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The *cctbx.xfel* GUI: processing serial crystallographic data at massive scales

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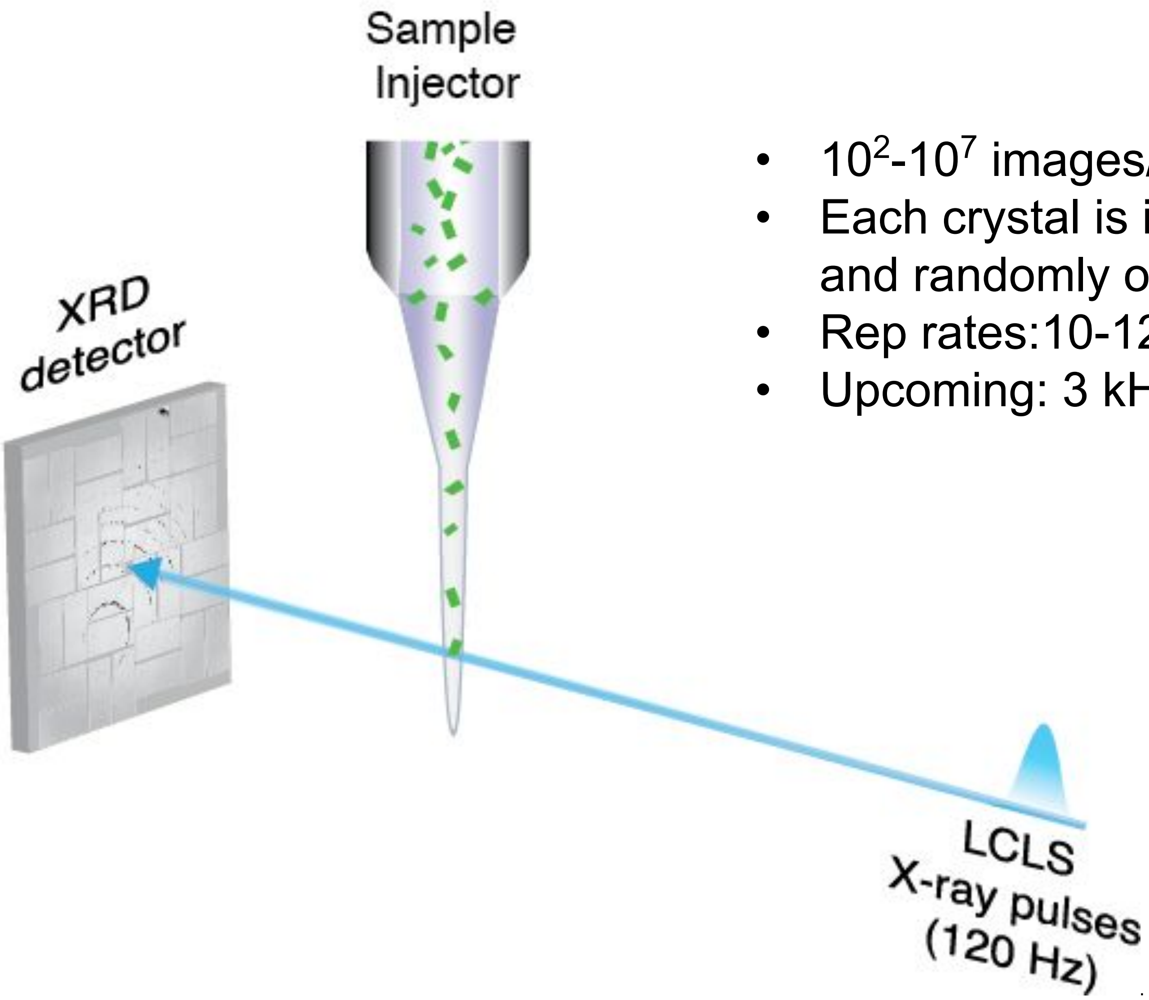
Serial crystallography



- 10^2-10^7 images/dataset
- Each crystal is independent and randomly oriented
- Rep rates:10-120 Hz
- Upcoming: 3 kHz

How much data do I need?

- What is my hitrate?
  - Solvent rate
  - Crystal rate
  - Indexing rate
  - High quality rate
- What is my completeness?
- Can I stop collecting data?

Beamtime is scarce! Fast feedback is critical!

cctbx.xfel GUI

- Built on *cctbx* and DIALS

Winter G. (2018). DIALS: implementation and evaluation of a new integration package. *Acta Crystallogr D Struct Biol* **74**, 85-97

- Full SX workflow
  - Each image: import, spot-find, index, integrate, scale, post-refine, merge
  - Monitor for new data and submit jobs
  - Organize processing many datasets
  - Massively parallel multiprocessing on the biggest computing clusters
  - MySQL backend allows scaling to the kHz regime

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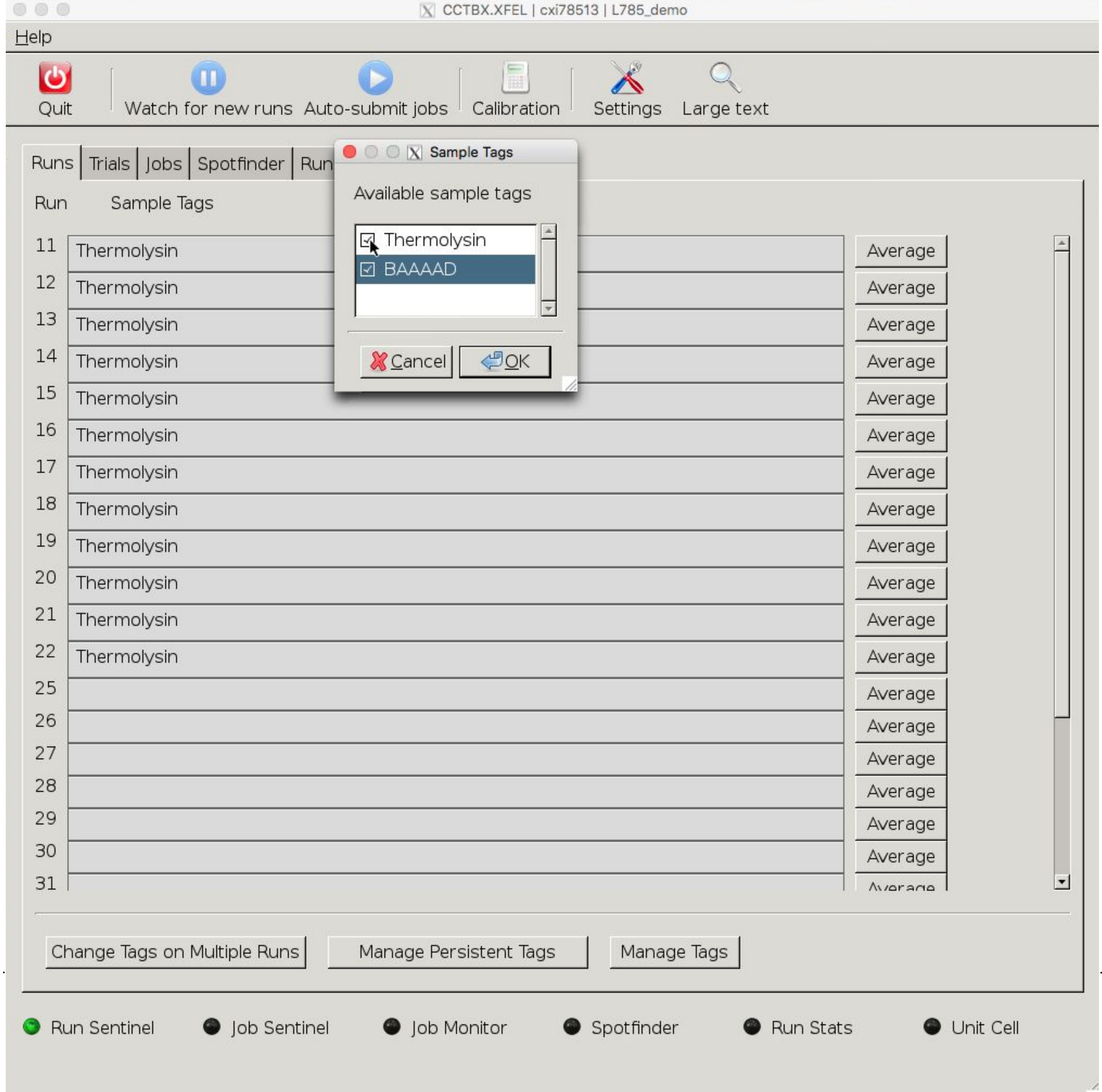
CCTBX.XFEL | cxi78513 | L785_demo
Help
Quit
Watch for new runs
Auto-submit jobs
Calibration
Settings
Large text
Runs
Trials
Jobs
Spotfinder
Run
Sample Tags
Available sample tags
Thermolysin
BAAAAD
Cancel
OK
Run
Sample Tags
11 Thermolysin
12 Thermolysin
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14 Thermolysin
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28
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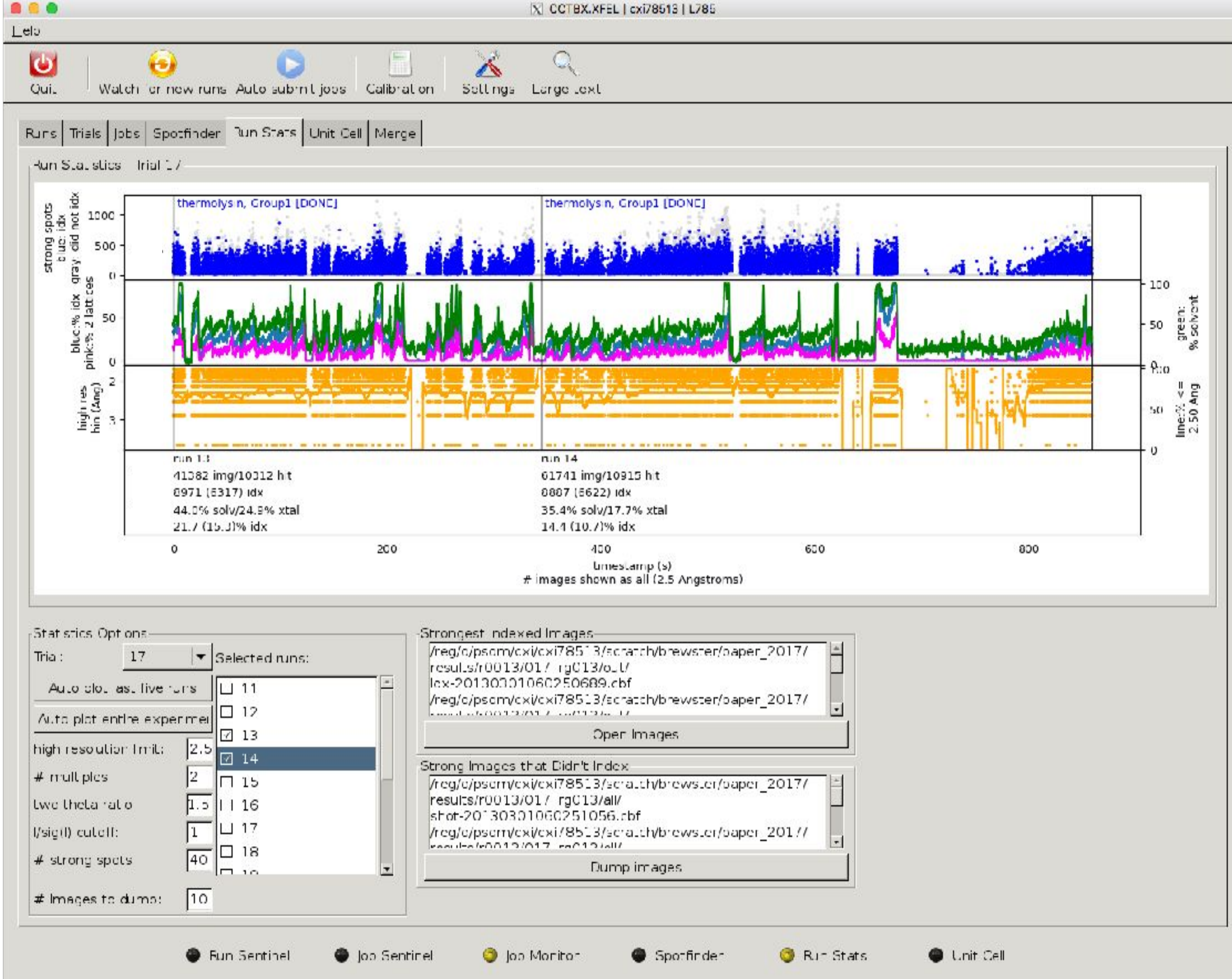
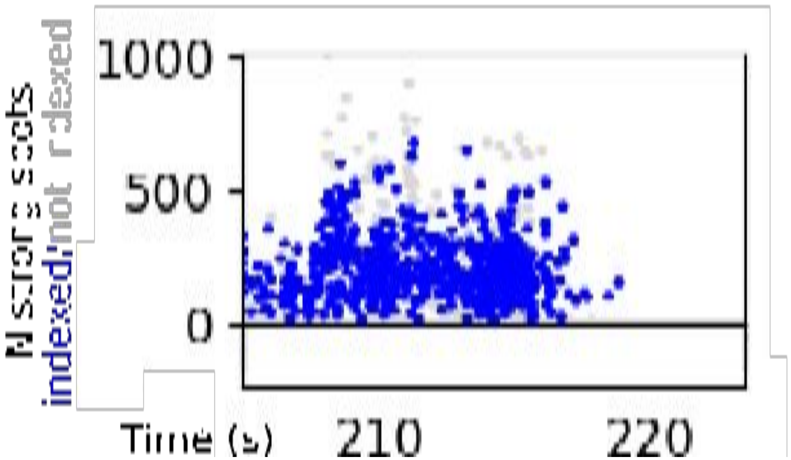
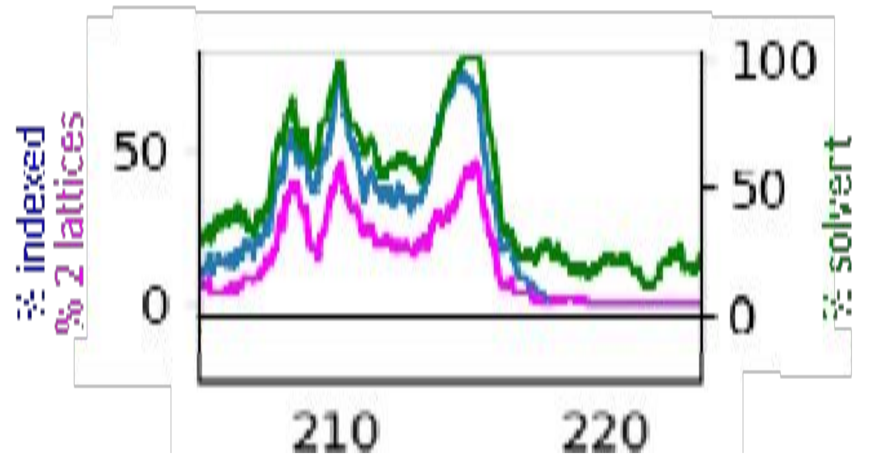
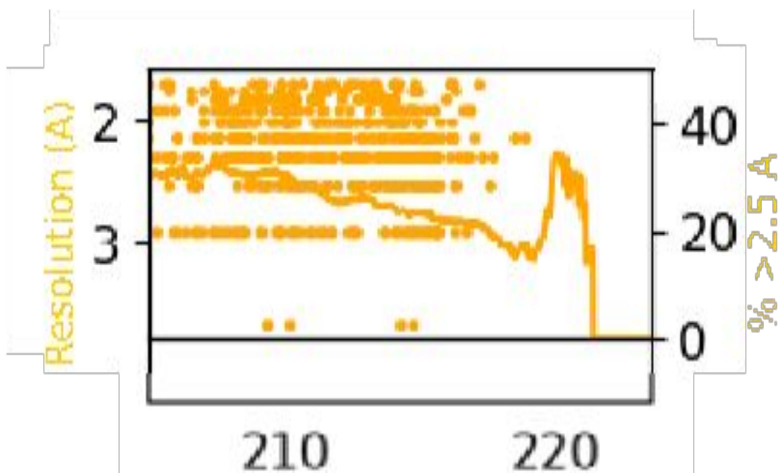
31
Average
Change Tags on Multiple Runs
Manage Persistent Tags
Manage Tags
Run Sentinel
Job Sentinel
Job Monitor
Spotfinder
Run Stats
Unit Cell


CCTBX.XFEL | cxi78513 | L785
Quit
Watch for new runs
Auto submit jobs
Calibration
Settings
Large text
Runs
Trials
Jobs
Spotfinder
Run Stats
Unit Cell
Merge
thermolysin, Group1 [DONE]
strong spots
blue: idx
gray: did not idx
blue:% idx
pink:% 2 lattices
green:
% solvent
high res
bin (Ang)
run 13
41382 img/10312 hit
8971 (6317) idx
44.0% solv/24.9% xtal
run 14
61741 img/10915 hit
8887 (6622) idx
35.4% solv/17.7% xtal
timestamp (s)
images shown as all (2.5 Angstroms)
Statistics Options
Trial:
Selected runs:
Auto plot last five runs
Auto plot entire experiment
high resolution limit:
multiples
two theta ratio
I/sig(I) cutoff:
strong spots
Images to dump:
Strongest indexed Images
Open Images
Strong Images that Didn't Index
Dump images
Run Sentinel
Job Sentinel
Job Monitor
Spotfinder
Run Stats
Unit Cell

Rate tracking

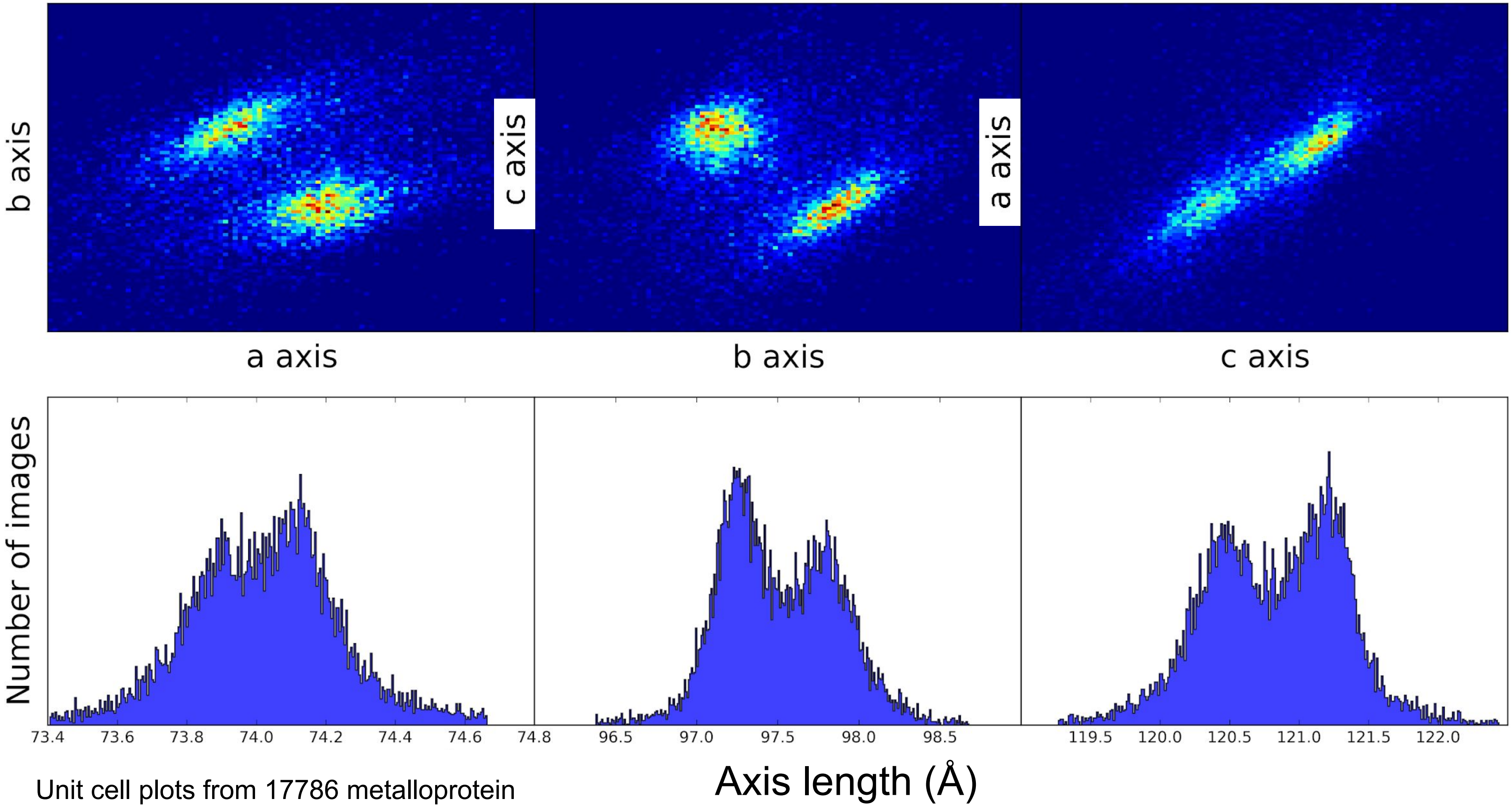






run 13
41382 img/10312 hit
8971 (6317) idx
44.0% solv/24.9% xtal
21.7 (15.3)% idx

Non-isomorphism: two clusters



Unit cell plots from 17786 metalloprotein crystals (space group $P2_12_12_1$) collected at LCLS beamline MFX.

Heuristics

- How much data do I need?
  - What is my hitrate?
  - What is my completeness?
  - Can I stop collecting data?

Easy answer (rule of thumb):

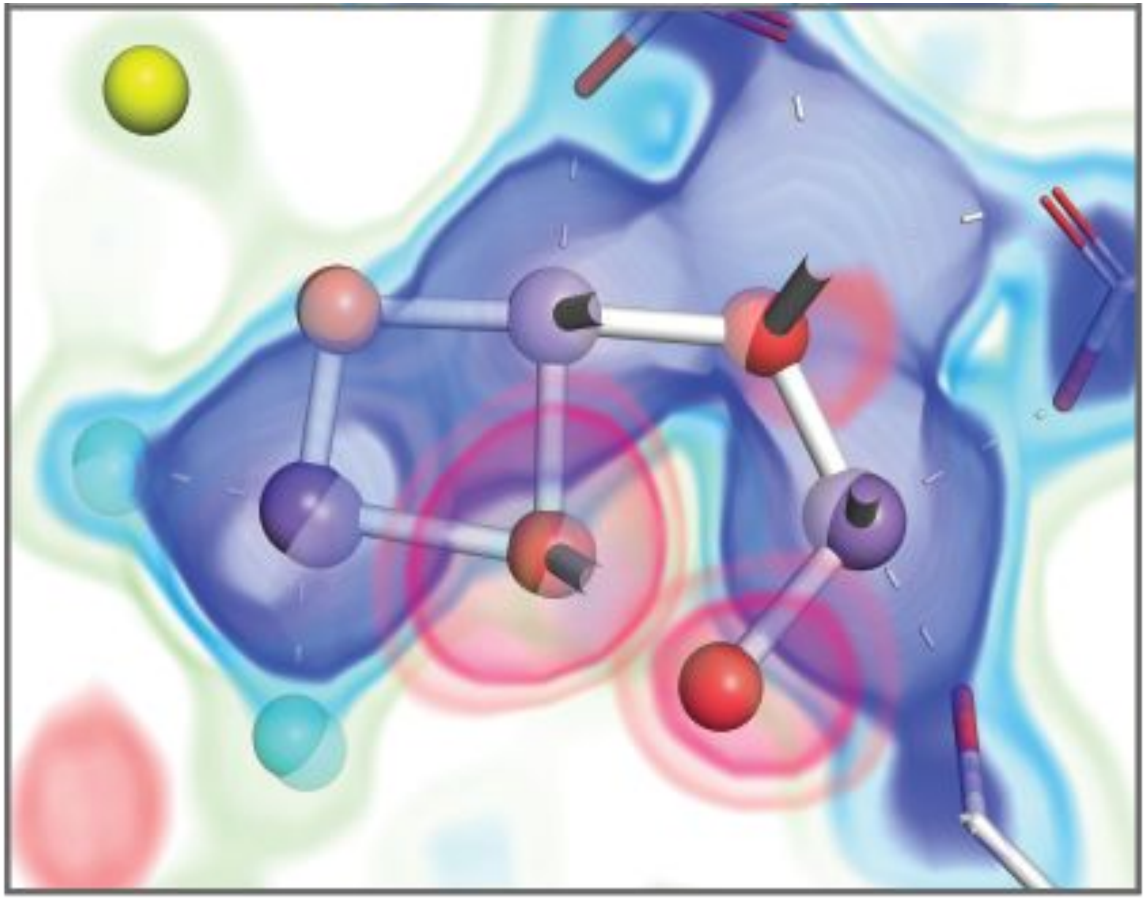
- 10-fold multiplicity at the resolution of interest
- Monotonically decreasing $CC_{1/2}$ to the resolution of interest

The easy answer lends itself to sampling the data

How much data do I need?

- How much data do I need to answer my biological questions?

How much data do I need?



PSII 2Fo-Fc and Fo-Fc at 2.07 Å, S3 state

Kern et al., 2018 Nature 563:421

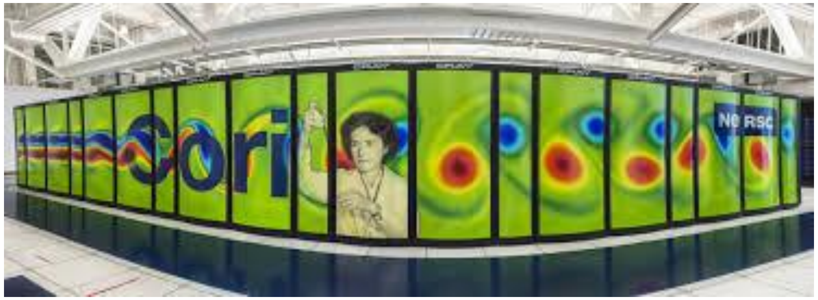
Data analytics at the petascale for free electron lasers

- Processing 1 image takes 30s per hit, 1s per miss, on average
- Vastly varies depending on protocol:
  - Multiple indexing methods
  - Multiple lattices
  - Large unit cell
  - Hit rate
- 30 Hz Rayonix at LCLS: only 288 cores available. Cannot keep up with good hitrates
  - 100% hitrate = 30s/image * 30 images/s = 900s to process 1s of data collection
  - Need 900 cores

Data analytics at the petascale for free electron lasers

Solution:

- Sample the data at LCLS for GUI (process 1 in 5 images). At the same time, transfer the data over 100 Gb-ESnet to NERSC, and process all images on Cori
  - 2388 Intel Xeon Haswell nodes
  - 9688 Intel Xeon Phi “Knight’s Landing” nodes (68 cores)
  - 1.8 PB burst buffer (keep the data on solid state drives)
- 9 TB example experiment; 861969 diffraction images (2.0 hrs’ data collection @ 120 Hz)
  - 150466 useful crystal patterns (17% hit rate)
  - Required 140 “Knight’s Landing” node-hours to process
  - Not counting I/O, 70 nodes in continuous use during data collection
  - About 1% of Cori



Four year Exascale Computing Project funding to scale this for

- bigger algorithms
- faster LCLS-II pulse rate
- exascale machines in a few years’ time
- Collaboration with Amedeo Perrazo, SLAC

Data collection at LCLS / MFX December 2018

- Four 12-hour shifts at MFX (LU50 / P143)
- 20 – 30 Hz overall collection rate (Rayonix 340)
- 594,230 total indexed images
- > 8.4 indexed images s^{-1} (31% of all shots)
- Overall 48% collection duty cycle
- ~ 54 tr-SFX + tr-XES data sets
- ~ 12 types of enzymes
- Typically ~ 1 mg protein per dataset
- Some data beyond 1.3 Å resolution

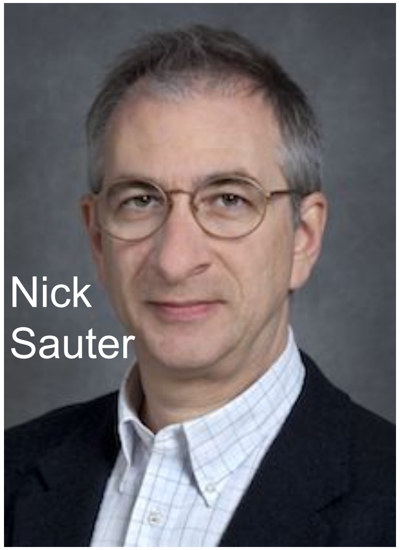
data se						x 340 r rate
1						lz
2						lz
3						lz
4						lz
5						lz
6						lz
7						lz
8						lz
9						lz
10						lz
11						lz
12						
13						lz
14						lz
15	Enz 01 oxidized | no run 20, no data in run	1.6	1.76	16851	45	30 Hz

Deployment: every XFEL

	LCLS	SACLA	PAL-XFEL	SwissFEL	EuXFEL
Location	Stanford, CA USA	Harima, Japan	Pohang, South Korea	Aargau, Switzerland	Schenefeld, Germany
Computing	NERSC or SDF	Local	KISTI	PSI	Maxwell
Detectors	CSPAD, ePix, Jungfrau, Rayonix	Octal-8 MPCCD, Rayonix	Rayonix	Jungfrau 16M	AGIPD

Supports LSF, SGE, Slurm, HTCondor, Docker/Shifter
New use of GUI: DLS beamline I24 (Pilatus3 6M)
Best current result: LCLS + NERSC, 5 minute turnaround for fully merged dataset

XFEL @ LBL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Elyse
Schriber


Aaron Brewster


Derek Mendez


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Zoom background: "Black Lotus" from Magic the Gathering

References

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http://www.phenix-online.org/newsletter

Brewster AS, et. al (2018): Improving signal strength in serial crystallography with DIALS geometry refinement. *Acta Crystallogr D Struct Biol* 74, 877-894.

http://cci.lbl.gov/xfel

http://dials.github.io