LCLS Run 23 Users Town Hall

January 30th 2024
## Agenda

<table>
<thead>
<tr>
<th>Time (PST)</th>
<th>Topic</th>
<th>Presenter</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Plenary Session - Join via Zoom &gt;&gt;</strong></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| 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

<table>
<thead>
<tr>
<th>Time</th>
<th>Session 1</th>
<th>Presenter</th>
</tr>
</thead>
</table>
| 10:10 am - 11:00am | • 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
  o Serious electrical accident at SLAC in December 2022
  o Site-wide power outage due to storms in March 2023
  o Run 21 restart delayed from January to July 2023

• **Run 22** (Jan – July 2024)
  o 177 proposals (back to historical high levels)
  o Increase in chemistry (CSD) and materials science (HCM)
  o Acceptance rate 23%, with 50 PRP experiments fielded

• **LCLS-II Project and SCRF operations**
  o Completed! (September 2023)
  o Slower-than expected initial commissioning
  o Focus on beam emittance, diagnostics to deliver useful beam
  o 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:

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

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

- **qRIXS**
  - Mono 250 – 1600 eV

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

- **HXR beam**
  - SurfSpec endstation
  - k-Microscope endstation

- **SXR beam**
  - 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: $3.0 \times 10^{10}$
- 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 14 operating months 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
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/lclsu](https://lcls.slac.stanford.edu/lclsu)

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)**

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

Linac gallery and new cryoplant viewed from Sector 0
Hard X-ray, Normal Conducting Linac Capabilities
### Beam Parameters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Cu-HXU x-rays</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( h \omega )</td>
<td>25000</td>
<td>eV</td>
</tr>
<tr>
<td>( \omega_{\text{max}} )</td>
<td>1000</td>
<td></td>
</tr>
<tr>
<td>( \omega_{\text{min}} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Photon Energy</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fundamental wavelength</td>
<td>( \lambda )</td>
<td>Å</td>
</tr>
<tr>
<td>Final linac e- energy</td>
<td>( \gamma m c^2 )</td>
<td>GeV</td>
</tr>
<tr>
<td>FEL 3-D gain length</td>
<td>( L_G )</td>
<td>m</td>
</tr>
<tr>
<td>Peak power</td>
<td>( P )</td>
<td>GW</td>
</tr>
<tr>
<td>Pulse duration range</td>
<td>( \Delta \tau )</td>
<td>fs</td>
</tr>
<tr>
<td>Nominal pulse duration</td>
<td>( \Delta \tau_f )</td>
<td>fs</td>
</tr>
<tr>
<td>Max Pulse Energy*</td>
<td>( U )</td>
<td>mJ</td>
</tr>
<tr>
<td>Photons per pulse*</td>
<td>( N_\gamma )</td>
<td>10^{12}</td>
</tr>
<tr>
<td>Peak brightness*</td>
<td>( B_{\text{pk, Cu-L}} )</td>
<td>10^{30} §</td>
</tr>
<tr>
<td>Average brightness (120Hz)*</td>
<td>( \langle B \rangle )</td>
<td>16</td>
</tr>
<tr>
<td>SASE bandwidth (FWHM)</td>
<td>( \Delta \omega / \omega )</td>
<td>eV</td>
</tr>
<tr>
<td>Photon source size (rms)</td>
<td>( \sigma )</td>
<td>μm</td>
</tr>
<tr>
<td>Photon far field divergence (FWHM)</td>
<td>( \Theta_{\text{FWHM}, x, \infty} )</td>
<td>μrad</td>
</tr>
<tr>
<td>Max. Beam Rate</td>
<td>( \varphi_{\text{FEL}} )</td>
<td>Hz</td>
</tr>
<tr>
<td>Avg. x-ray beam power</td>
<td>( P_x )</td>
<td>W</td>
</tr>
<tr>
<td>Linear Polarization (100%)</td>
<td>( \langle P \rangle )</td>
<td>Vertical</td>
</tr>
</tbody>
</table>

*Assuming nominal duration and undulator strength

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

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

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

https://lcls.slac.stanford.edu/machine/parameters
Hard X-ray Self-Seeding (HXRSS)

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

Spectral brightness enhancement for narrow bandwidth experiments

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photon energy</td>
<td>4.5 – 11 keV</td>
</tr>
<tr>
<td>Bandwidth (FWHM)</td>
<td>0.35 – 1.5 eV</td>
</tr>
<tr>
<td>Max pulse energy</td>
<td>0.2 – 0.5 mJ</td>
</tr>
<tr>
<td>Duration</td>
<td>30 fs</td>
</tr>
</tbody>
</table>

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

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

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)

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)
## Advanced Multi-Pulse/Color Modes

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

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

Discuss special requirements with your LCLS POC
Soft X-ray, Superconducting Linac Capabilities
SC Linac Rate Ramp-Up

- Beam Power related to \([\text{Repetition Rate} \times \text{Charge}]\), 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
## Beam Parameters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>SC-SXU x-rays</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hbar\omega_{\text{max}}$</td>
<td>1300</td>
<td>eV</td>
</tr>
<tr>
<td>$\hbar\omega_{\text{nominal}}$</td>
<td>800</td>
<td></td>
</tr>
<tr>
<td>$\hbar\omega_{\text{min}}$</td>
<td>200</td>
<td></td>
</tr>
</tbody>
</table>

### Photon Energy
- $\hbar\omega$ 1300 800 200 eV

### Fundamental wavelength
- $\lambda_r$ 9.5 15.5 62.0 Å

### Final linac e- energy
- $\gamma m c^2$ 3.5-4.0 GeV

### FEL 3-D gain length
- $L_{\text{bg}}$ 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*
- $B_{\text{pk,SASE}}$ 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)
- $\sigma_s$ TBD µm

### Far field divergence (FWHM)
- $\Theta_{\text{FWHM},x,\infty}$ TBD µrad

### Max. Beam Rate
- $\varphi_{\text{FEL}}$ 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
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

<table>
<thead>
<tr>
<th>Technique</th>
<th>Min Pulse Duration</th>
<th>Linac (Max Rate)</th>
<th>Energy range</th>
<th>Energy/Pulse</th>
<th>Single Spike rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laser Heater Shaping</td>
<td>&lt; 8 fs</td>
<td>SC (1 kHz+)</td>
<td>SXR</td>
<td>10-20 uJ</td>
<td>TBD</td>
</tr>
<tr>
<td>XLEAP</td>
<td>TBD</td>
<td>SC (1 kHz+)</td>
<td>SXR</td>
<td>TBD</td>
<td>TBD</td>
</tr>
</tbody>
</table>

fs and sub-fs pulses to be demonstrated w/ SC linac during Run 22
## Photon Energy Scanning

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

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 \textit{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
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
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
Performance Expectations

Transmission-XAS

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

TFY-XAS

x10 SNR improvement at 33 kHz

RIXS

33 kHz

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

<table>
<thead>
<tr>
<th>Concentration (mM)</th>
<th>$\mu_{\text{solute}}/\mu_{\text{total}}$</th>
<th>Total count rate (1/s)</th>
<th>Tr-RIXS?</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>1/2</td>
<td>$10^4$</td>
<td>Yes</td>
</tr>
<tr>
<td>100</td>
<td>1/20</td>
<td>$10^3$</td>
<td>Possible</td>
</tr>
<tr>
<td>10</td>
<td>1/200</td>
<td>$10^2$</td>
<td>Hard</td>
</tr>
</tbody>
</table>
# chemRIXS Run 23 Key Parameters

## X-ray

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Repetition rate (Hz)</td>
<td>Up to 33 kHz</td>
</tr>
<tr>
<td>Energy Range (eV)</td>
<td>250 - 1600 eV</td>
</tr>
<tr>
<td>Pulse Duration (fs)</td>
<td>20 fs (nominal, 5ASE)</td>
</tr>
<tr>
<td>Energy per pulse at the IP (monochromatic)</td>
<td>&gt;100 nJ (250 - 1000 eV)</td>
</tr>
<tr>
<td></td>
<td>&gt;10 nJ (1000 - 1300 eV)</td>
</tr>
<tr>
<td></td>
<td>&gt;1 nJ (1300 - 1600 eV)</td>
</tr>
<tr>
<td>Beamline Resolving Power</td>
<td>&gt;2000</td>
</tr>
<tr>
<td>Spot Size, FWHM (range)</td>
<td>10 - 1000 (µm) diameter</td>
</tr>
<tr>
<td>Polarization</td>
<td>Linear, Horizontal</td>
</tr>
</tbody>
</table>

## Laser

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

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
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.**

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**.

Instrument Lead: Takahiro Sato
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
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 multi crystal spectrometer.

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

Instrument Lead: Leland Gee
**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.
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

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

Instrument Lead: Eric Galtier
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](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/LCLSIIaData/LCLS-II+Data+Acquisition+and+Analysis](https://confluence.slac.stanford.edu/display/LCLSIIaData/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/anapsana1/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)
# S3DF Quick Reference

**S3DF Quick Reference:** [https://s3df.slac.stanford.edu/public/doc/#/](https://s3df.slac.stanford.edu/public/doc/#/)

<table>
<thead>
<tr>
<th>Service</th>
<th>URL</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSH</td>
<td>s3dflogin.slac.stanford.edu</td>
</tr>
<tr>
<td>NoMachine</td>
<td>s3dfnx.slac.stanford.edu</td>
</tr>
<tr>
<td>OnDemand</td>
<td><a href="https://s3df.slac.stanford.edu/ondemand">https://s3df.slac.stanford.edu/ondemand</a></td>
</tr>
<tr>
<td>Globus Endpoint</td>
<td>slac#s3df</td>
</tr>
<tr>
<td>Help (slack channel)</td>
<td>slac.slack.com#comp-sdf</td>
</tr>
<tr>
<td>Help (email)</td>
<td><a href="mailto:s3df-help@slac.stanford.edu">s3df-help@slac.stanford.edu</a></td>
</tr>
<tr>
<td>Banking &amp; Accounting</td>
<td><a href="https://s3df.slac.stanford.edu/coact">https://s3df.slac.stanford.edu/coact</a></td>
</tr>
<tr>
<td>S3DF Dashboard &amp; Monitoring</td>
<td><a href="https://s3df.slac.stanford.edu/monitoring">https://s3df.slac.stanford.edu/monitoring</a></td>
</tr>
<tr>
<td>Time (PST)</td>
<td>Topic</td>
</tr>
<tr>
<td>-----------</td>
<td>------------------------------------------------------------</td>
</tr>
<tr>
<td>9:00 am</td>
<td>Current LCLS Status &amp; Plans</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>9:23 am</td>
<td>User Executive Committee Update</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>9:27 am</td>
<td>Accelerator Plans for Run 23</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>9:40 am</td>
<td>New instrument Update (introduce breakouts)</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>9:50 am</td>
<td>Hard X-ray instruments brief overview (introduce breakouts)</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>9:55 am</td>
<td>Data systems</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Breakout Sessions/Office Hours by Instrument</td>
<td>Session 1</td>
</tr>
<tr>
<td>10:10 am - 11:00 am</td>
<td>TMO [Join via Zoom &gt;&gt;]</td>
</tr>
<tr>
<td></td>
<td>MEC [Join via Zoom &gt;&gt;]</td>
</tr>
<tr>
<td></td>
<td>MFX [Join via Zoom &gt;&gt;]</td>
</tr>
<tr>
<td></td>
<td>qRIXS [Join via Zoom &gt;&gt;]</td>
</tr>
<tr>
<td></td>
<td>XCS [Join via Zoom &gt;&gt;]</td>
</tr>
<tr>
<td></td>
<td>ChemRIXS [Join via Zoom &gt;&gt;]</td>
</tr>
<tr>
<td></td>
<td>CXI [Join via Zoom &gt;&gt;]</td>
</tr>
<tr>
<td></td>
<td>XPP [Join via Zoom &gt;&gt;]</td>
</tr>
<tr>
<td></td>
<td>TXI [Join via Zoom &gt;&gt;]</td>
</tr>
</tbody>
</table>
Run 23:

- **HXR undulator** to continue steady delivery with **NC Linac**

- **SXR undulator** devoted to ramp of new, high-rate **SC Linac**
LCLS-II SC Linac: A New Frontier for XFEL Science