LCLS UEC Meeting Minutes

February 1, 2024

Present

• Mike Dunne, Alfred Zong, Artem Rudenko, Brandon Tan, Cathy Knotts, Chitra Rajendran, Dominik Oberthür, Elisa Biasin, Leilani Conradson, Margaret Doyle, Marius Schmidt, Martin Centurion, Matteo Mitrano, Nick Hartley, Natalia Powers-Riggs, Paul Jones, Rebecca Boll, Sam Teitelbaum, Silvia Pandolfi, Siqi Li, Uwe Bergmann

Opening remarks

Nick Hartley: For the next meeting at the end of February 2024, a major discussion topic is user outreach and expansion. Matthias Kling and Meng Liang will be joining. Members of the UEC are encouraged to think about suggestions before the next meeting. [Note added: this will be moved to the March meeting due to staff availability]

Mike Dunne: Rebecca Boll is co-organizing the FELs@Ringberg workshop in mid-February. He wishes the workshop a success and asks that the UEC is briefed on the outcomes of the meeting (progress with FEL facilities and user community scientific directions).

Director's updates from Mike Dunne

1. Instrument status

LCLS Run 22 has been going for a couple of weeks so far. MeV-UED is also running gas-phase experiments at the moment.

2. Looking into the future: The DOE Office of Science is driving an update to the "Facilities for the future of science" roadmapping process. Details of the charge from Dr Asmeret Berhe are at: https://science.osti.gov/-/media/bes/besac/pdf/Charges/2023-Berhe-Facilities-Charge.pdf

DOE Office of Science

- "Facilities for the future of science"
- Projects pre-CD2 and >\$100M
- DOE-BES includes:
 - LCLS-II-HE
 - HE Low Emittance Injector
 - LCLS-X
 - "Future Light Source"
- DOE-FES includes:
 - MEC-Upgrade (webinar 15th Feb 1pm PT)
- DOE-ASCR includes:
 - High Performance Data Facility (HPDF)



This is DOE Office Science's planning for the next 10 to 20 years. Key questions that need input from the user community include:

- What facilities and instruments would we like to build?
- Strategically what scientific directions would we like to go?

Here are Mike's explanations of the bullet points in the slide:

- As we envision the future facilities, two questions are being asked by DOE Office of Science:
 - What's the potential for world-leading science?
 - What's the construction readiness?
- The type of projects under consideration are pre-CD2 (critical decision 2) i.e. projects that are pre-baseline (regarding a firm timeline and budget), and >\$100M
 - For example, SSRL and LCLS instrument improvement projects (Major Items of Equipment, MIE) are generally <\$100M so do *not* fall under this category
 - LCLS-II-HE meets the criterion (budget ~\$710M) and expects to meet CD2 within the next 6 months
 - HE Low Emittance Superconducting Injector also meets the criterion, ~\$200–250M
 - It would allow the X-ray energy to be increased to a harder regime: from a limit of 13 keV to 20 keV
 - A full list of projects under consideration within DOE-BES (Basic Energy Sciences) can be found at: <u>https://science.osti.gov/-/media/bes/besac/pdf/Charges/2023-</u> <u>BES-Facilities-Charge-Project-Description-rev-02-01-2024.pdf</u>



Figure 14 Preconceptual layout of a representative LCLS-X facility in which a suite of X-ray undulators are populated in a newly constructed tunnel to feed a series of new instruments.

LCLS-X would deliver a step-change in XFEL science – a suite of optimized beamlines and instruments (with examples shown in Figure 15(a)) provided to a large user community, allowing full exploitation of each scientific area. This would allow different communities to push instrumentation relevant to their field rather than forced to make compromises. The increased capacity would further permit more innovative experiments, which are not accepted by the proposal panels today because outcome can't be guaranteed.

Operationally, the population of the full set of undulators enabled by LCLS-II will bring XFEL science into a synchrotron-like mode, with a large number of parallel experiments that support a broad critical mass of PI's across the community, and with an associated reduction in cost per experiment - as outlined in Figure 15(b).

- LCLS-X: This is still an early-stage concept, where multiple (on the order of 10, and thus the name "X") independent beamlines (and thus ~30 end-stations) can run simultaneously (schematic shown above)
 - With the upgrade to MHz LCLS-II (eventually up to 2 MHz), it is possible to fan out the X-ray beam and feed into individual end-stations, where each end-station will

have ~100 kHz repetition rate. If a particular experiment needs much more than 100 kHz, then special scheduling will be needed

- Some end-stations will have semi-permanent or dedicated instruments, e.g., those specialized in attosecond beams, extremely high-brightness beams, inelastic X-ray scattering, in operando measurements, etc.
- Of course, a lot of details need to be filled in, and we as a community are invited to help identify the scientific cases and needs as the plan develops
 - Workshops are expected to be organized to address the above details, and some of which can certainly fall into the annual LCLS/SSRL Users' Meeting
- "Future Light Source" (FLS): this is again an open book at present, and such a light source is expected to serve the scientific demands in mid- to late-2030s that are not met by the current set of facilities.
 - The need for the light source can be from a scientific perspective or from an instrumentation point of view (e.g. new storage rings)
- DOE-FES (Fusion Energy Sciences)
 - Similarly, DOE-FES (Fusion Energy Sciences) are running a parallel process to input into the Roadmap. This includes MEC-Upgrade and ITER as the two existing projects, plus a range of potential future opportunities. Details are at: https://science.osti.gov/-/media/fes/fesac/pdf/2023/2023-Facilities-Charge-Fusion-Energy-Sciences_final.pdf
 - There will a community webinar on February 15th at 1 pm (PST) about MEC-Upgrade
 - Leilani Conradson will help announce the webinar information to the LCLS community
 - There will be some test projects running, e.g., fusion prototypic neutron source, reactor-scale materials test facilities
- DOE-ASCR (Advanced Scientific Computing Research): it is of interest to the computing teams at LCLS
 - HPDF is led by Jefferson Lab on the east coast and mirror-hosted by Lawrence Berkeley National Laboratory on the west coast
 - LCLS has a strong partnership with HPDF team that will facilitate massive-scale online processing, offline data analysis and storage for the experiments at LCLS-II, to be realized towards the later part of this decade

3. Looking into the past: updates from DOE regarding LCLS strategic plan and review



Here is the strategic plan:

https://lcls.slac.stanford.edu/sites/default/files/2023-12/LCLS%20Strategic%20Plan%202023-2028.pdf

Here is the science review:

https://lcls.slac.stanford.edu/sites/default/files/2024-01/lcls_assessment_final.pdf

DOE asked the five lightsources (ALS, APS, LCLS, NSLS-II, SSRL) along with the neutron sources (SNS, HFIR) to work together and to take SWOT analysis (strengths, weaknesses, opportunities, and threats) for the DOE complex as a whole

• This process kick-started last week and will report out in six months

In the LCLS Science Impact Assessment, a panel chaired by Antoinette (Toni) Taylor (Los Alamos National Laboratory) took a retrospective look at where LCLS Science has been impactful.

4. Q&A with Mike Dunne

If we want to be a part of the LCLS-X workshops, whom do we contact? Could some of the workshops be part of the user meeting? What about the funding sources for the workshops?

• We haven't set out the details of the workshop yet and we are looking into filling them in the summer/next two months. Workshops can be a part of the LCLS Users' Meeting, and funding for attendance at the workshops will be looked into by Mike Dunne

The vision for LCLS-X end-stations is to have semi-permanent instruments, so will there be overall more beamtime available?

• With ~10 beamlines and 30 parallel instruments, the capacity is increased significantly: but how we schedule the beamtime is a completely open question and that's something we'll need to work together. One important point of semi-permanent instruments is that we can avoid the setup time that can be quite long (e.g., many hours). Having dedicated and specialized instruments set up in the end-station helps to realize a mode of operation akin to a synchrotron, and/or as a next-generation version of "standard configurations". This approach will also enable a much more expansive approach to LCLS Scientific Campaigns.

As DOE is very familiar with the mode of operation of synchrotrons, DOE really loves the metric of "up time". How will this mode of thinking impact the operation of LCLS-X?

• At the present stage of discussion, we will strive for a balance between speculative vs. investigative science, having both exploratory science as well as measurements that need long-term stability (e.g., accumulating statistics for days/weeks to get very good resolutions)

Is it fair to say that LCLS-X is more like a synchrotron so that instruments will be more independent? And with more instruments running simultaneously, will there be opportunities for speculative science?

• Yes, that's exactly the goal

Currently the operational cost per hutch of an FEL is one order of magnitude higher than that of the synchrotron. Is the reduction of the operational cost also part of the planning for LCLS-X? Will there also be a large level of staff scientists support at LCLS-X?

• With more experiments running at the same time in LCLS-X, the cost per experiment is estimated to be reduced such that it is only about 2 times the cost of running at a synchrotron. As for the staff support, it varies for the experiments. For more exploratory type of experiments, the anticipated support will be higher. For routine/standard measurements, the staff support will be lower.

For LCLS-X, the plan is to have all end-stations running all at the same time. Right?

• Yes. The kicker works so that you can fan it back and forth in real time to get an individual repetition rate of around 100 kHz for about 10 beamlines. 100 kHz also looks like the optimal point as this is where the average power peaks out.

Is there an advantage of having two FELs in the US instead of one LCLS-X with 10 beamlines?

• There are pros and cons. One disadvantage for two FELs is that the buy-in cost for the FEL infrastructure is very high (~\$3B for LCLS so far), and the support team has to be local. We need to evaluate what are the benefits of duplicating the infrastructure and human resources vs. enhancing the existing resources

The next LCLS proposal is due in about three weeks, but we don't have the scheduling/feedback of the previous one yet for the soft X-ray experiments seeking to use the SCRF beam

• This is an important feedback and Mike Dunne will look into this today and talk to Sebastien Boutet with a view to issuing the feedback this week [note: this was done].

Updates about 2024 Users' Meeting by Chitra Rajendran

Members of the UEC are encouraged to think about the following two items before the next meeting, and email Chitra Rajendran (<u>Chitra.Rajendran@biologie.uni-regensburg.de</u>) or discuss in the next UEC meeting about their feedbacks:

- 1. The option to publish the meeting proceedings as a special issue of a journal for the Bio session. Chitra will let us know more details about the scheduling in the next UEC meeting
- 2. New topics for workshop and tutorial sessions for the meeting

Any other feedback about the meeting (e.g., food choice) are welcome.

Feedback from the LCLS Virtual Town Hall Meeting, Tuesday, January 30, 2024

Leilani Conradson reported that there were 334 registrants and 307 attendants. Paul Jones mentioned about 20–30 people attended most of the breakout rooms.

Paul Jones reminded us that all sessions can be accessed through the LCLS website.

There was less interaction in the MEC breakout room but it seems that other breakout rooms were quite interactive with Q&A between the staff scientists and the audience. Silvia Pandolfi was surprised that the MEC upgrade was not mentioned in the breakout session, probably because there will be an upcoming webinar on February 15th about it (Mike Dunne just got the information yesterday; Leilani Conradson will help disseminate this webinar information).

Mike Dunne affirmed that TMO is taking proposals this round, which was not very clear from the townhall meeting.