Biological Science Capabilities at LCLS

Mark Hunter
LCLS Biology and Sample Environment and Delivery Departments

LCLS Biology Department personnel and associates

Experimental Structural Biology

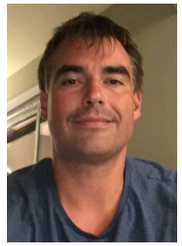

Andy Aquila


Maithri Kashipathy

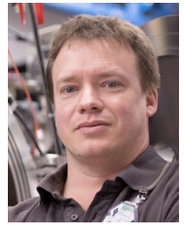

Alex Batyuk


Chris Kupitz


Frank Moss


Mark Hunter

Sample Delivery


Dan DePonte


Stella Lisova


Christina Hampton


Ray Sierra

BioChemistry


Roberto Alonso-Mori

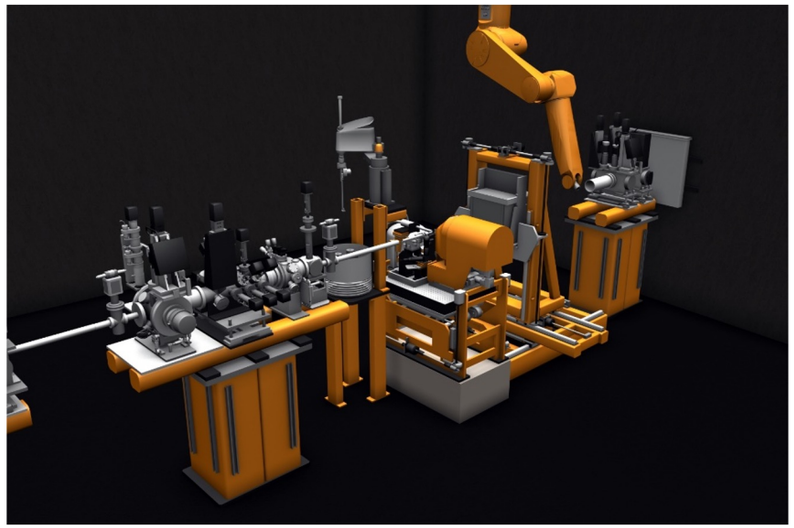

Leland Gee

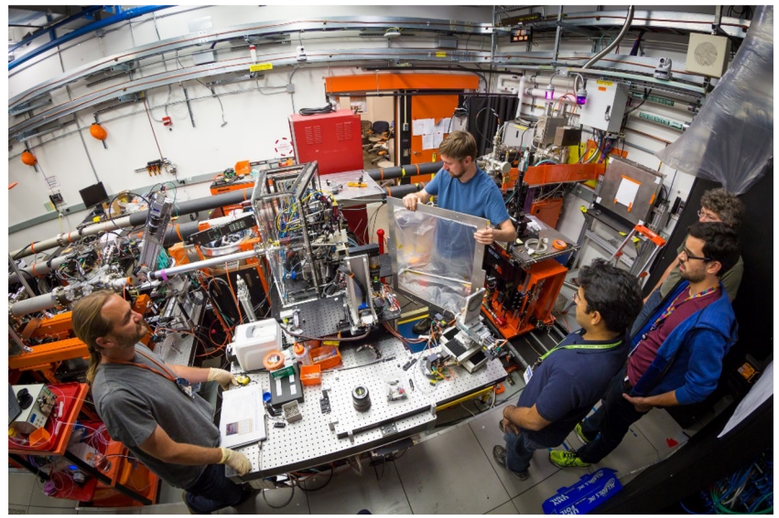

Brandon Hayes


Jeppe Ormstrup

MFX: Macromolecular Femtosecond Crystallography

- High power density atmospheric pressure sample environment
- Versatile system, configurable for specific needs



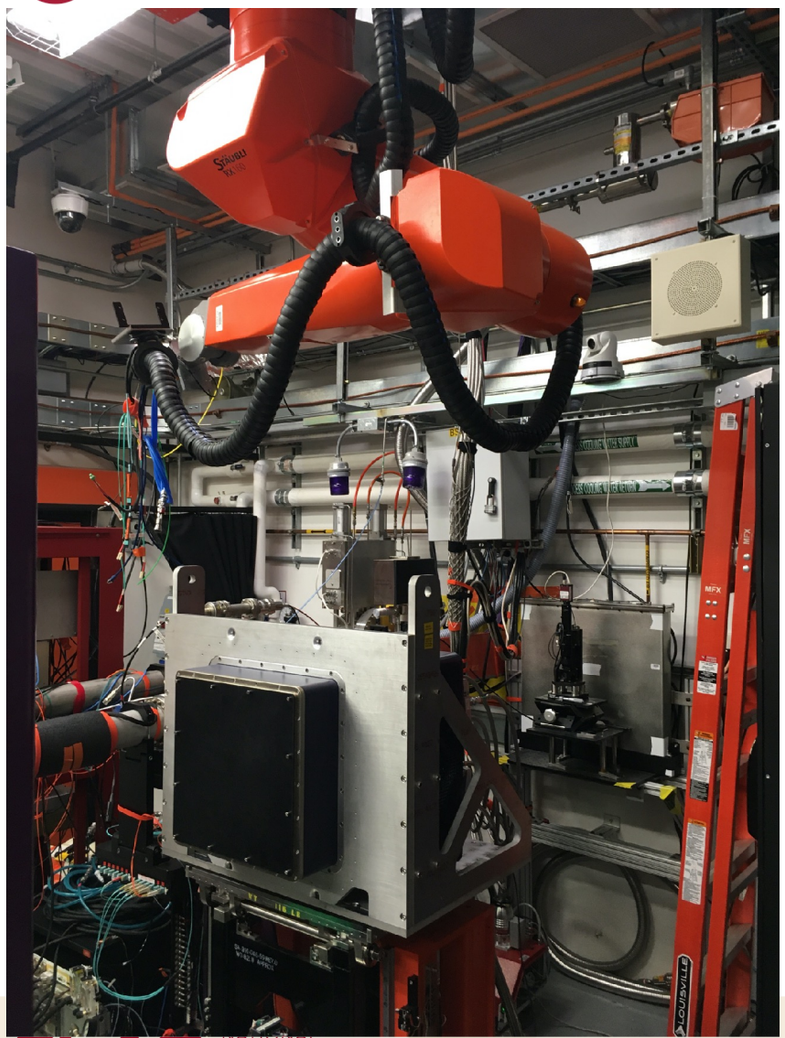


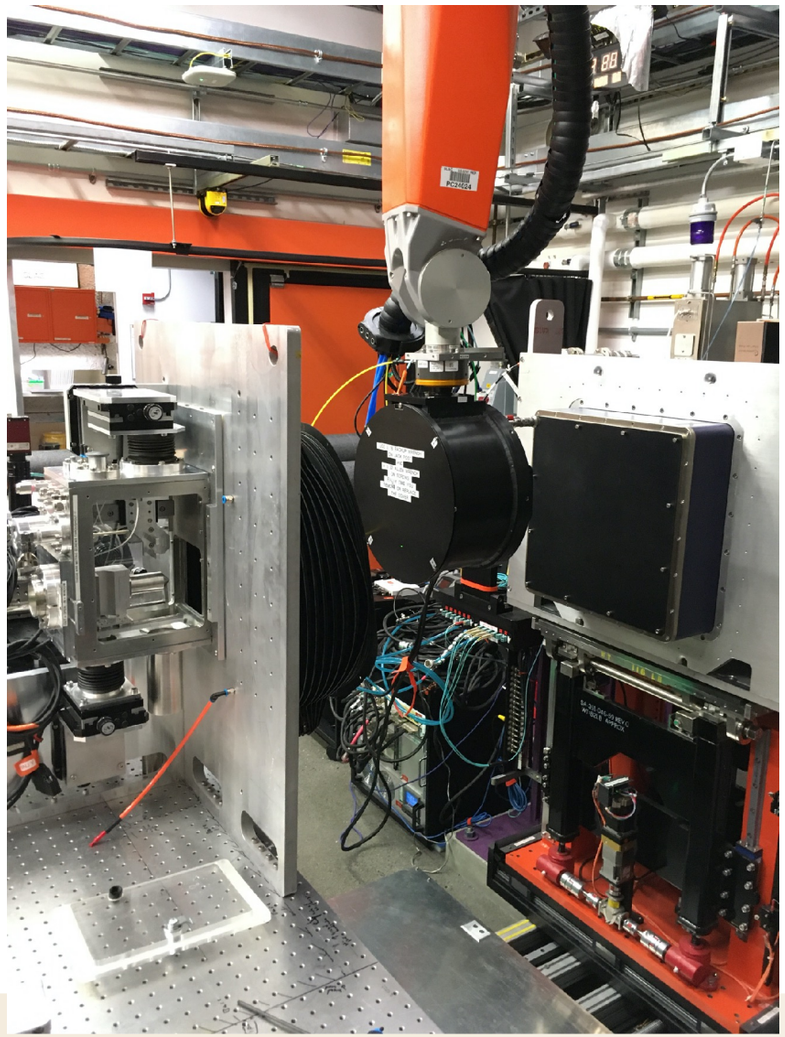
Standard Configurations

- Goniometer system with sample mounting robot
- Helium-Rich Ambient (HERA) instrument for time-resolved liquid jet crystallography

https://lcls.slac.stanford.edu/standard-configurations#mfx

MFX Detectors



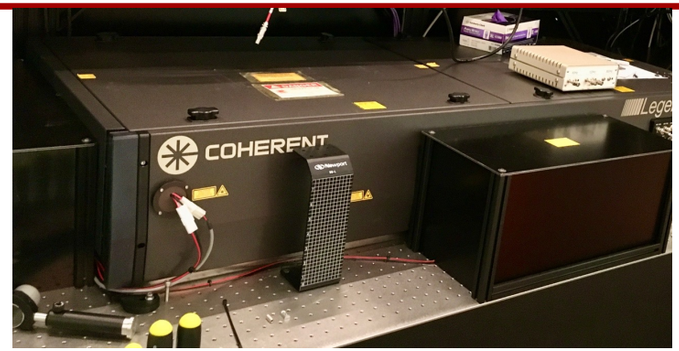


- Rayonix on the mover
- ePix10k-2M and other smaller detectors on the robot arm
- ePix100
- Jungfrau 0.5M and 1M

MFX New(ish) Capabilities

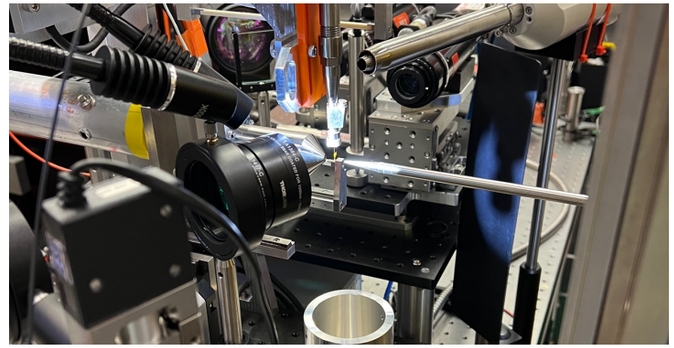
fs Ti:Sapphire optical pump laser

- Fundamental (800 nm) or 2nd harmonic, ~ 50 fs pulse
- Beam delivered to the sample collinearly with X-rays
- TOPAS-Prime OPA capable of 480-2400 nm



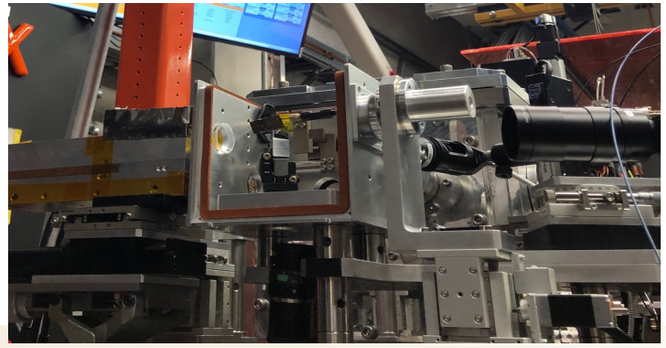
AirA standard configuration

- In Air environment and not He enclosure (HERA)
- Multiple sample delivery modes permitted
- Compatible with optical pumping



Liquid Jet Endstation (LJE)

- He environment compatible with spectroscopy and forward scattering
- Horizontal sample delivery



CXI - Coherent X-ray Imaging Standard Config

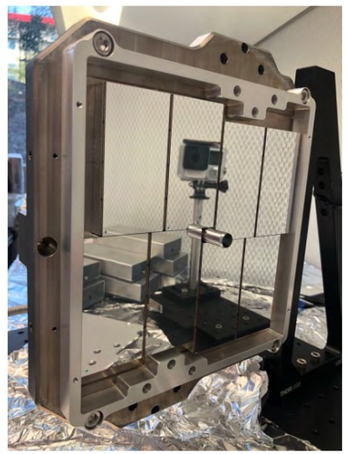
Forward scattering – high power density, optimal signal to noise (vacuum)

two interaction regions:

- 1 micron focus
- “parasitic” Chamber uses a refocused beam from microfocus
- Unfocused or CRL focused beam – photon energies >10keV

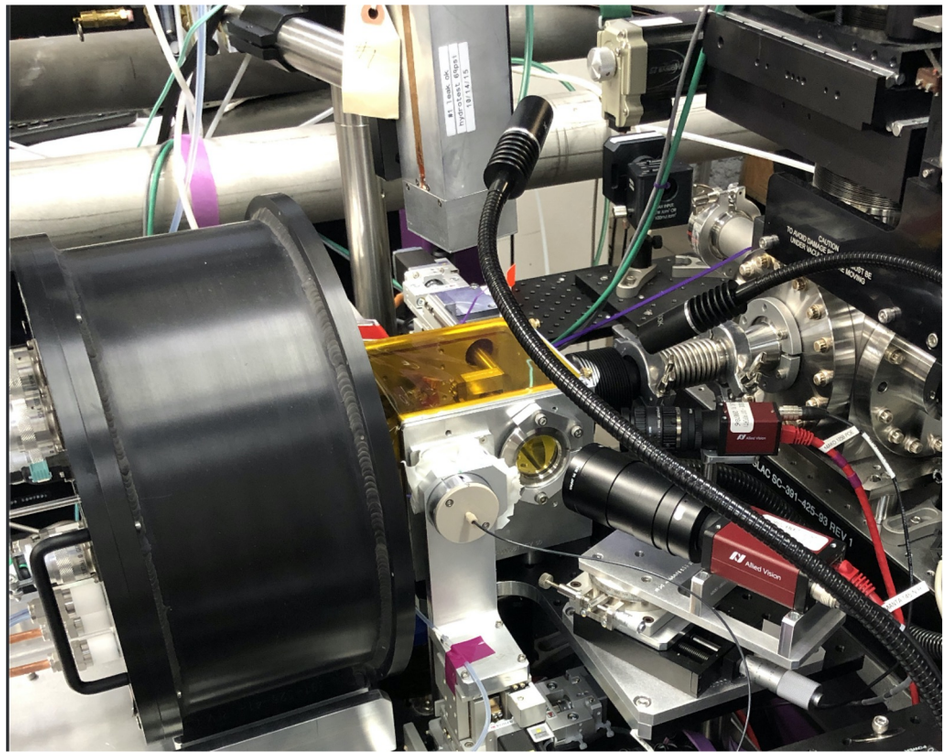
Jungfrau 4M

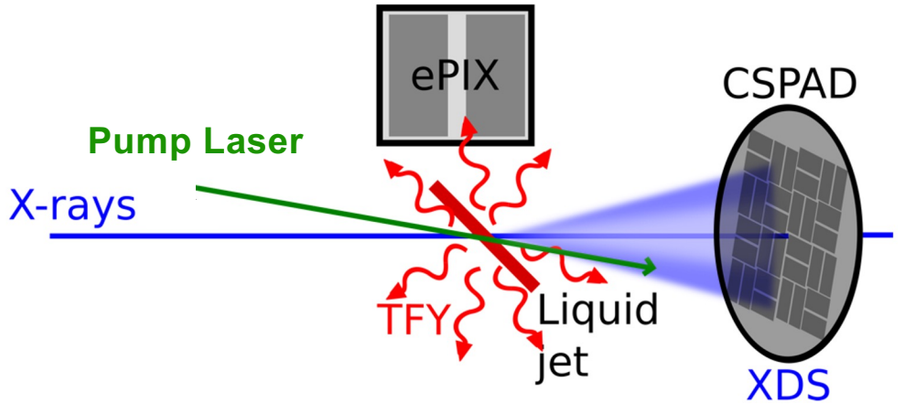
- Microfocus
- Adaptive gain
- Higher dynamic range
- Up to 1kHz repetition rate
- CSPAD for Parasitic Experiments

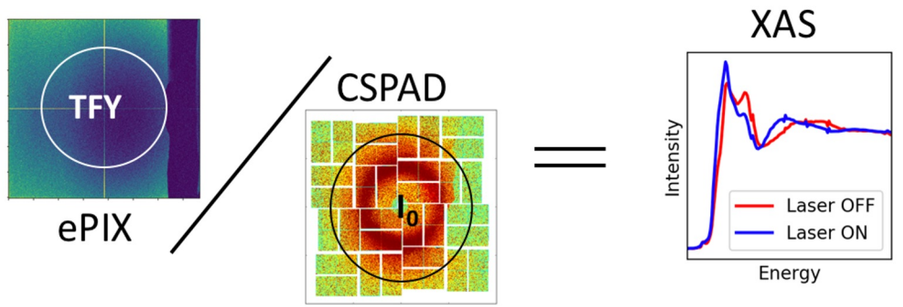


XPP Standard Configuration #2: Liquid Phase XAS

Time Resolved Hard X-ray XAS



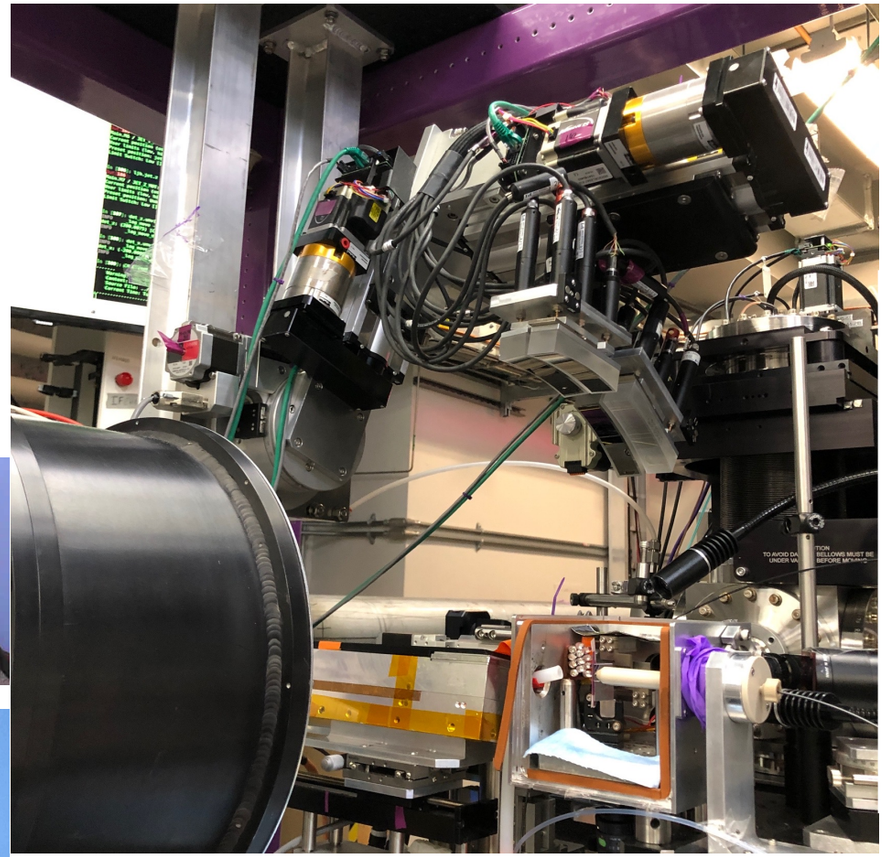


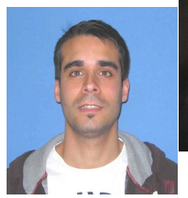


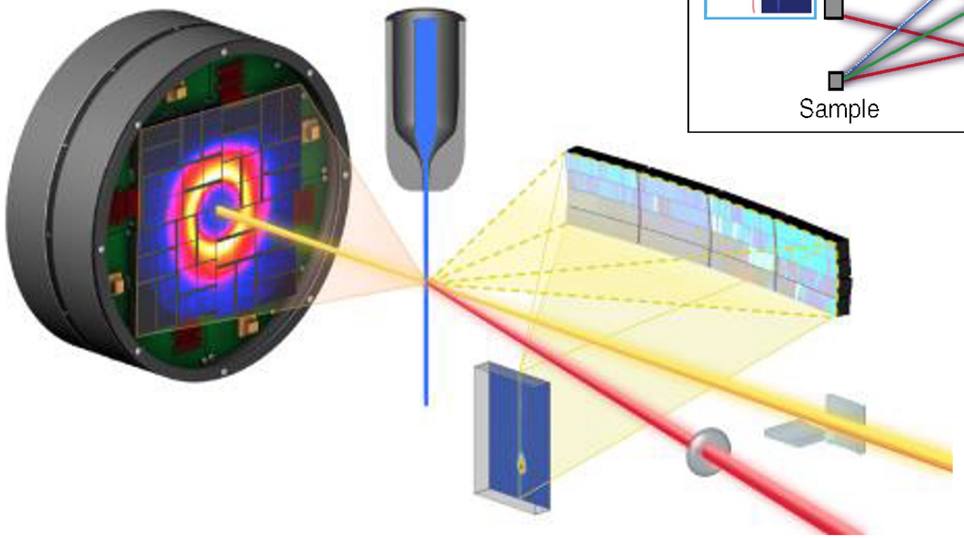
https://lcls.slac.stanford.edu/instruments/xpp/standard-configurations

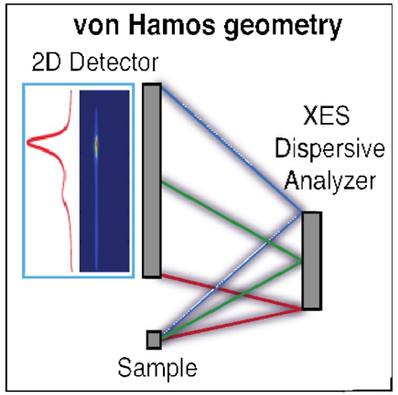
XCS Standard Configuration #1: Liquid Phase XES/XDS

Time Resolved Hard X-ray XES +XDS





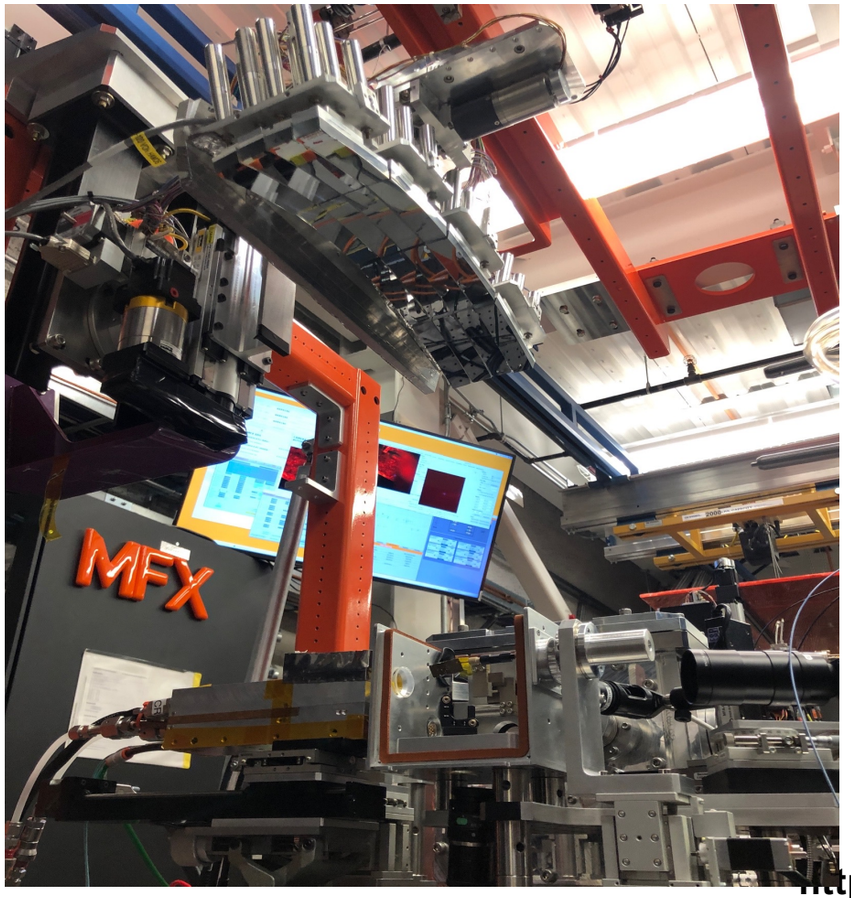


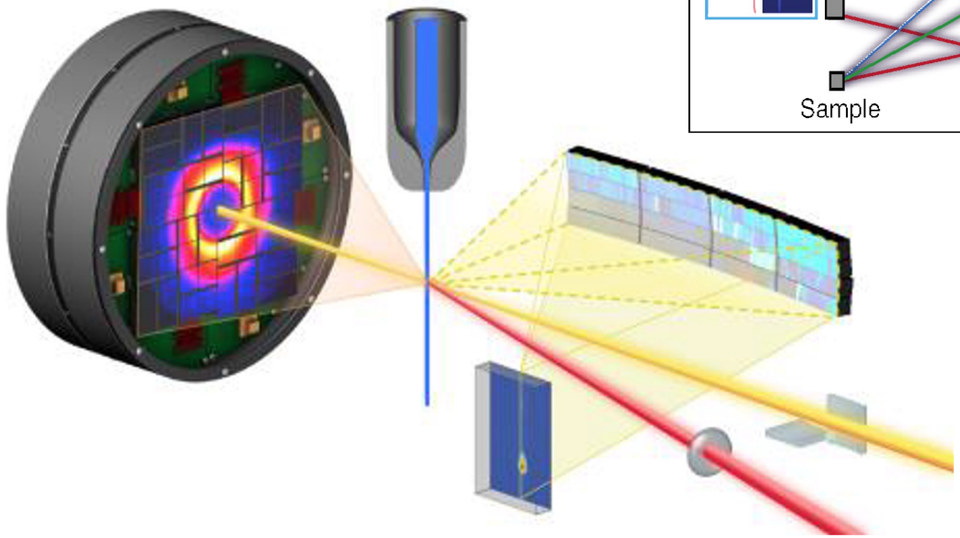


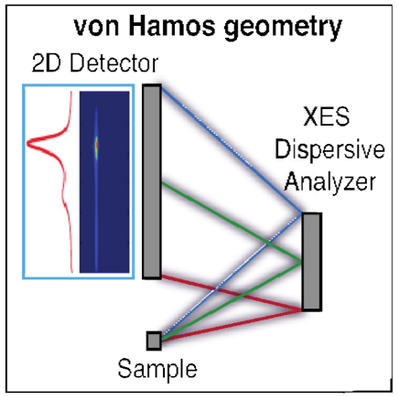
https://lcls.slac.stanford.edu/instruments/xcs/standard-configurations

MFX Standard Configuration #3: XRD/XES

Hard X-ray XES+XRD: Damage-free atomic and electronic structure of metalloproteins at RT

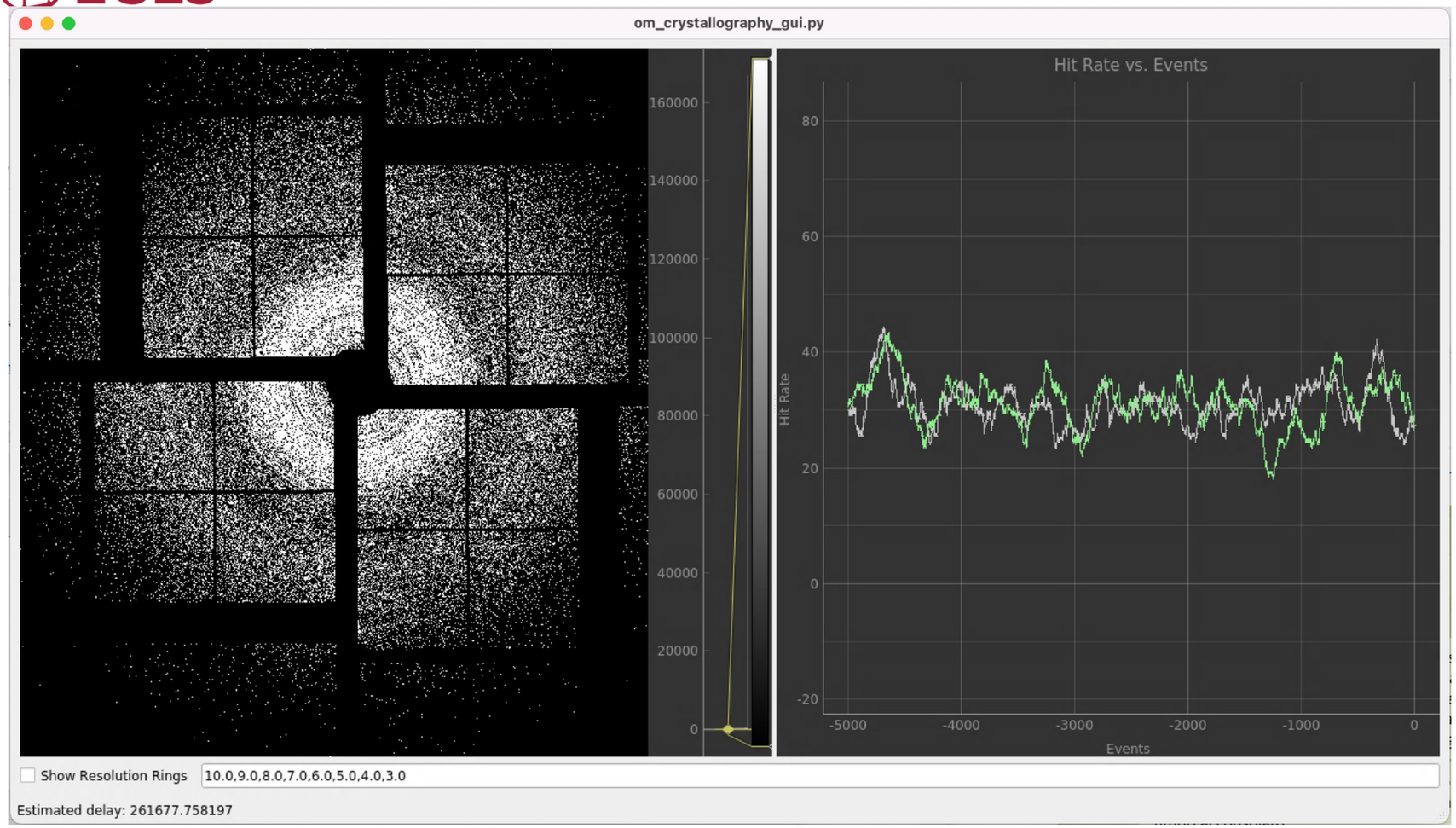






https://lcls.slac.stanford.edu/instruments/mfx/standard-configurations

Online Monitoring Upgrades



New in OM:

Preliminary support for pump-probe serial crystallography experiments:

- Separate statistic (hit-rate) for laser-on and laser-off events
- Separate hit-rate history for laser-on and laser-off events

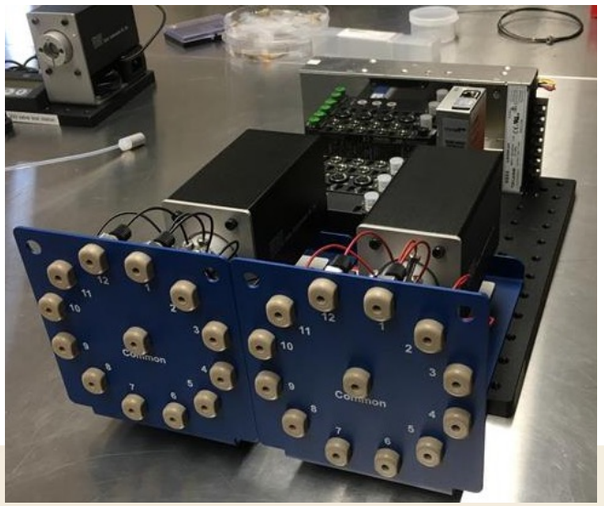
Standard sample delivery hardware

Proportionairs

Bronkhorst gas mass flow controllers

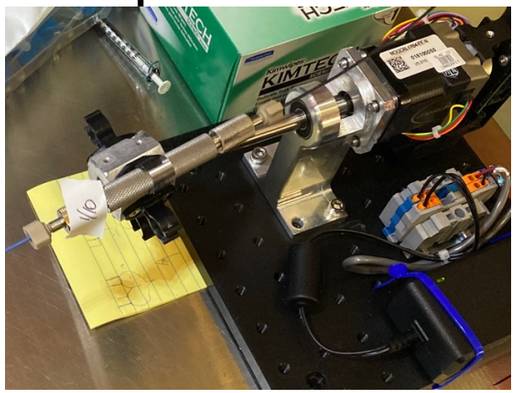
Shimadzu LC-20 and LC-40 series HPLCs

Sample selector boxes



Sensirion liquid flow meters

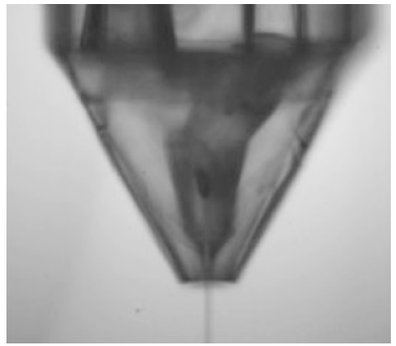
Compact anti-settlers



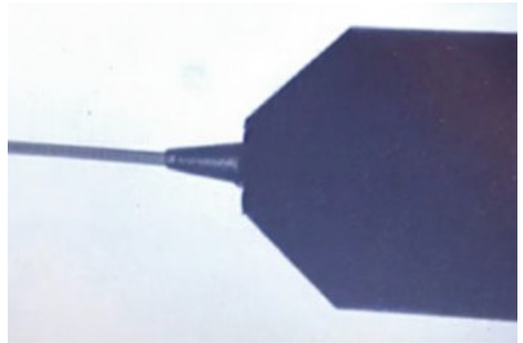
High pressure reservoirs

Currently supported sample delivery methods and formats for Bio

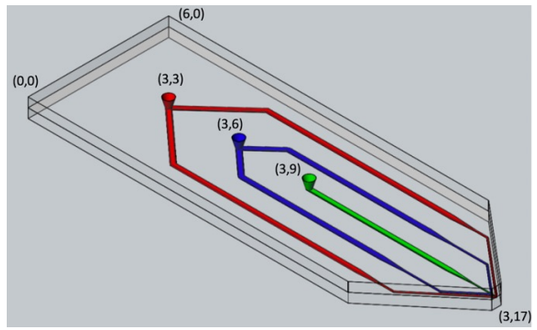
Several injection formats are supported across the hutches



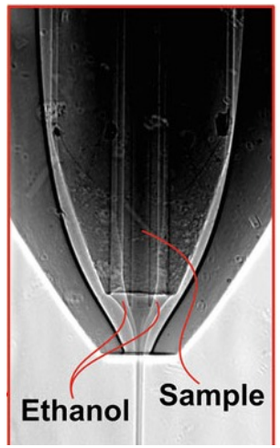
3D printed GDVN (above) and DFFN (below) (Kirian Group ASU)

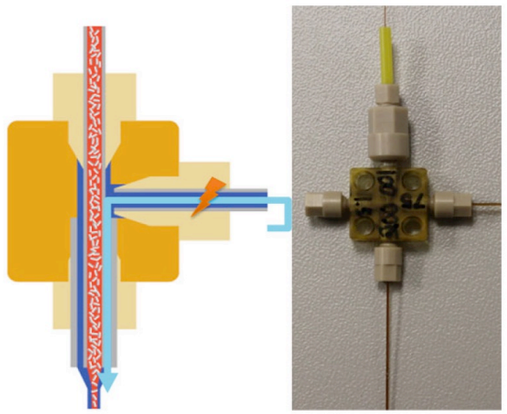


LCP and HVE sample injector (Weierstall group ASU)

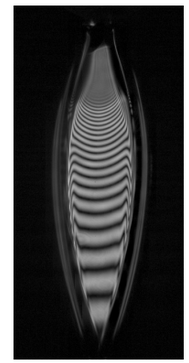


Chip nozzles and chip interfaces





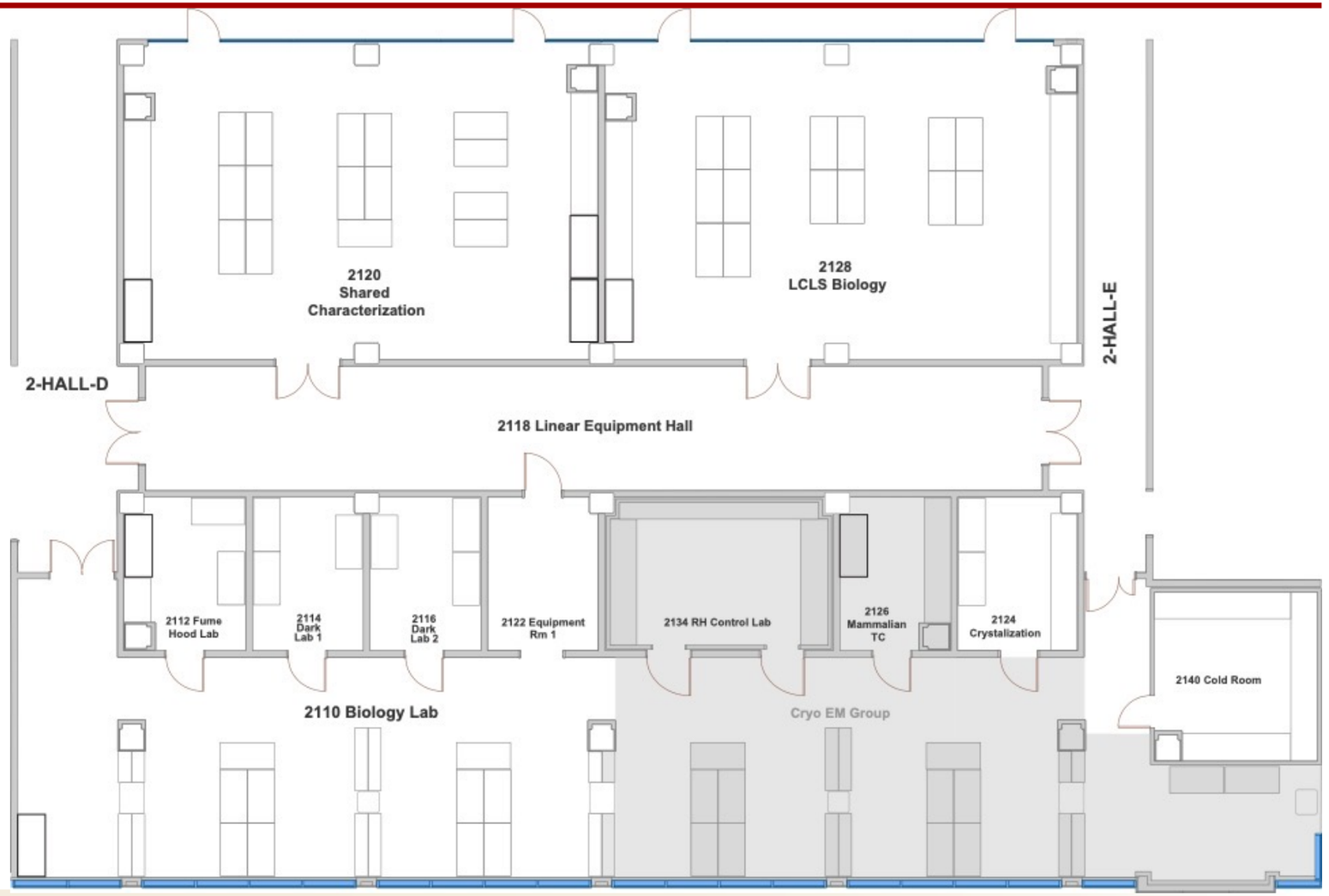
Electrokinetic (MESH/coMESH)



Sheet jets*

Biolabs at the Arrilliaga Science Center

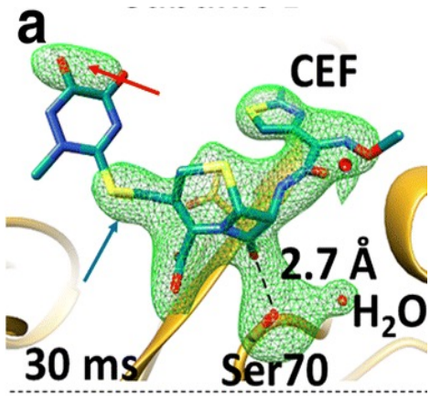
- ~7,000 sqft of usable space
- 300 sqft of coldroom
- Two darklabs
- BSL1 and BSL2 zones
- Equipment to go from cell growth through protein purification and crystallization

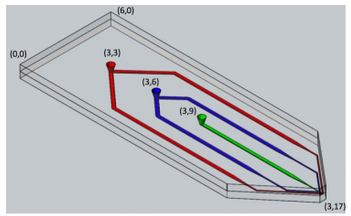


NIGMS Center for Structural Dynamics in Biology

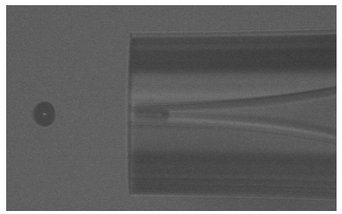
LCLS

NIH National Institute of General Medical Sciences

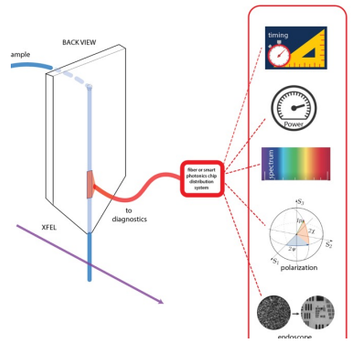




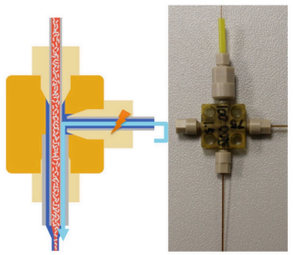
Standardized (chip) nozzles*



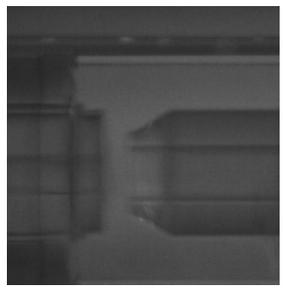
Droplet on Demand*



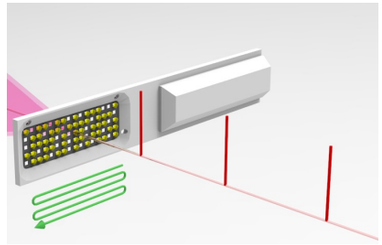
Integrated diagnostics*



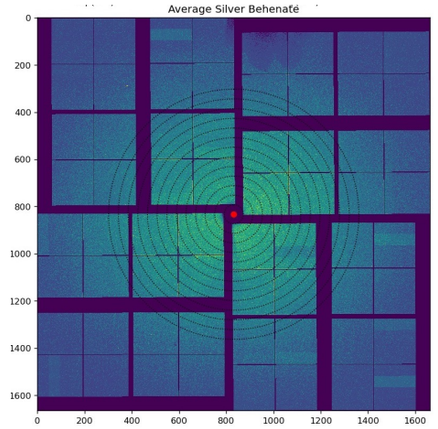
Electrokinetic (MESH/coMESH)



Short time point mixers



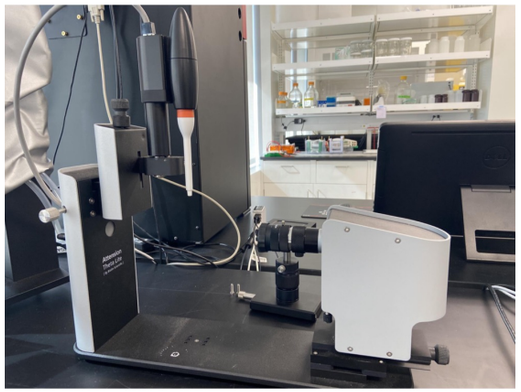
Fast fixed target



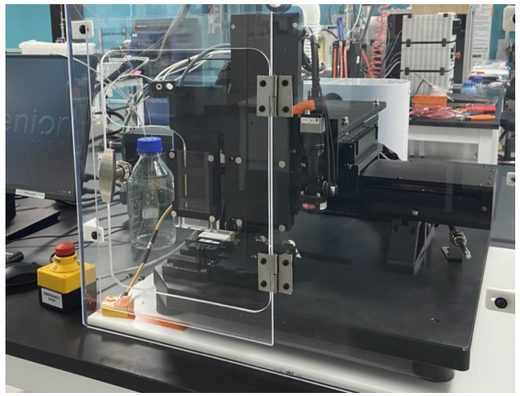
New equipment at the Biolabs at the Arrillaga Science Center

Anaerobic Glove Box

- ppm O2 levels
- Nanosight, microscope in box
- Schlenk line available

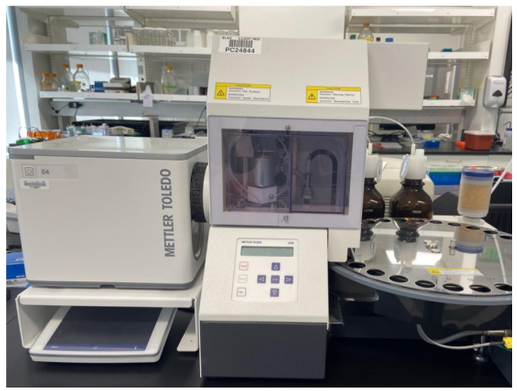


Surface Tensiometer



Automated Droplet on Demand

Automated Viscometer



Automated Densiometer

Thank you!

Rapid Access and Biology at LCLS Website
- https://biology-lcls.slac.stanford.edu/

Biolabs at ASC Website
- https://lcls.slac.stanford.edu/biolabs-asc

LCLS Sample Prep Labs Website
- https://lcls.slac.stanford.edu/spl

Injector Characterization Labs Website
- https://lcls.slac.stanford.edu/sed/lab

Christopher Kupitz: Sample Environment
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Ray Sierra: Sample Delivery
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Mark Hunter: Rapid Access, Bio, SED
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Bio@LCLS

Bio-Bloopers

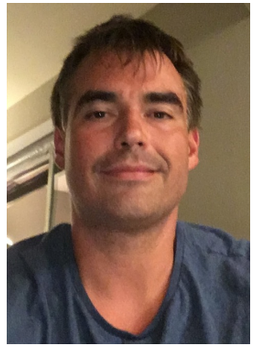
XFELs for Bio Book

Backup Slides

Sample environment and delivery (SED) team

Dan DePonte

Christina Hampton



Mark Hunter

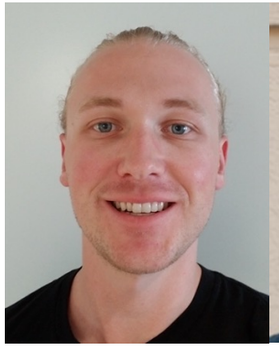
Jake Koralek

Mason Landrum

Cynthia Melendrez

Ray Sierra

Tim B van Driel



Brandon Hayes

DJ Hoffman

Maithri Kashipathy

Chris Kupitz

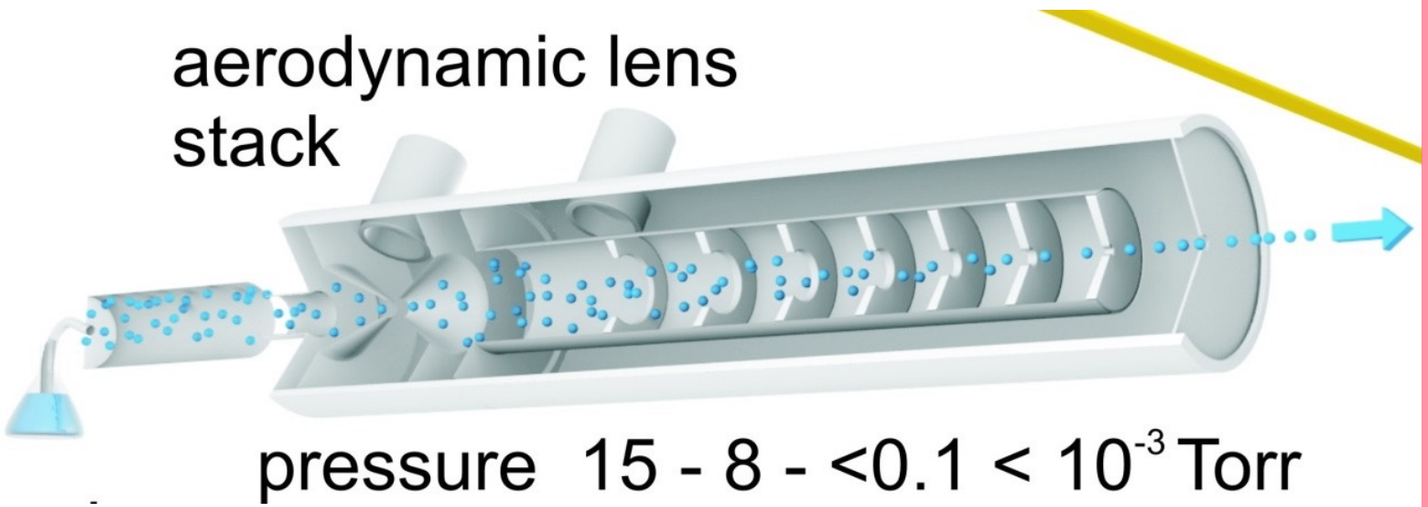
Stella Lisova

Tyler Pennebacker

Bob Sublett

Peter Walter

Aerosol Delivery (ALS) is back at LCLS



Main R&D areas

- Aerosolization
- Focusing
- Sample preparation/state

Hutches/Instruments

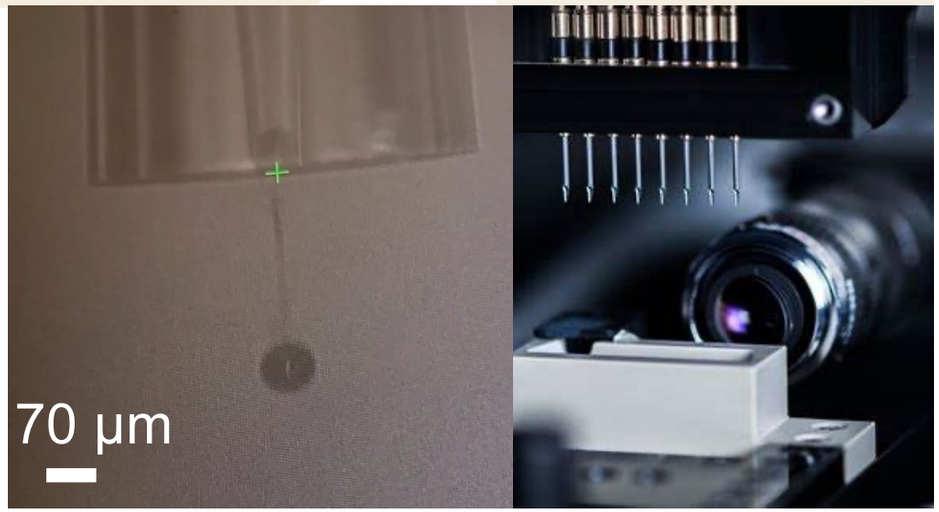
- TXI
- CXI
- TMO
- UED?

Science Areas

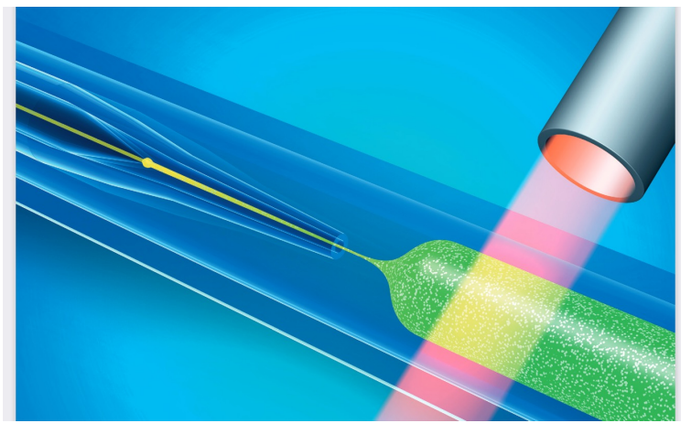
- Materials Science
- AMOS
- Bio
- Chem?

Future: Chips, Drops, and More Access

- Drop on demand capabilities to enable forward scattering and crystallography experiments in ambient conditions (commissioning Run 19, EOY)
- Characterizing chip and delivery methods to make sample delivery more of a science rather than an art (NIH P41 Grant: Boutet, Cohen, Hunter)
- New flexible Rapid Access program
  - lab testing and characterization
  - SSRL times
  - parasitic LCLS shifts
  - *5 star user support!*



K. Karpos and R. Alvarez (Kirian@ASU, Scienion and SLAC)



Huyke *et al. Anal. Chim. Acta* 2020