LCLS Call for Data Set Collection (DSC) Proposals

Closing Date: March 2, 2018

SUBMIT NEW PROPOSALS BY 4 pm PACIFIC on **March 2, 2018**.

This DSC beamtime is to be awarded during LCLS Run 17, and is expected to be between September 2018 and December 2018.

Due to the one-year shutdown of LCLS after Run 17, the Protein Crystal Screening (PCS) program will be temporarily supplanted by a Data Set Collection (DSC) program. The focus of DSC will be to facilitate data collection for projects that are close to completion or only need a short amount (1-2 shifts max) of beam time at LCLS to reasonably achieve a full data set. The PCS program will resume for Run 18.

The LCLS DSC program aims to allot LCLS beamtime for biological structure determination by making use of short, 6-24 hour runs to collect a full data set under good running conditions. To enable measurements within such a short time frame and maximize efficiency and the chances of success, these studies must be carried out with limited instrumentation flexibility to minimize the time impact of setup changes. The following configurations will be supported for DSC in this current call for proposals: liquid and high viscosity jet systems as well as fixed targets in vacuum at CXI and at atmospheric pressure at MFX. Other liquid jet systems supplied by user groups compatible with the basic CXI and MFX systems will also be considered if the schedule allows it and at the discretion of LCLS. Schedule constraints are unpredictable and no guarantees can be made that any of the mentioned experimental setups will be available for DSC in this run. Use of optical lasers is outside the scope of the DSC program.

DSC at CXI

DSC experiments at CXI will be carried out using the standard CXI configuration, using the refocused X-ray beam from the 1 µm focus as a parasitic measurement to a primary experiment, depending on scheduling constraints and at the discretion of LCLS. Sample delivery will be via liquid and high viscosity jet systems as well as fixed targets in vacuum. User-supplied sample delivery systems or modifications to the existing system are allowable only if they are compatible with the existing systems and can be exchanged with the other systems used for DSC beamtime within a time frame compatible with 12-hour parasitic runs and rapid turnaround between groups. Decisions on using alternative sample delivery systems are entirely at the discretion of the LCLS facility.

DSC at MFX

DSC experiments at atmospheric pressure are expected to be available. The home of such experiments is now the MFX instrument with multiple options likely to be available, including a goniometer system, allowing scanning of fixed-mounted crystals, and a liquid jet system compatible with various types of jets. These systems can also be modified in principle for use of a variety of atmospheric pressure sample delivery systems. User-supplied systems may also be available. The availability of all these systems will depend on scheduling constraints and is entirely at the discretion of LCLS.

Other Experimental Geometries or Capabilities

Time-resolved studies and spectroscopy are currently not within the scope of DSC beam time.

Proposal Review and Beamtime Award

These DSC proposals will be reviewed by the PRP BIO-C panel together with the regular proposals. It is desirable to shorten the period between DSC proposal submission and beam time allocation to maximize flexibility and the ability to be reactive to novel samples or ideas. LCLS will aim to pre-allocate blocks of beamtime on CXI and/or MFX based on the overall demand. Proposals will be awarded beam time by LCLS based on the scientific recommendation of the Proposal Review Panel and other technical considerations by LCLS, including sample readiness, technical feasibility and scheduling constraints. A minimum 2 months notice will be given to the selected user groups to allow for appropriate preparation.

Overlap with Regular LCLS Proposals

DSC proposals should differ in some significant way to a regular proposal by, for example, focusing on a reduced scope since the DSC and regular proposals will be reviewed during the same review panel.

Proposal Format

DSC proposals follow a similar format as regular proposals. They must be submitted separately.

DSC proposals are evaluated on the impact, originality, need for LCLS, scientific risk, prior results, as well as technical feasibility.

LCLS DSC proposals should be submitted through the User Portal.

Provide a descriptive title of your proposed experiment that you would be willing to be made public if awarded beam time.

The proposal text is limited to 2 pages in PDF format. Pages should have at least 1 inch margins and not less than 10 pt font. It should include the following information:

- **Experimental Team**: In a table, list the names, institution, email address of PIs and collaborators who would participate in the proposed experiment (e.g., sample prep, theory, data collection, data analysis). This section could also briefly mention directly-relevant previous work done by the team members.
- **Scientific Case**: Briefly explain the background and significance of your experiment. In particular, why is LCLS required for this experiment? Itemize the specific aims and particular questions you want to answer. Focus on the specific experiment and avoid broad discussions in general terms.
- **Experimental Procedure**: If the DSC proposal is related to one or more regular LCLS proposals that have been submitted or already received beam time, state this in the proposal. Tell us if you plan or have carried out supporting experiments at other facilities. Have simulations of the experiment been performed? What are the anticipated data rates? Provide a beam time plan, indicating what could be accomplished in less than 6 hours of beam time. Describe any additional equipment you plan to bring to LCLS for the experiment. We strongly recommend that you contact LCLS Scientist Mark Hunter (mhunter2@slac.stanford.edu) before proposal

submission to discuss capabilities, to identify possible problems in integrating external equipment with LCLS instrumentation and to determine possible solutions.

- **Technical Feasibility**: Proposals must contain sufficient information for LCLS to review the proposal for technical feasibility. This information should include:
    - Equipment
      Which elements of the proposed instrument do you require for the proposal?
      What additional equipment is needed, including detector, sample delivery/environment, temperature, pressure, etc.?
      How do you plan to provide/organize the additional equipment?
    - Experimental protocol
      Describe the experimental geometry.
      Calculate the expected signal rate/background.
      Describe samples and concentrations, sample preparation and storage.
      Describe local facilities that may be required.

* Safety related documents must be submitted during the safety management portion of the LCLS proposal submission process in the user portal. List and describe any safety concerns that may arise with samples you will examine, equipment you will use, or techniques you will perform (including any physical, chemical or biological hazards) and how these issues will be addressed in the experiment design.