

Operation Discussions

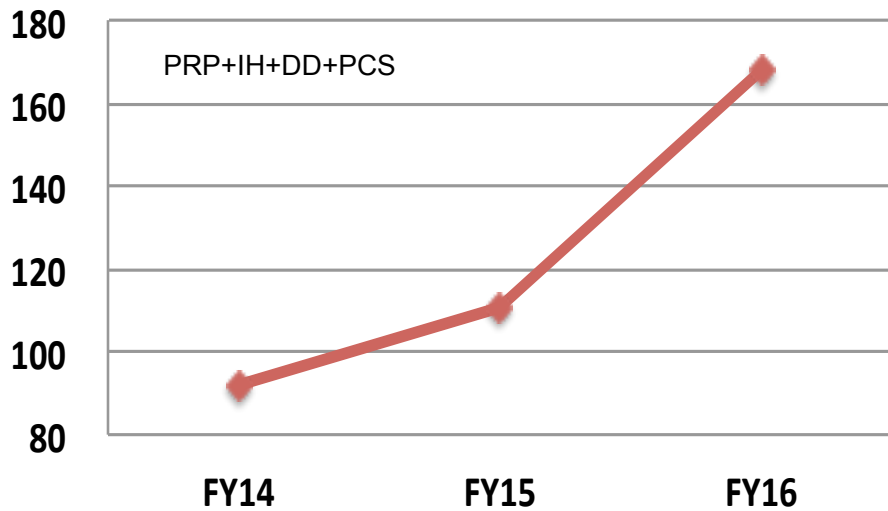
Diling Zhu, on behalf of LCLS

8th Hard X-ray FEL Collaboration Meeting, 2016

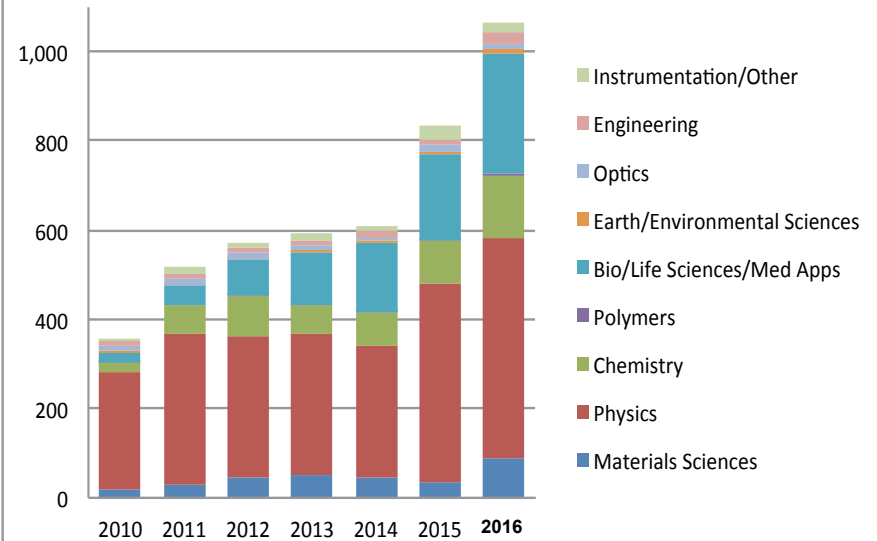
- Increase multiplexing flexibility
- Implement standard configuration
- Opportunities for automation

Increase user access to LCLS (FY16)

Total number of LCLS experiments



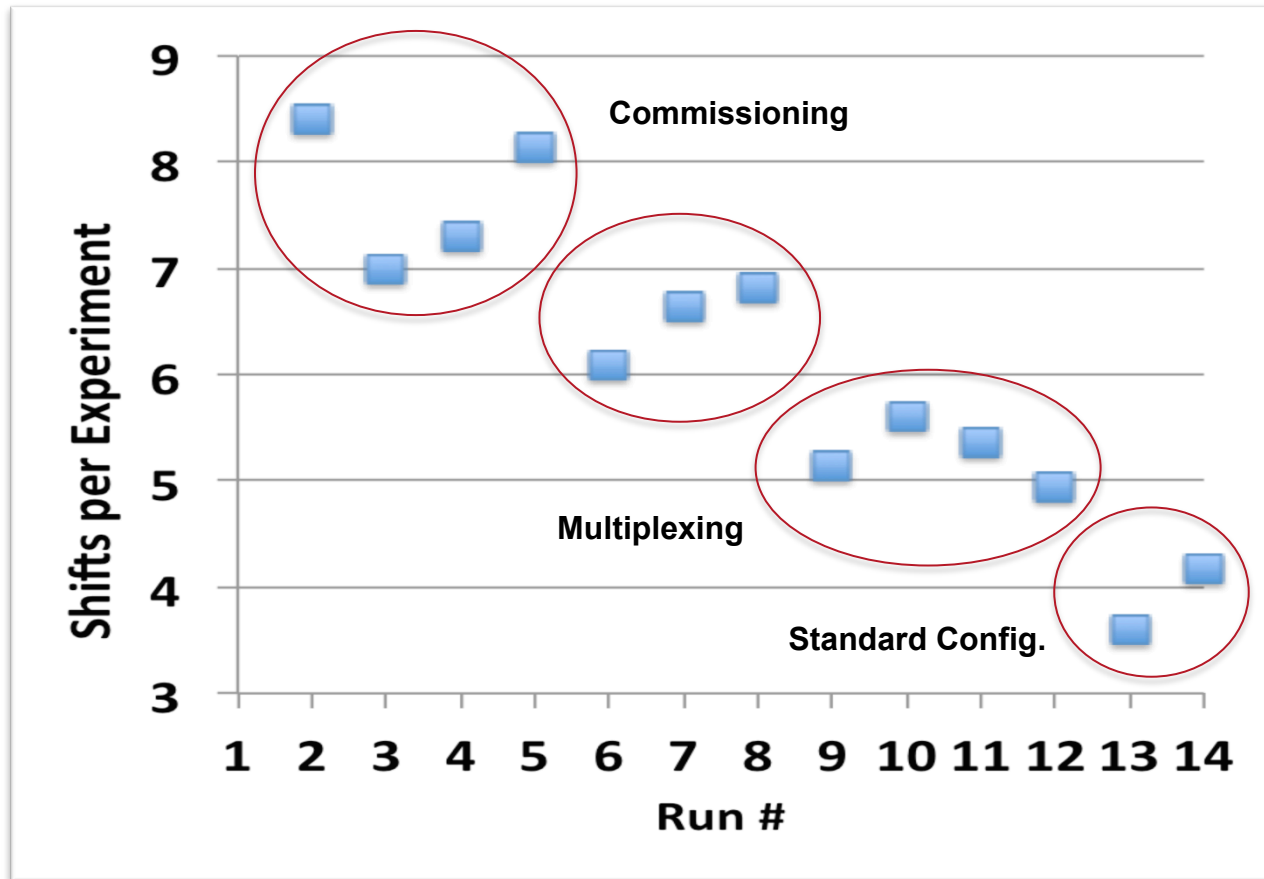
Unique Onsite Users for LCLS by Discipline



50% increase in user experiments

27% increase in onsite users

Average duration of LCLS user experiments



Implementation of “standard configurations” has been well received by the user community, representing ~30% of all proposals

Before Multiplexing (2011.11 – 2012.05)

Scheduling LCLS Run V

Ver 8: CB 10/27/11

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| Nov 11 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | | |
| Day | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | | |
| Night | PPS checkouts & start-up | | | | | | | | | | | | | | | | Com | Com | Com | Com | Com | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | | L477 Robinson | | | | | L421 Coffee | | | | | Gruebel (L304, run 4) | | | | | |

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| Dec 11 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
| Day | Thur | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat |
| Night | L498 Yachandra | | | | | | | L487 Sokoloski-Tinten | | | | | IH Botek | | L447 Harmand | | SLAC holidays | | | | | | | | | | | | | | |
| | IH Lemke | | | L396 Scherz | | | L396 Scherz | | | | | L409 Boeglin | | | | | | | | | | | | | | | | | | | |

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| Jan 12 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
| Day | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue |
| Night | SLAC holidays | | PPS contingency | | | | | | | | | | | | | | Start-up | | | | | L399/433 Fromme/Neutze | | | | | L467 Madsen | | | | |
| | | | | | | | | | | | | | | | | | Com Com Com L467 Mad | | | | | L399/433 Fromme Com Com | | | | | | | | | |

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| Feb 12 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 |
| Day | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed |
| Night | L432/490 Fromme/Stevens | | | | | L430 Foerst | | | | | L391/398 Miao | | | | | L390 Staub | | | | | L431 Frank | | | | | | | | |
| | Com Com Com Com Com | | | | | Com Com L445 Hajdu | | | | | Com Com Com Com Com | | | | | Com | | | | | | | | | | | | | |

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| Mar 12 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
| Day | Thur | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat |
| Night | L443 Gruebel | | | L435 Gaffne | | | L407 Beye | | | L417 L417 | | | L419 L407 | | | L419 Chen | | | IH Milathianaki | | | L489 Stephenson | | | L439 Glowina | | | | | | |
| | L443 | | | Com Com Com | | | L407 | | | L417 | | | L419 | | | L417 | | | IH | | | L489 | | | L439 | | | | | | |

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| Apr 12 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 |
| Day | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon |
| Night | L439 | | L441 Graber | | | Com | | | IH Krupin | | | L387 Trabert (Ebit) | | | Com Com L497 Wark | | | L497 | | | L463 Leheny | | | L401 Abbey | | | Com | | | |
| | | | L441 | | | Com | | | IH | | | L387 | | | Com Com | | | L497 | | | L463 | | | L401 | | | Com | | | |

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| May 12 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
| Day | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu | Fri | Sat | Sun | Mon | Tue | Wed | Thu |
| Night | IH Feng | | L431 Frank | | | CXI in-house | | | CXI inhouse | | | L481/494 | | | L405 Berrah | | | L456 Krasniq | | | L481/ L481/ Com | | | IH MEC | | | L434 Fuchs | | | | |
| | IH | | L431 | | | CXI | | | CXI | | | L481/494 | | | L405 | | | L456 | | | L481/ L481/ | | | IH | | | L434 | | | | |

AMO
SXR

XPP
XCS

CXI
MEC

unscheduled

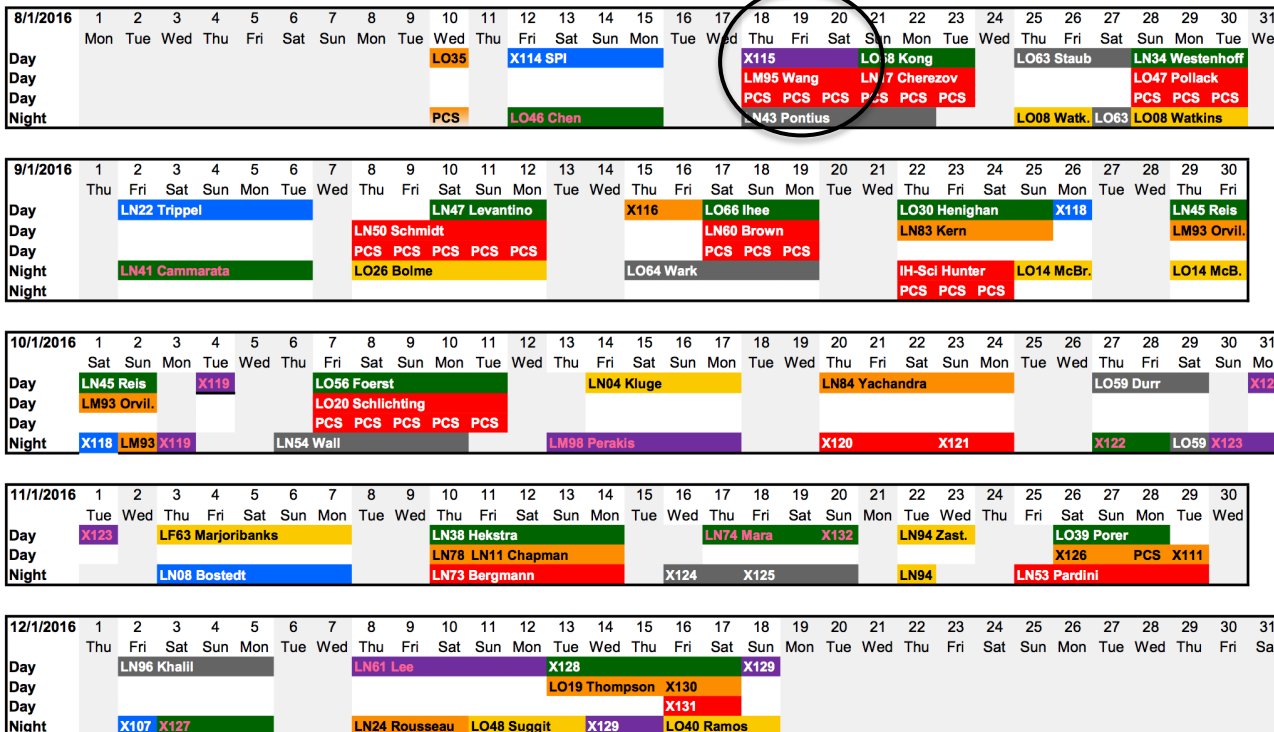
Day 9 am - 9 pm
Night 9 pm - 9 am

12 hour shift structure: Day/Night split between two instruments

After Multiplexing (2016.08 – 2016.12)

LCLS Run 14 Schedule
Ver 1: 5/2/16

First XCS 'mono' Multiplexing Shifts



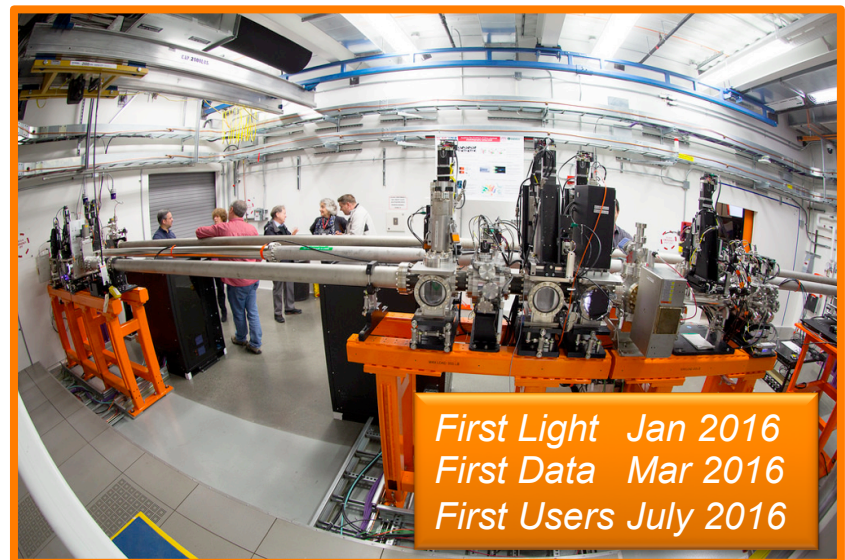
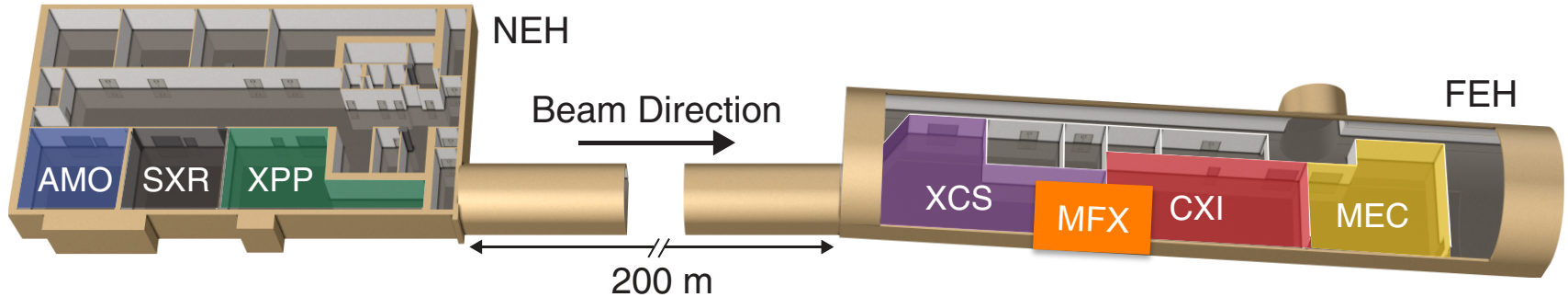
AMO SXR XPP XCS MFX CXI MEC

Day 9 am - 9 pm
Night 9 pm - 9 am

From 2 rows to 4 rows: A fairly significant increase in number of shifts.

New instrument area: “MFX” in hutch “4.5”

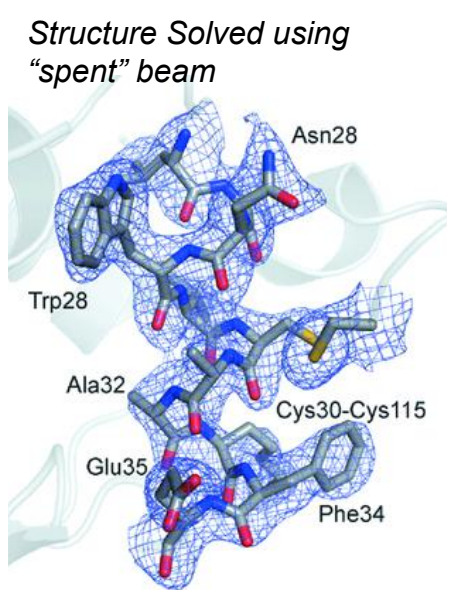
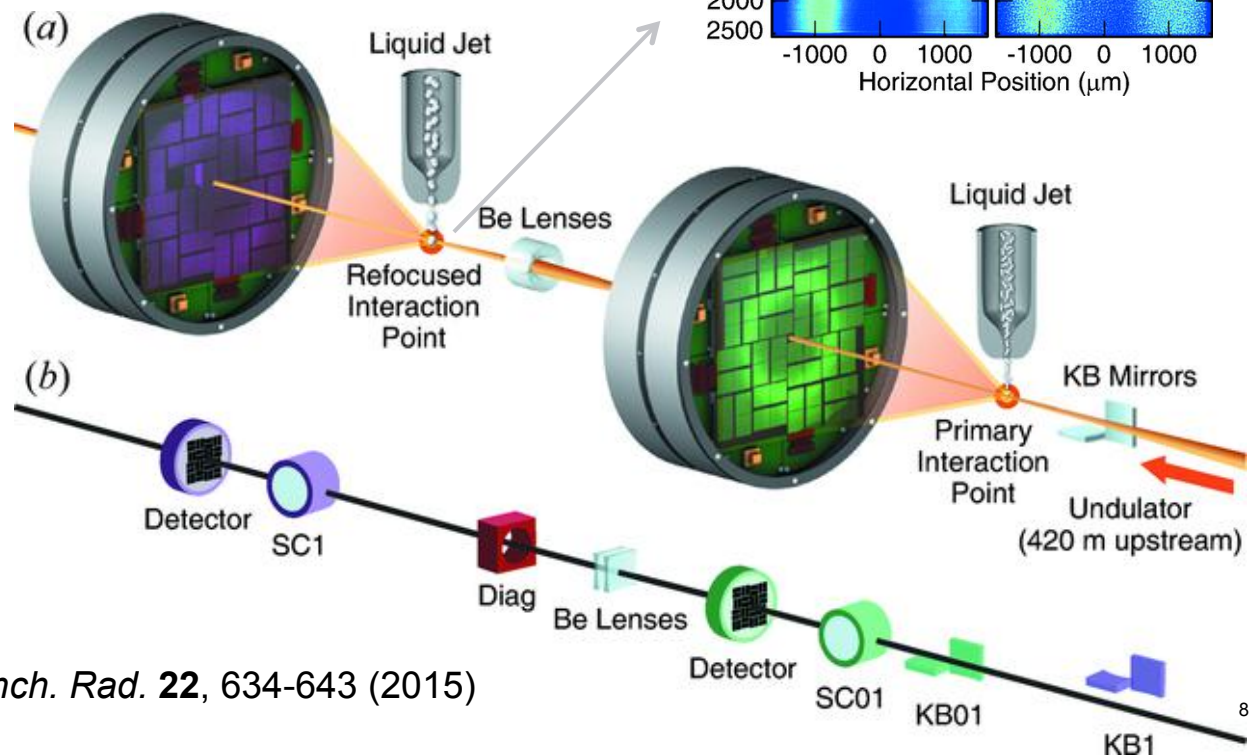
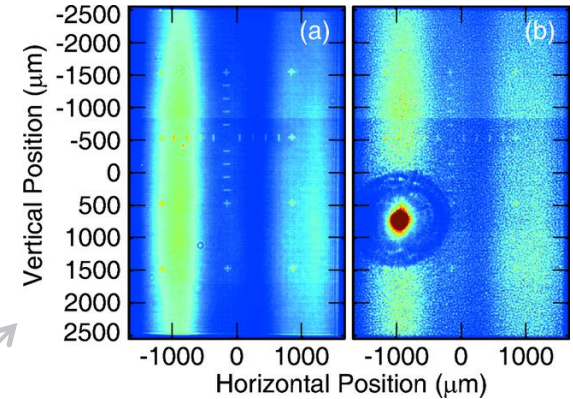
Macromolecular Femtosecond Xtallography



Serial Serial Femtosecond Crystallography

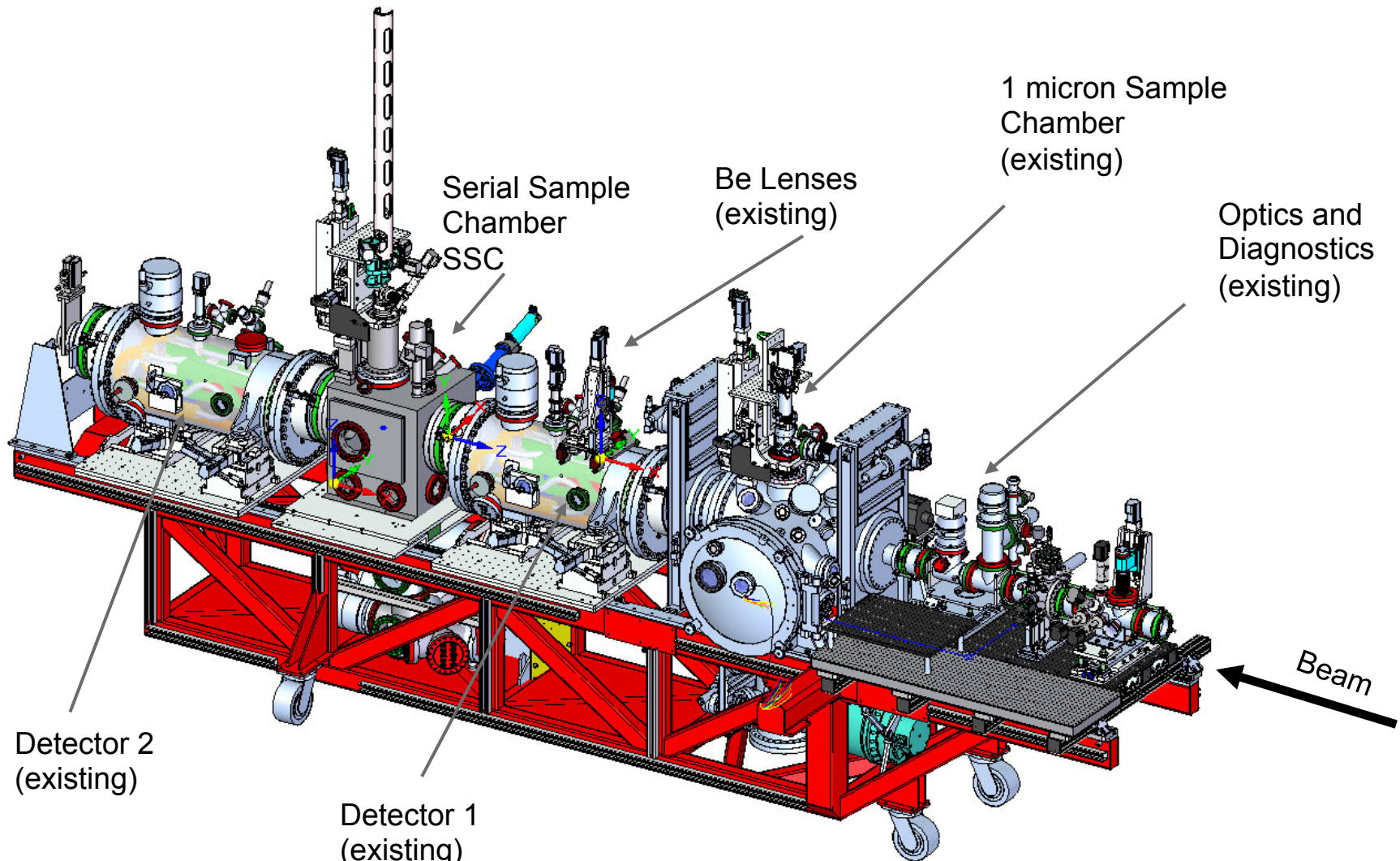
- Reuse the “spent” beam from the upstream experiment into a second independent experiment.
- Structures were obtained from each of the data sets from the independent experiments.

Beam without Lenses Beam After Lenses

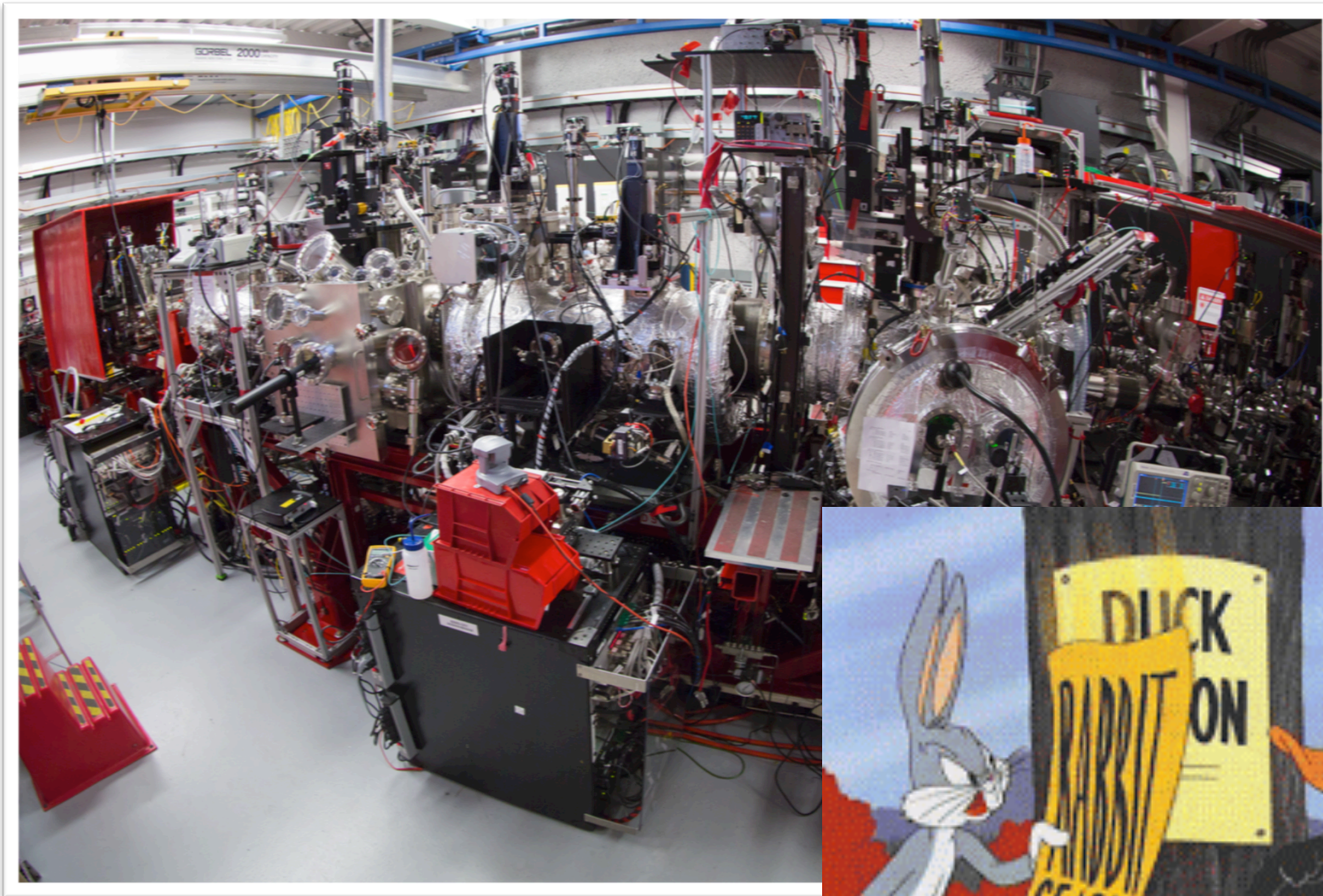


Boutet et al., *Jour. Synch. Rad.* **22**, 634-643 (2015)

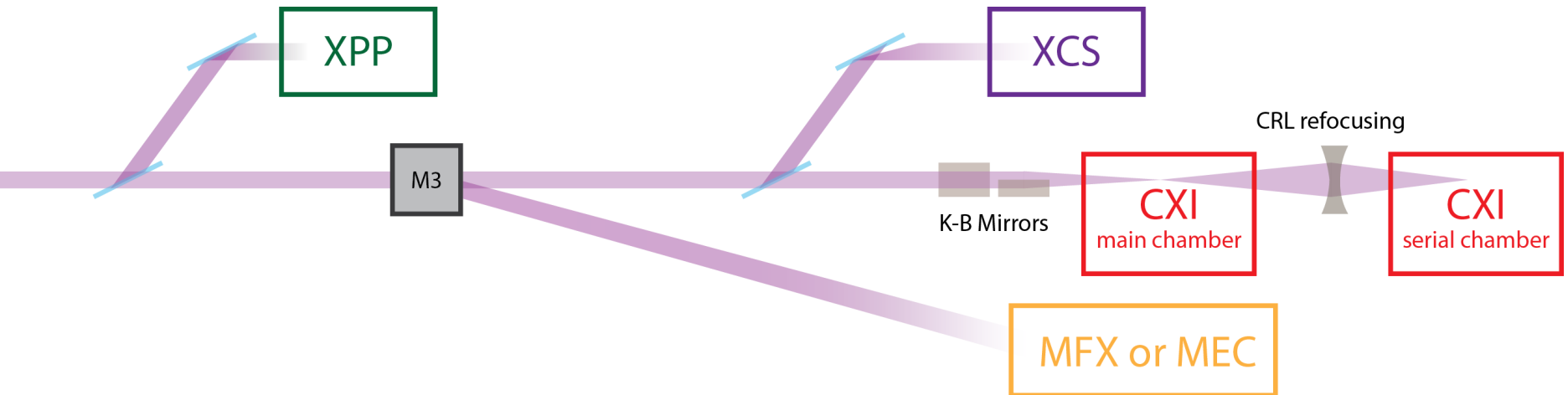
CXI Serial Sample Chamber – Installed June 2015



Challenges of SSC Operation



5-Way Multiplexing



- Modification to M3 mirror now serves both MFX and MEC.
- 60 um diamond commissioned for XCS Large Offset Mono.
- Serial Sample Chamber commissioned at CXI.

Standard Configurations

AMO: gas phase molecular dynamics with LAMP. VMI, eTOF, iTOF detectors.

SXR: Resonant soft x-ray scattering endstation. Liquid jet endstation.

XPP: Time-resolved in-air diffraction of solid samples, low T with cryostream.

XCS: Time-resolved solution scattering and emission spectroscopy.

CXI: 1 um KB, SFX and scattering, various injectors to choose from.

MEC: X-ray diffraction and Thomson scattering on shocked material by ns laser.

PCS at **CXI** & **MF**: Protein screening time, SFX.

Quote from Call for Proposal

“ Selected areas will operate ~25% of Run 15 (possibly more if user demand is high) in a contiguous block of time during which the instrument will be in a Standard Configuration.”

Further Standardize Standard Configurations

Example: 6 experiments in 5 weeks for the liquid scattering and spectroscopy standard configuration. How similar are they?

| | Primary technique | No. of Shifts | X-ray photon energy | Laser wavelength | detector | Sample delivery | Analysis | New group |
|------|-------------------|---------------|---------------------|------------------|----------|------------------|--------------|-----------|
| LO46 | XAS | 4 | Pink, 7.1 keV | 520 nm | CSPAD | Liquid jet | Matlab | N |
| LO58 | WAX | 3 | Mono, 9.5 keV | 400 nm | CSPAD | Liquid jet | Matlab, Igor | Y |
| LN34 | WAX | 3 | Mono, 9.5 keV | 266 nm | CSPAD | Liquid jet | Python | Y |
| LN41 | XAS | 5 | Pink, 7.1 keV | 540 nm | CSPAD | Liquid jet | Python | N |
| LN47 | SAX | 3 | Mono, 9.5 keV | 540 nm, 580 nm | Rayonix | Capillary Ver. 1 | Python | N |
| LO66 | SAX | 3 | Mono, 9.5 keV | 530 nm | CSPAD | Capillary Ver. 2 | C++ | Y |

Need new setup: fixed experimental procedure based on well established hardware is the starting point for the implementation of automation.

Automation Example: Timing Diagnostics & Feedback



Standard hardware

XPP - LAS:FS3:VIT Details...

LASER TIME SETTING

4457.341335 ns Target Time
+ 0.000000 ns Offset
4457.341335 = 4457.3 ns

TIMETOOL DRIFT CONTROL

Accumulation Correction

Current Correction [ns] -0.001097
Zero Re-Center - +

IPM -0.000195 HIGH 20.000 LOW 0.500
TTAMP 33.883891 HIGH 1.000 LOW 0.020

NOISE ANTI-ELIMINATOR

0V MIN 0.000 0.000 V
5V MAX

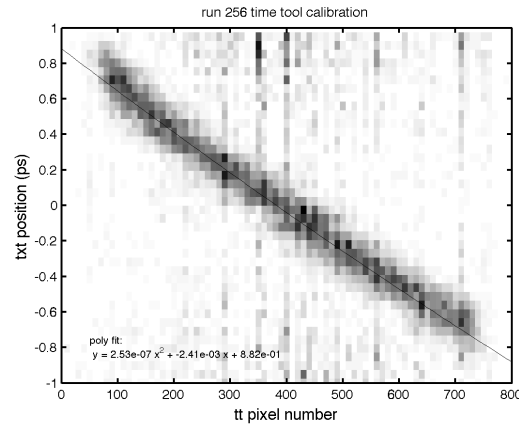
TIMING SYSTEM STATUS

responder not stable 200

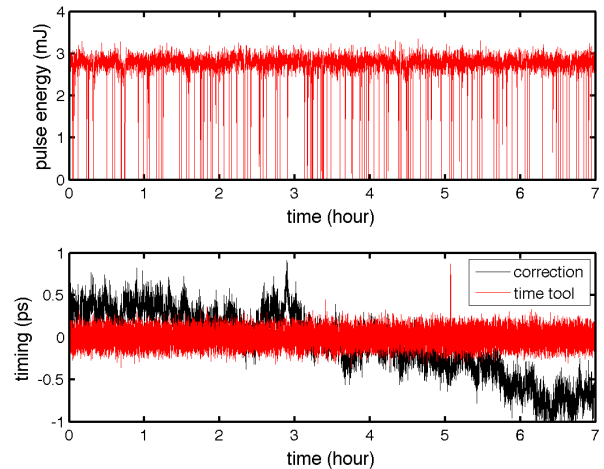
4457.341335 ns 49.0 Hz Locked
200.000000 ns -0.007 Hz 120.0 Hz

Laser EVR Event Sequencer

high level control interface



Automatic calibration routine



Feedback implementation to enable robust maintenance free operation

Standard Configuration

- Discuss/Collaborate on the designs and implementation of standard configurations to make life easier for users who performs similar experiments at different facilities.
- Common intermediate data format, common data analysis routines.

Operation Automation

- Identify best implementation of in-situ diagnostics for beam pointing stabilization.
- K-B alignment, need to develop diagnostic implementation and optimization routines for the 10s of K-B systems across all facilities.
- Automatic sample injection monitoring and tracking via advanced image recognition algorithms.