
# SSRL and LCLS
## Facility
## SSX and SFX

Clyde Smith
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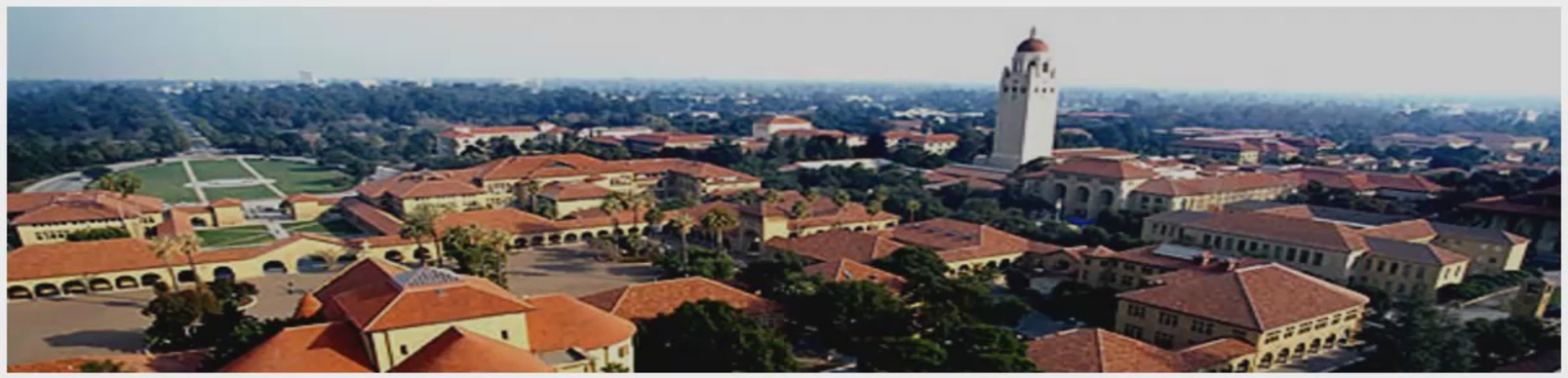
Structural Molecular Biology
Stanford Synchrotron Radiation Lightsource



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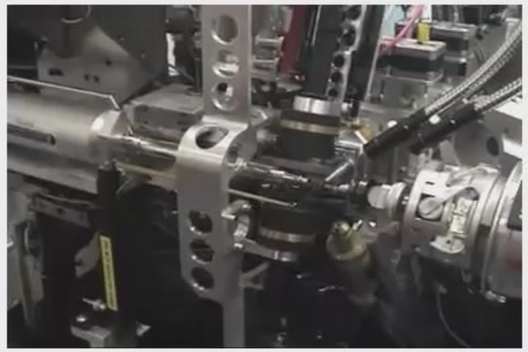
# Automation and Remote Access


Full automation
- all beam line functions motorized

Sample changing robot (SAM) (since 2004)
- automated sample mounting

Remote access (since 2005)

High-throughput crystal screening (since 2005)
- real-time results and analysis



Automated data collection and analysis (2011)
- Autodrug

X-ray rastering (2012) and shutterless rastering on BL12-2 (2014)
- Rastering now included in crystal screening

UV-vis microspectrophotometer on BL11-1 (2013) and BL9-2 (2016)
- Raman spectrometer to come (2019)

Faster robot (2015)
- increased robot speed, crystal pre-fetching
- 25 sec crystal exchange


Remote access at room temperature (2018)
- robotic mounting and humidity control

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# The SSRL PX Resource


| Beamline | Capability | Flux (p/s)[a] @ 500 mA | Availability for general users | Special equipment | Detector |
|---|---|---|---|---|---|
| 12-2 | MAD (6-17keV) Microfocus | $4x10^{12}$ | 60% | Microcollimator, Microdiffractometer, On-axis camera | PILATUS 6M |
| 9-2 | MAD (6-15keV) | $8x10^{11}$ | 100% | UV-Vis absorption Microspec, Microdiffractometer | PILATUS 6M |
| 14-1 | MAD (6-13keV) | $2x10^{11}$ | 50% | Microdiffractometer | EIGER 16M |
| 7-1 | MAD (7-12.7keV) | $2x10^{11}$ | 100 % | Kappa diffractometer | Q315 |
| 12-1 | MAD (5-15keV) Microfocus | $4x10^{12}$ | 50% | Microcollimator, Microdiffractometer, On-axis camera | Rayonix 325 |

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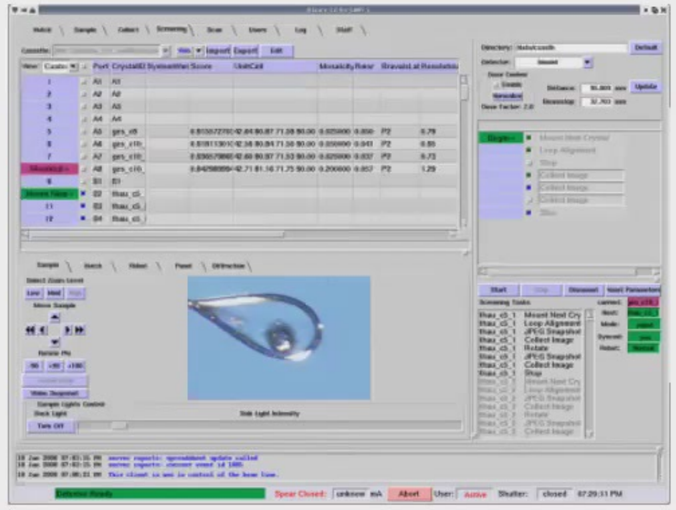
# Data processing


EIGER 16M, currently running on a bend magnet beamline

- cbf files
- will be moved to BL12-1
- conventional and SSX

For all beamlines

- screening (2 images)
- analysis server in background
- data returned to spreadsheet
- Web-Ice for data collection strategy
- data collection run exported to Blu-Ice

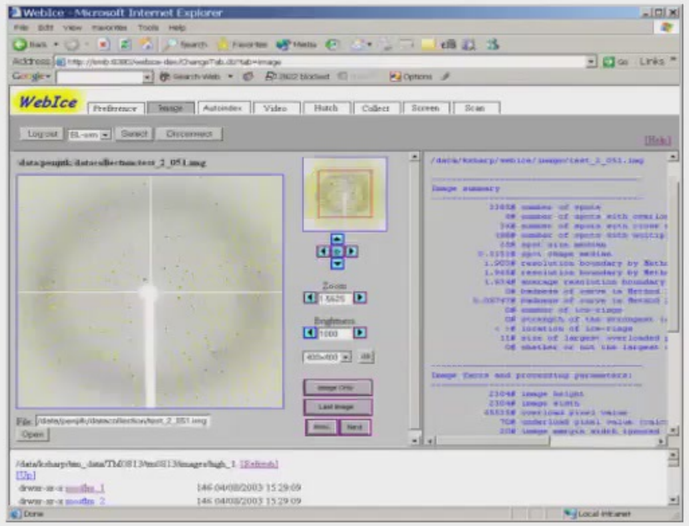


Data collection

- 0.1 or 0.2º
- 360º
- autoprocessed with xds

2 PB storage

- users can connect after their beamtime to process



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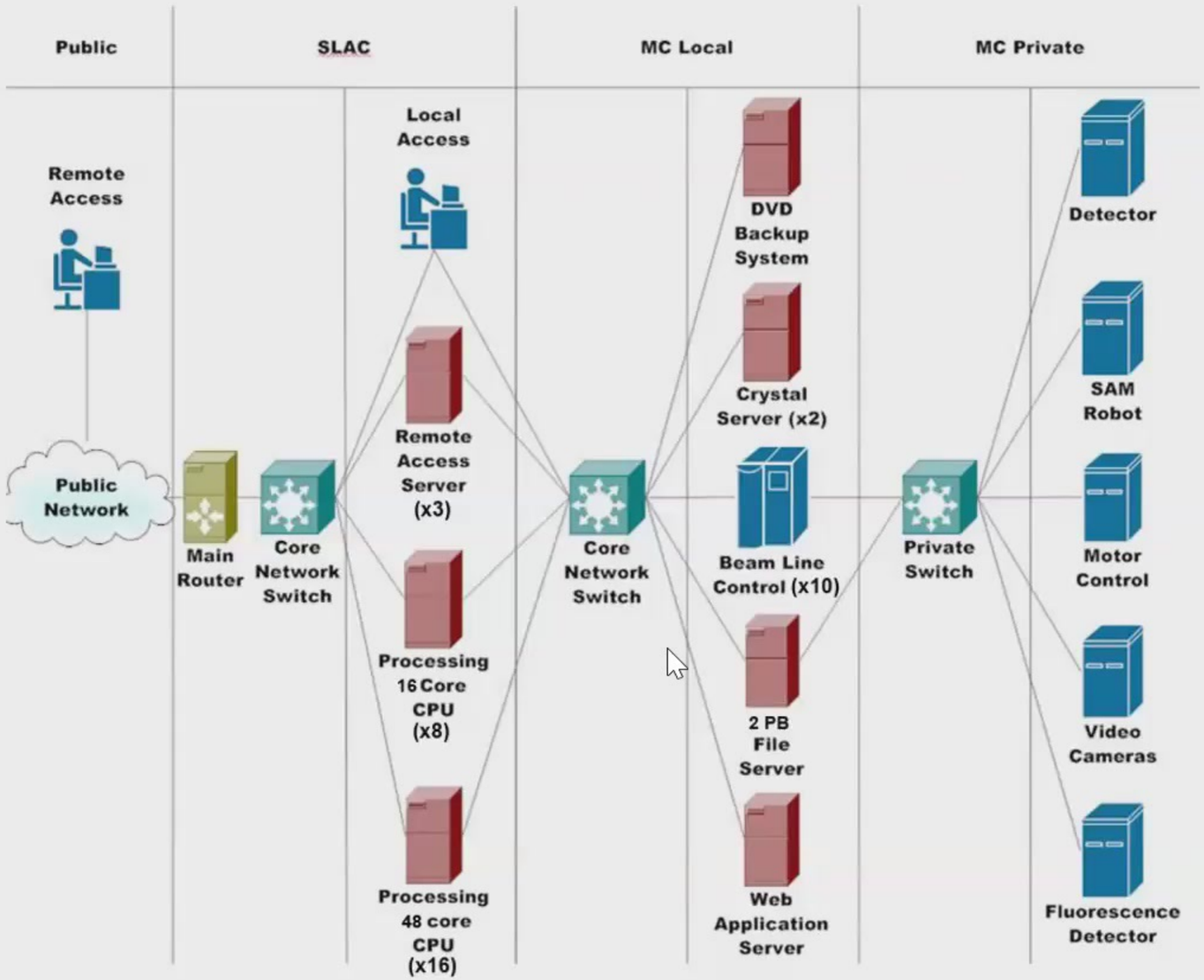
# SSRL PX Computing Environment

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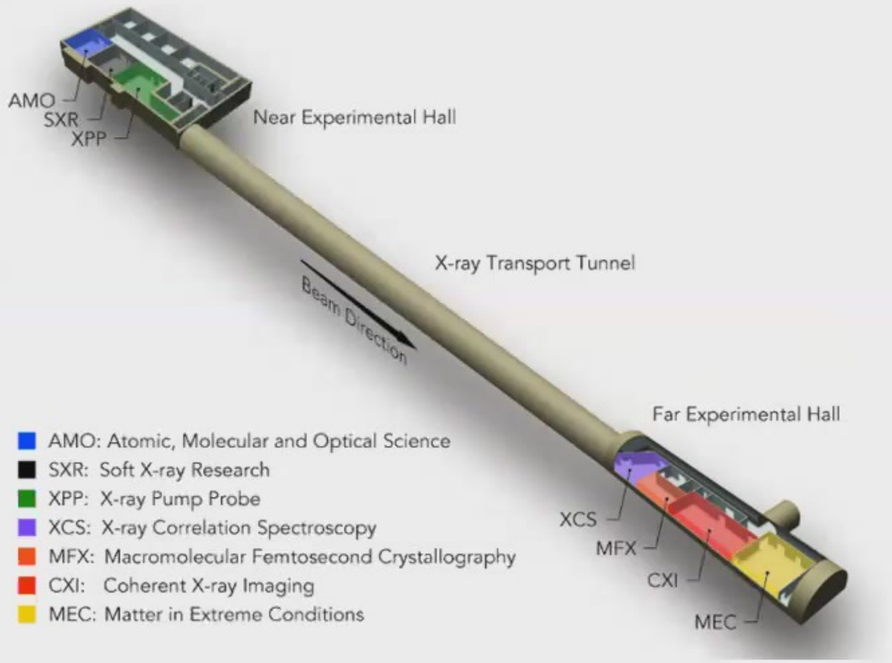
# LCLS X-ray Free Electron Laser





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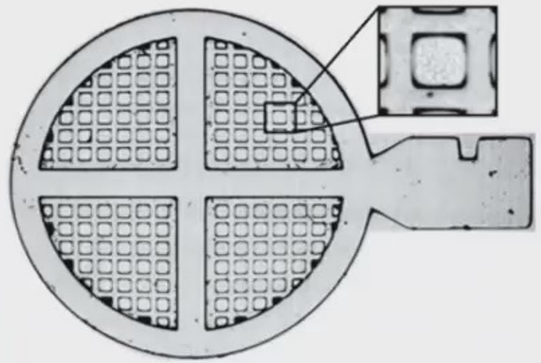
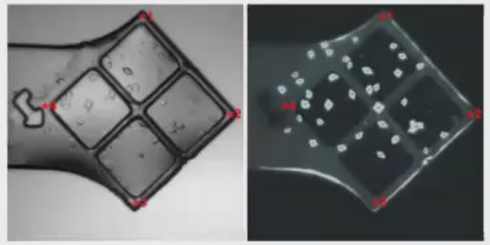
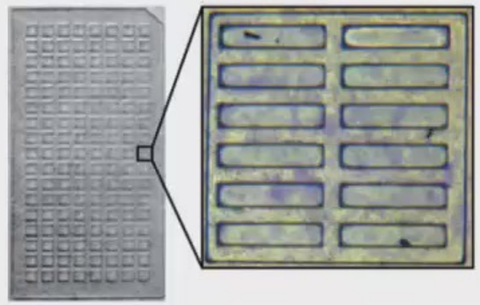
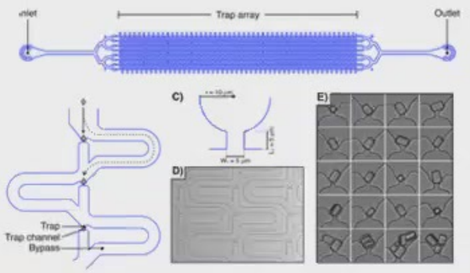
# Fixed Target Serial Crystallography





http://www.mitegen.com/






If it has known dimensions and fiducials, we can use it!


Cohen, *et al.*, *PNAS* (2014)
Roedig, *et al.*, *Sci Rep* (2015)
Feld, *et al.*, *J Appl Cryst* (2015)
Lyubimov, *et al.*, *Acta Cryst D* (2015)
Murray, *et al.*, *Acta Cryst D* (2015)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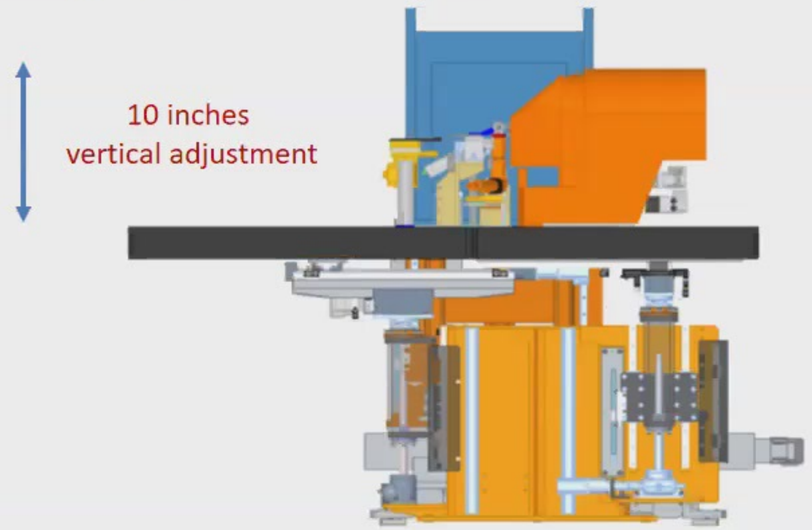
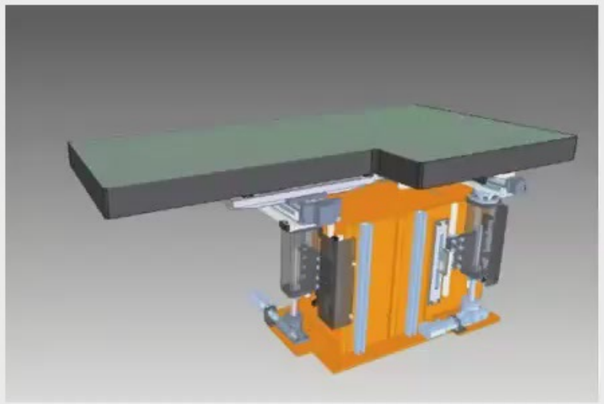
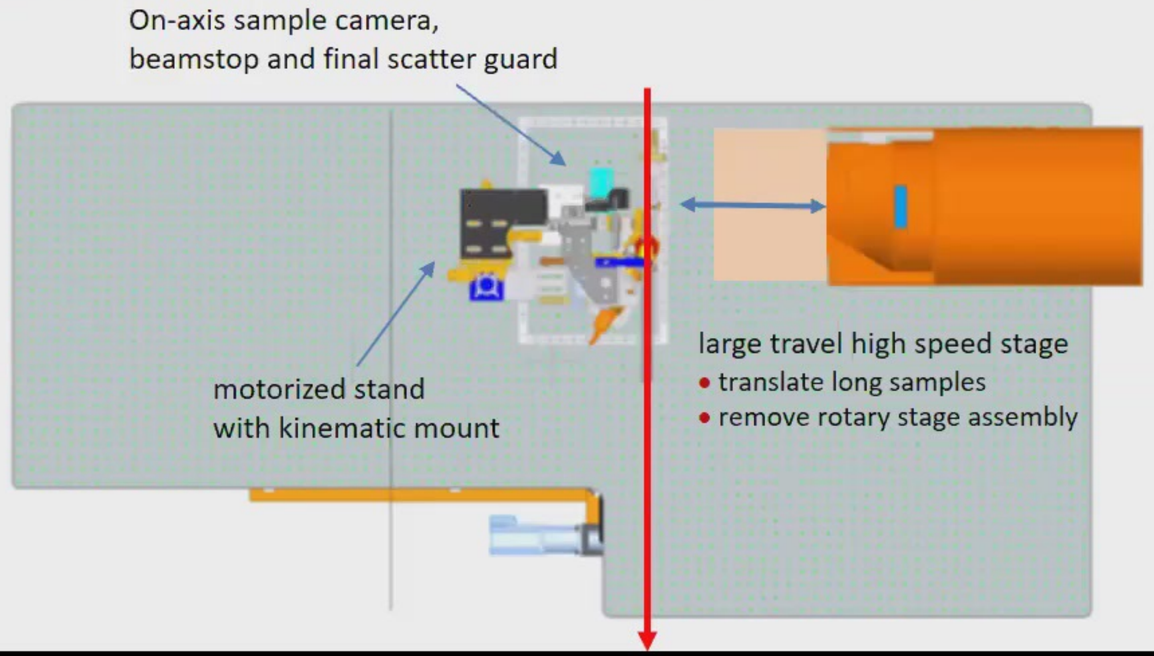
# MFX Experimental Table


## Rapidly switch between experimental setups

- Large table horizontal adjustment so the goniometer setup may remain while a different experiment is setup on other side of table
- All motions fully encoded (0.5 μm repeatability) for rapid repositioning of hardware
- The goniometer moves back to clear space for other experiments that may use the same on-axis microscope, beamstop and scatter guard
- Motorized stand has kinematic mount to easily swap from a cryo-cooler, humidity control device or other sample delivery device.





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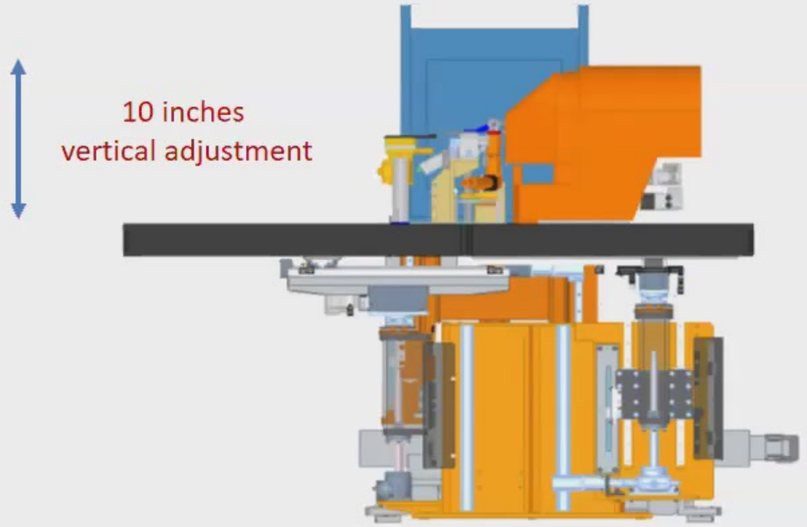


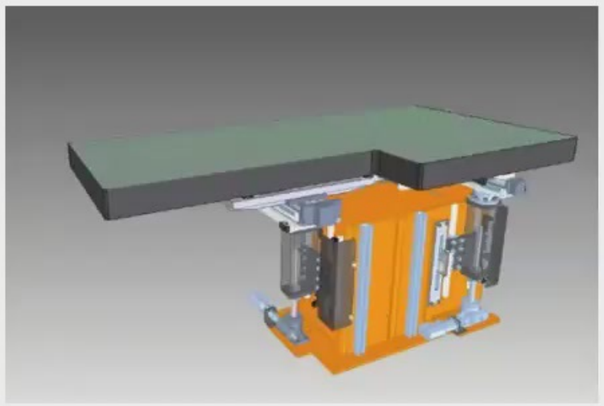

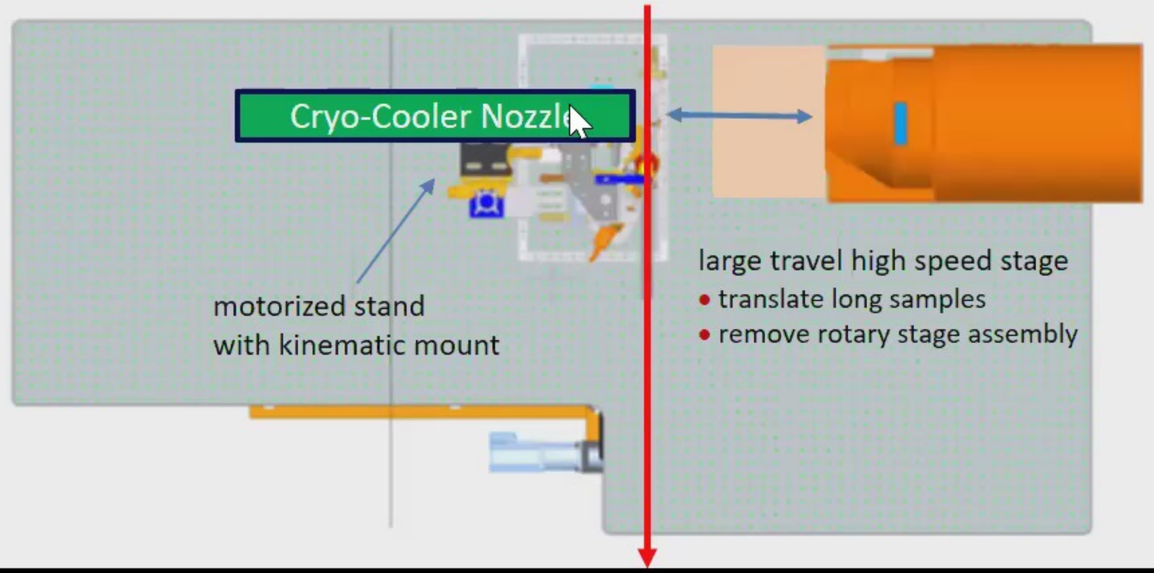

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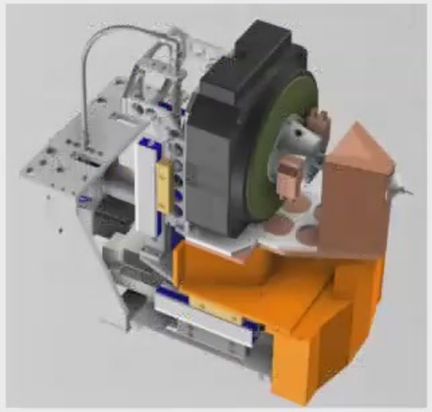
# LCLS-MFX Standard Goniometer Setup

## Developments and Upgrades



Air-bearing phi-axis (360 deg/sec)
Air-bearing sample z stage (up to 300 mm/s)
Low profile SMARACT stages

### High Performance Micro-crystal Goniometer

- Closer detector approach
- Faster sample translations and concerted motions for rapid multi-crystal data collection using mapped high density mounts at 120 Hz
- Design completed Jan 2018 – fabrication in progress

### Improved Sample Visualization

- Upgrade for visualization of light sensitive samples in low light and IR conditions – 2017
- *in-situ* UV-tryptophan fluorescence microscope - in development

### Automated Data Collection at Room Temperature with Humidity Control

- Commissioned in October 2017 – released to general users in 2018 (run 17)

### High-end X-ray Detector System for Femtosecond Crystallography - Rayonix MX340-HS-C2

**Rayonix 340-HS-C2 detector delivered for LCLS run 17 (Sept 2018)**

- Larger area and higher dynamic range than the CSPAD (large unit cells, higher resolution data)
- Supports 40 Hz operation
- Center hole passes direct beam.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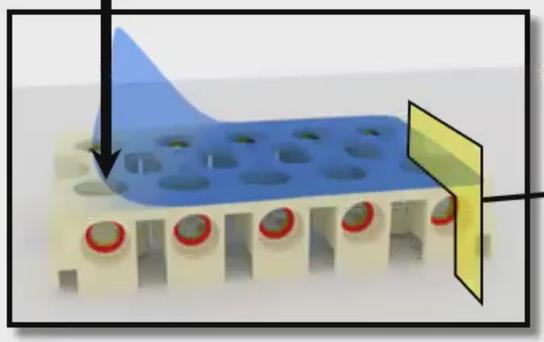
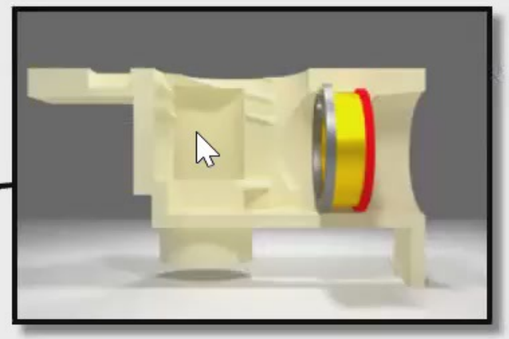
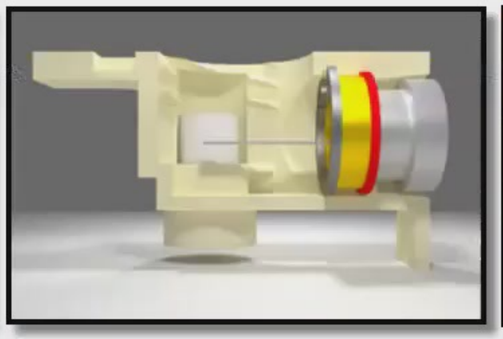
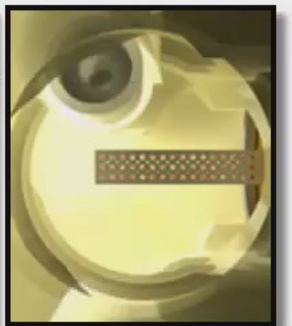
# Crystallization, Storage and Shipping Plate

Compatible with Qiagen screw-caps





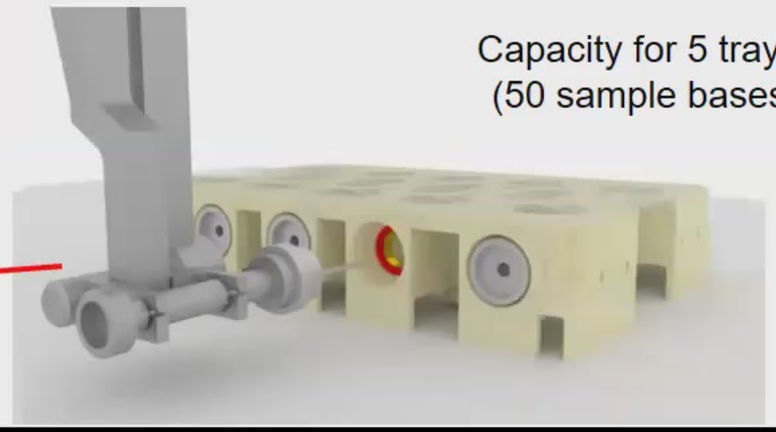




Ring magnet holds sample base inside

Sample delivery device in hydrated environment

Automated sample exchange with SAM



Capacity for 5 trays
(50 sample bases)

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# New Microfocus Beamline SSRL BL12-1


## BL12-1 First Light 2018

### Specifications

**5-15 keV** range, S-SAD phasing optimized

Intense X-ray micro-beams: **1 μm²** to **100 μm²**

**>2x10¹² photons/sec flux into 5 x 5 μm²** (~6x BL12-2)

**Multilayer monochromator option for SSX**

1% energy bandpass (similar to LCLS)

**4.3 x 10¹⁴ photons/sec to focal plane**

EIGER PAD detector

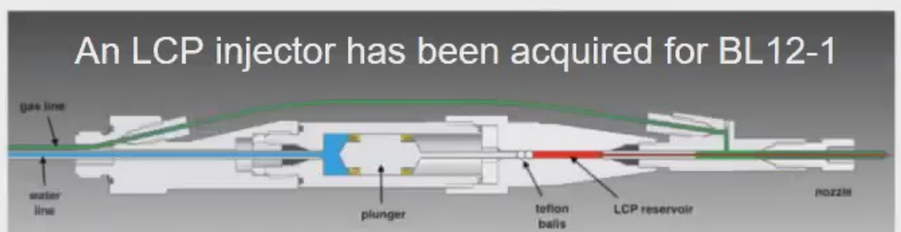
**133 Hz** frame rate

or **750 Hz** region of interest

Complete remote access capability including room temperature collection at controlled humidity

### Time Resolved Studies - Liquid-Crystal Injectors

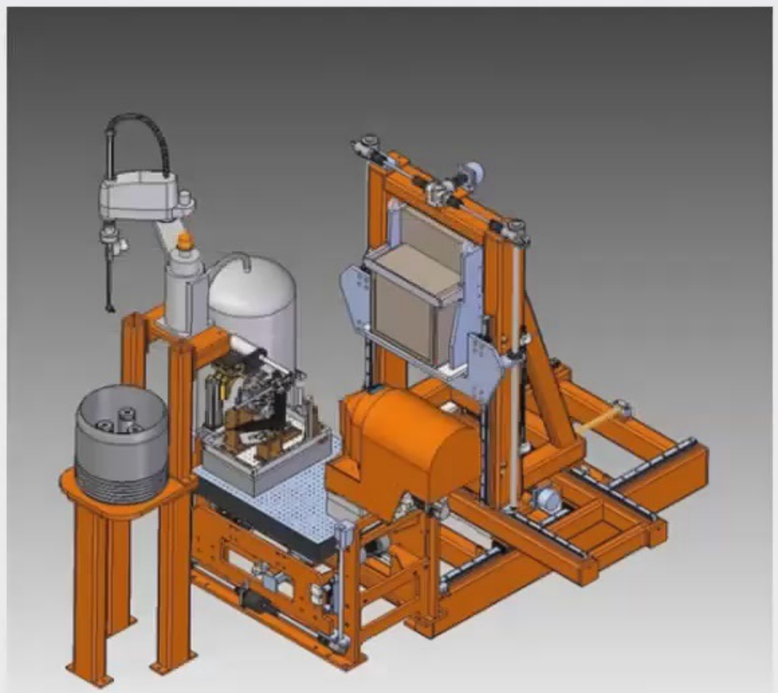
An LCP injector has been acquired for BL12-1




Weierstall, et al. Nature Comm. 5 (2014)

### Synergistic Operation with LCLS-MFX

Similar equipment and control software



Stanford and Scripps Funding

50% of beam time to the general user community

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# New Microfocus Beamline SSRL BL12-1