruments brief overview (introduce breakouts)	**Sebastien Boutet** Experimental Operations Director
9:55 am	Data systems	**Jana Thayer** Data Systems Dept. Head
Breakout Sessions/Office Hours by Instrument		
10:10 am - 11:00am	Session 1	
	•TMO Join via Zoom >>	James Cryan
	•MEC Join via Zoom >>	Eric Galtier
	•MFX Join via Zoom >>	Leland Gee
	•qRIXS Join via Zoom >>	Georgi Dakovski
	•XCS Join via Zoom >>	Matthieu Chollet
	•ChemRIXS Join via Zoom >>	Kristjan Kunnus
	•CXI Join via Zoom >>	Meng Liang
	•XPP Join via Zoom >>	Takahiro Sato
	•TXI Join via Zoom >>	Andy Aquila

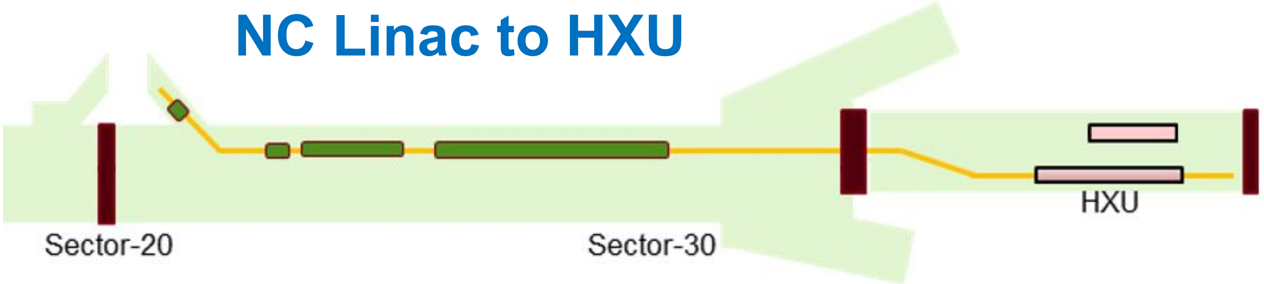
Backup Accelerator Slides

LCLS NC/SC Linac FEL Complex

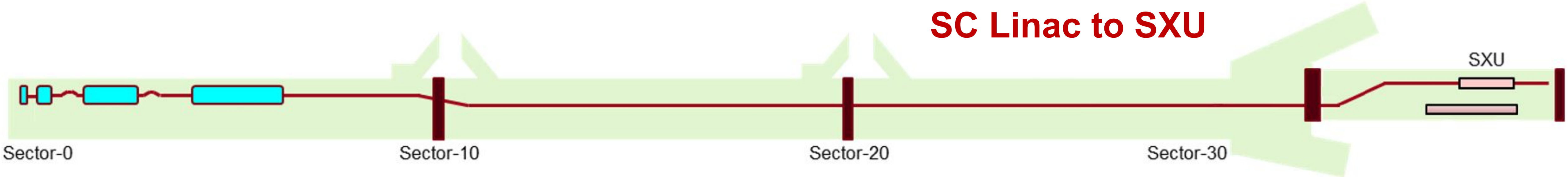
Run 23:

- HXR undulator to continue steady delivery with NC Linac
- SXR undulator devoted to ramp of new, high-rate SC Linac

NC Linac to HXU



SC Linac to SXU



LCLS-II SC Linac: A New Frontier for XFEL Science