09:00

Welcome to DESY — *MNICH, Joachim*
Seminar Room 4, DESY Hamburg — 09:00 - 09:10

Willkommen, Einführung — *JUNG, Christopher*
Seminar Room 4, DESY Hamburg — 09:10 - 09:20

Licht-optische Nanoskopie — *KEPPER, Nick*
Seminar Room 4, DESY Hamburg — 09:20 - 09:55

10:00

Selective Plane Illumination Microscope — *KOBITSKIY, Andrey*
Seminar Room 4, DESY Hamburg — 09:55 - 10:30

Kaffee
Seminar Room 4, DESY Hamburg — 10:30 - 10:55

11:00

X-Ray Imaging for Life Sciences: Challenges in Data Analysis — *VAN DE KAMP, Thomas*
Seminar Room 4, DESY Hamburg — 10:55 - 11:30

Die digitalen Handschriftenbeschreibungen des "Virtuellen Skriptoriums St. Matthias" — *VANSCHEIDT, Philipp*

12:00

Services und Datenfluss in BioQuant LSDF — *THIEMANN, Christian*
Seminar Room 4, DESY Hamburg — 12:05 - 12:40

Mittagessen

13:00

Seminar Room 4, DESY Hamburg — 12:40 - 13:40

Human Brain Projekt — *MOHLBERG, Hartmut*

14:00

Seminar Room 4, DESY Hamburg — 13:40 - 14:15

Center for Free Electron Laser - Datenanalyse — *BARTY, Anton*
Seminar Room 4, DESY Hamburg — 14:15 - 14:50

15:00

LHC Computing in der Hochenergiephysik — *STADIE, Hartmut*
Seminar Room 4, DESY Hamburg — 14:50 - 15:25

Kaffee
Seminar Room 4, DESY Hamburg — 15:25 - 15:55

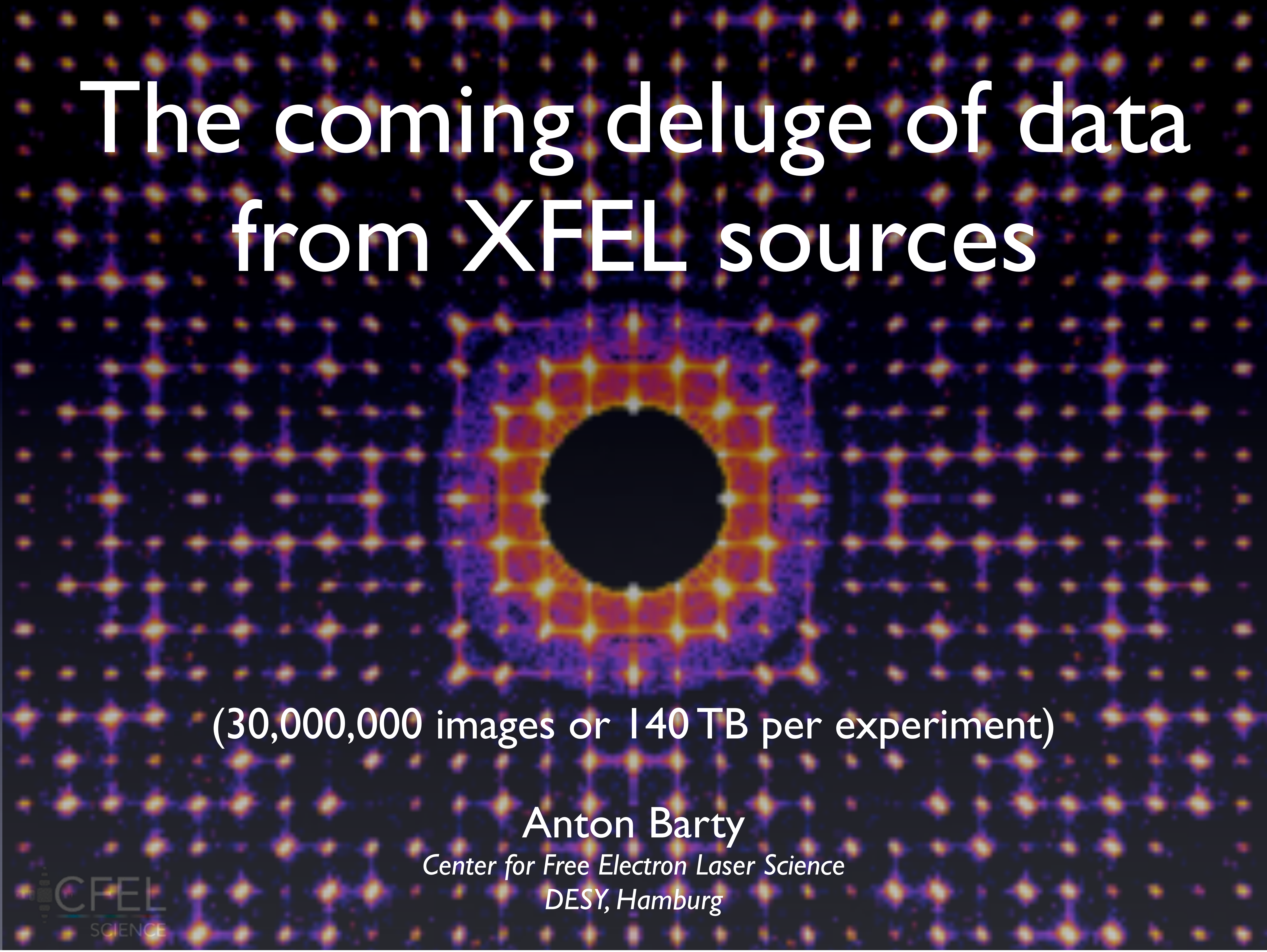
16:00

Verteiltes Datenmanagement für Klimadaten — *EHBRECHT, Carsten*
Seminar Room 4, DESY Hamburg — 15:55 - 16:30

From ground shaking to timely earthquake information and seismological research - challenges for data handling in seismology — *HANKA, Winfried*

17:00

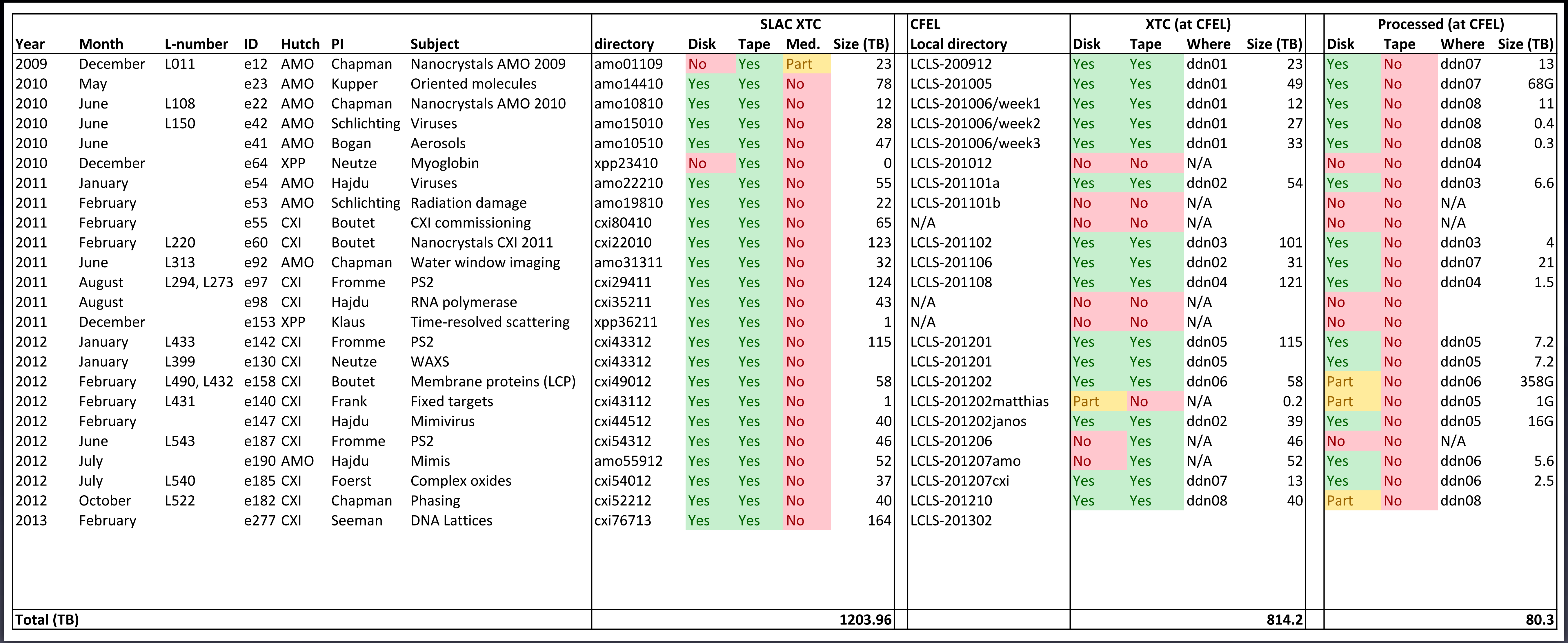
The coming deluge of data from XFEL sources



(30,000,000 images or 140 TB per experiment)

Anton Barty
Center for Free Electron Laser Science
DESY, Hamburg

In three years, our research group has taken analysed over 1.2 PB of data from LCLS



							SLAC XTC					CFEL	XTC (at CFEL)				Processed (at CFEL)			
Year	**Month**	**L-number**	**ID**	**Hutch**	**PI**	**Subject**	**directory**	**Disk**	**Tape**	**Med.**	**Size (TB)**	**Local directory**	**Disk**	**Tape**	**Where**	**Size (TB)**	**Disk**	**Tape**	**Where**	**Size (TB)**
2009	December	L011	e12	AMO	Chapman	Nanocrystals AMO 2009	amo01109	No	Yes	Part	23	LCLS-200912	Yes	Yes	ddn01	23	Yes	No	ddn07	13
2010	May		e23	AMO	Kupper	Oriented molecules	amo14410	Yes	Yes	No	78	LCLS-201005	Yes	Yes	ddn01	49	Yes	No	ddn07	68G
2010	June	L108	e22	AMO	Chapman	Nanocrystals AMO 2010	amo10810	Yes	Yes	No	12	LCLS-201006/week1	Yes	Yes	ddn01	12	Yes	No	ddn08	11
2010	June	L150	e42	AMO	Schlichting	Viruses	amo15010	Yes	Yes	No	28	LCLS-201006/week2	Yes	Yes	ddn01	27	Yes	No	ddn08	0.4
2010	June		e41	AMO	Bogan	Aerosols	amo10510	Yes	Yes	No	47	LCLS-201006/week3	Yes	Yes	ddn01	33	Yes	No	ddn08	0.3
2010	December		e64	XPP	Neutze	Myoglobin	xpp23410	No	Yes	No	0	LCLS-201012	No	No	N/A		No	No	ddn04	
2011	January		e54	AMO	Hajdu	Viruses	amo22210	Yes	Yes	No	55	LCLS-201101a	Yes	Yes	ddn02	54	Yes	No	ddn03	6.6
2011	February		e53	AMO	Schlichting	Radiation damage	amo19810	Yes	Yes	No	22	LCLS-201101b	No	No	N/A		No	No	N/A	
2011	February		e55	CXI	Boutet	CXI commissioning	cxi80410	Yes	Yes	No	65	N/A	No	No	N/A		No	No	N/A	
2011	February	L220	e60	CXI	Boutet	Nanocrystals CXI 2011	cxi22010	Yes	Yes	No	123	LCLS-201102	Yes	Yes	ddn03	101	Yes	No	ddn03	4
2011	June	L313	e92	AMO	Chapman	Water window imaging	amo31311	Yes	Yes	No	32	LCLS-201106	Yes	Yes	ddn02	31	Yes	No	ddn07	21
2011	August	L294, L273	e97	CXI	Fromme	PS2	cxi29411	Yes	Yes	No	124	LCLS-201108	Yes	Yes	ddn04	121	Yes	No	ddn04	1.5
2011	August		e98	CXI	Hajdu	RNA polymerase	cxi35211	Yes	Yes	No	43	N/A	No	No	N/A		No	No		
2011	December		e153	XPP	Klaus	Time-resolved scattering	xpp36211	Yes	Yes	No	1	N/A	No	No	N/A		No	No		
2012	January	L433	e142	CXI	Fromme	PS2	cxi43312	Yes	Yes	No	115	LCLS-201201	Yes	Yes	ddn05	115	Yes	No	ddn05	7.2
2012	January	L399	e130	CXI	Neutze	WAXS	cxi43312	Yes	Yes	No		LCLS-201201	Yes	Yes	ddn05		Yes	No	ddn05	7.2
2012	February	L490, L432	e158	CXI	Boutet	Membrane proteins (LCP)	cxi49012	Yes	Yes	No	58	LCLS-201202	Yes	Yes	ddn06	58	Part	No	ddn06	358G
2012	February	L431	e140	CXI	Frank	Fixed targets	cxi43112	Yes	Yes	No	1	LCLS-201202matthias	Part	No	N/A	0.2	Part	No	ddn05	1G
2012	February		e147	CXI	Hajdu	Mimivirus	cxi44512	Yes	Yes	No	40	LCLS-201202janos	Yes	Yes	ddn02	39	Yes	No	ddn05	16G
2012	June	L543	e187	CXI	Fromme	PS2	cxi54312	Yes	Yes	No	46	LCLS-201206	No	Yes	N/A	46	No	No	N/A	
2012	July		e190	AMO	Hajdu	Mimis	amo55912	Yes	Yes	No	52	LCLS-201207amo	No	Yes	N/A	52	Yes	No	ddn06	5.6
2012	July	L540	e185	CXI	Foerst	Complex oxides	cxi54012	Yes	Yes	No	37	LCLS-201207cxi	Yes	Yes	ddn07	13	Yes	No	ddn06	2.5
2012	October	L522	e182	CXI	Chapman	Phasing	cxi52212	Yes	Yes	No	40	LCLS-201210	Yes	Yes	ddn08	40	Part	No	ddn08	
2013	February		e277	CXI	Seeman	DNA Lattices	cxi76713	Yes	Yes	No	164	LCLS-201302								
Total (TB)											**1203.96**					**814.2**				**80.3**

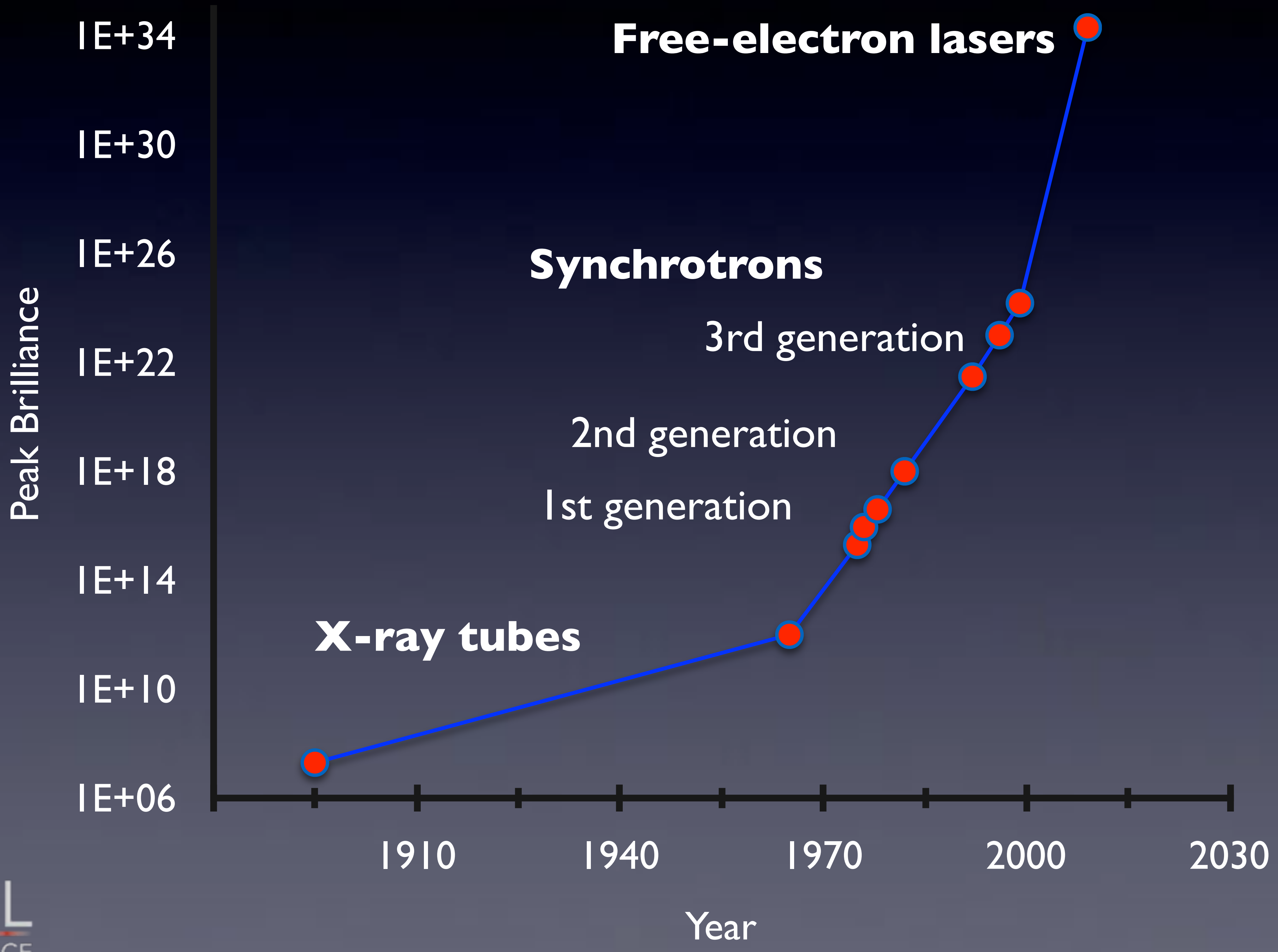
LCLS 2009-2012
(3 years)

Data analysed:
1202 TB

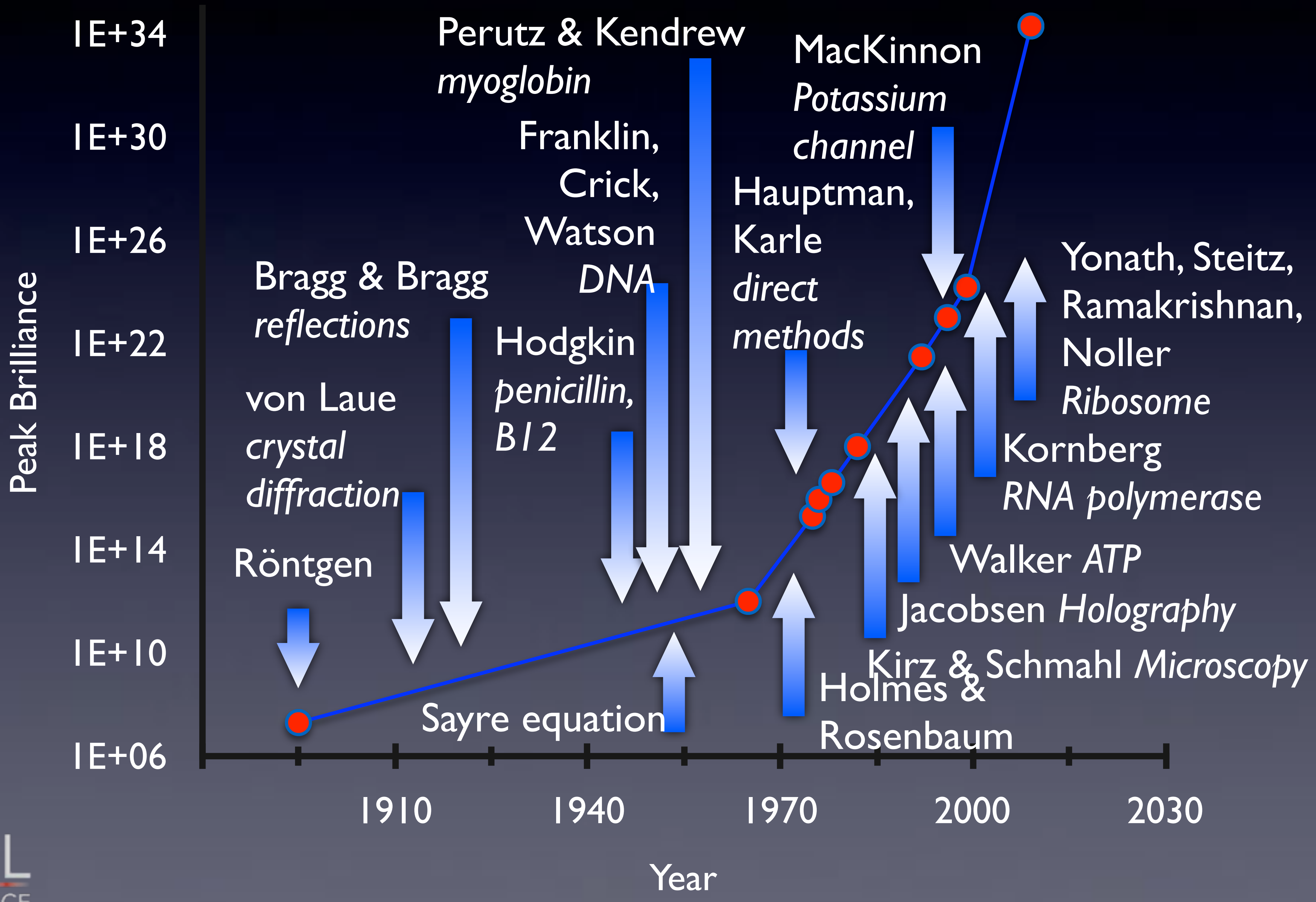
Data taken home:
814 TB

Reduced data:
80 TB

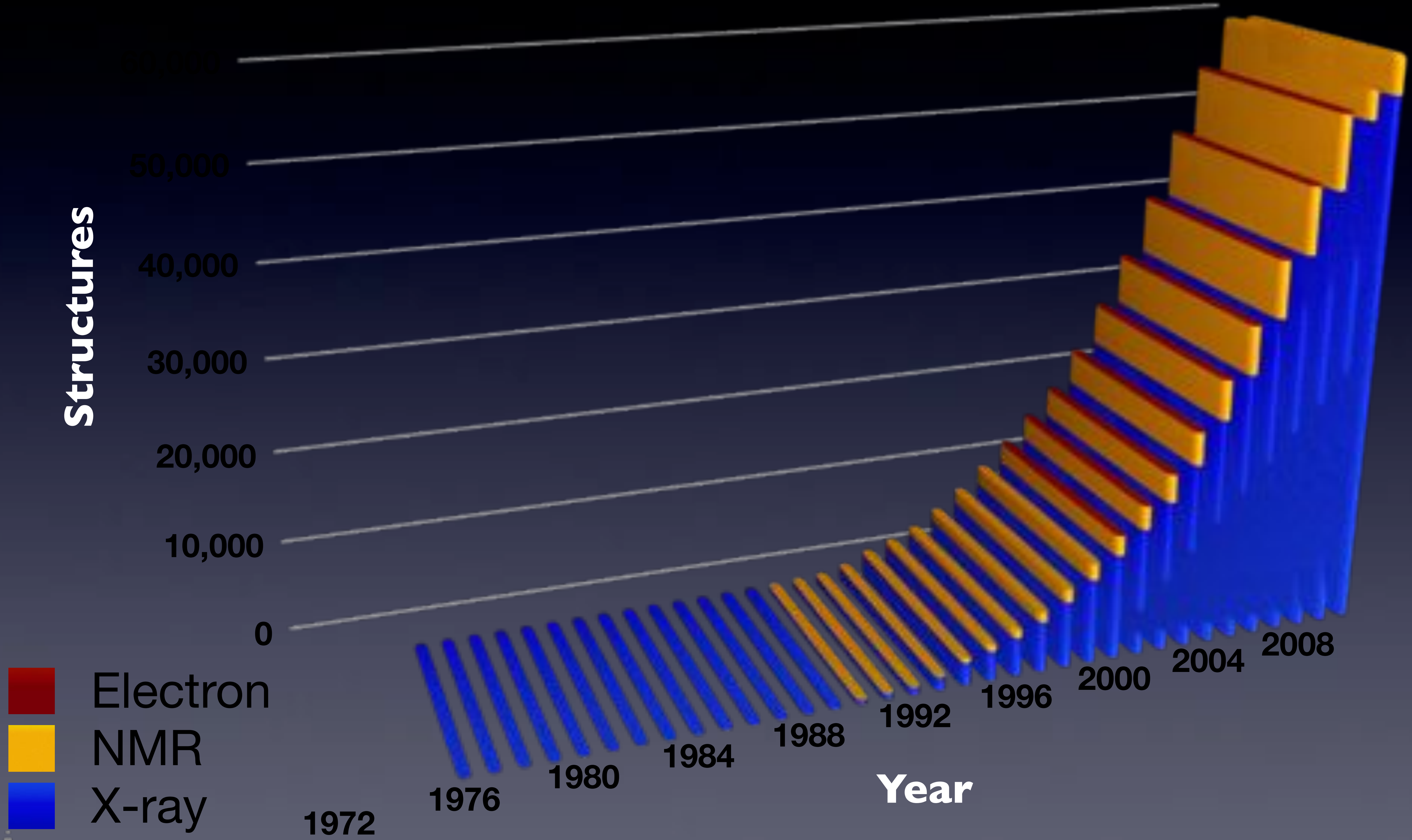
X-ray sources have developed at a staggering pace since their discovery in 1895



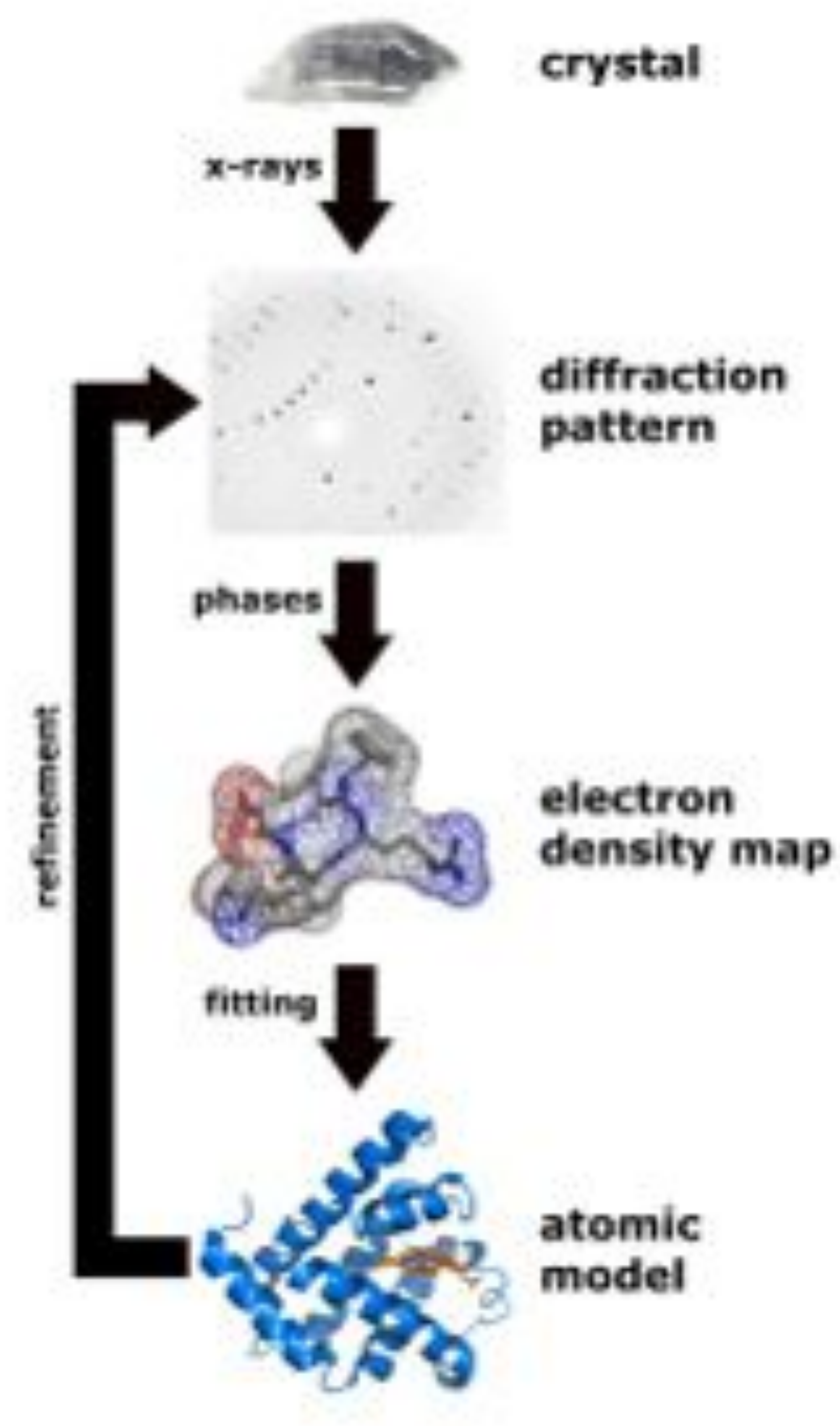
X-rays have been responsible for many significant discoveries in biological science



The bulk of protein structures have been solved using X-ray crystallography



X-ray crystallography requires large, well ordered crystals to overcome radiation damage



http://en.wikipedia.org/wiki/Image:X_ray_diffraction.png

- >52,684 PDB entries
- but only
  - ~10,000 *distinct* structures
  - 114 integral membrane proteins

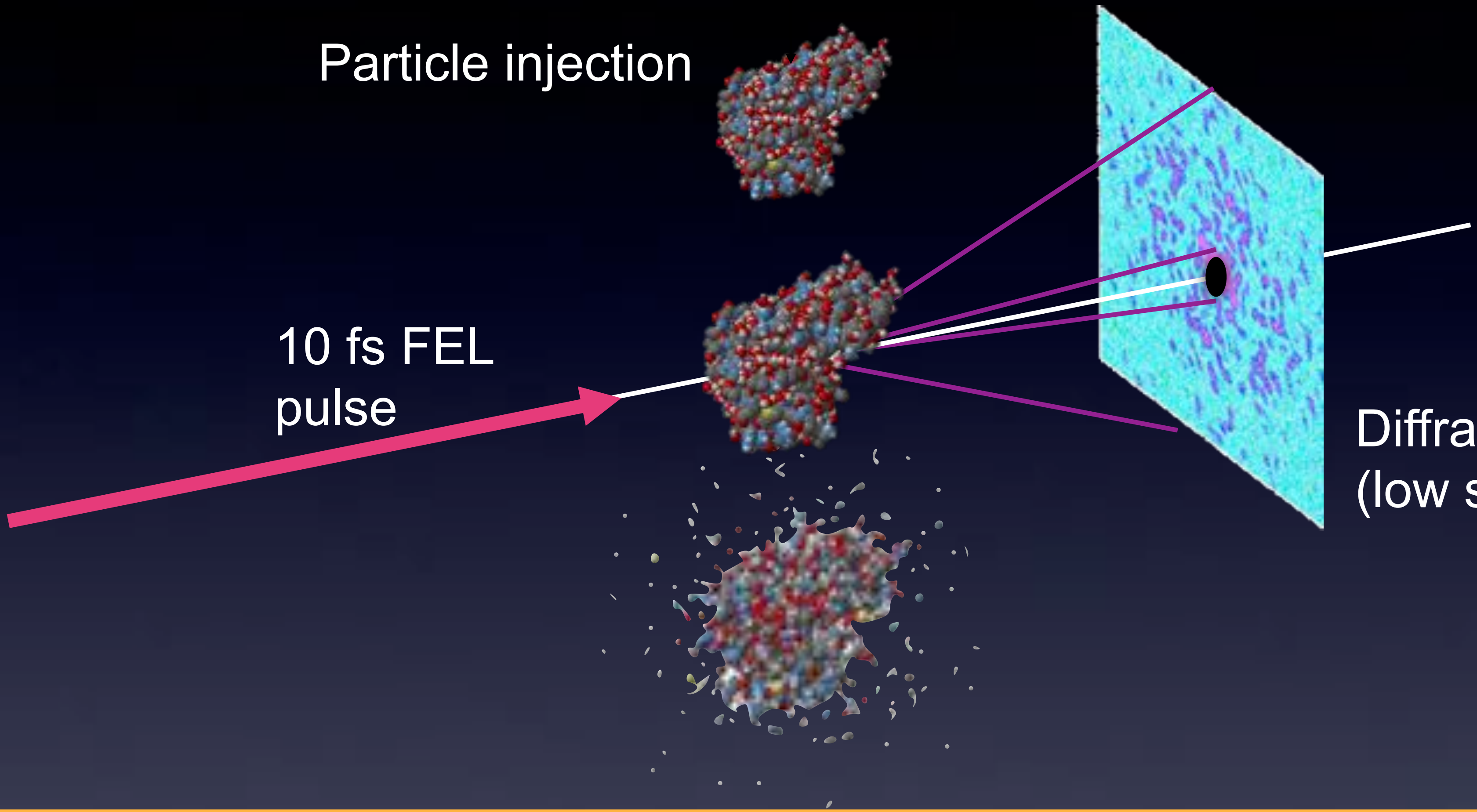
- **The bottleneck is in growing good crystals**

- Membrane proteins are especially important (eg: for drug delivery)

- *Grand challenge:*
  Can we revolutionise molecular biology by imaging isolated molecules ?

CFEL SCIENCE

X-ray free-electron lasers may enable atomic-resolution imaging of macromolecules without the need to grow large crystals



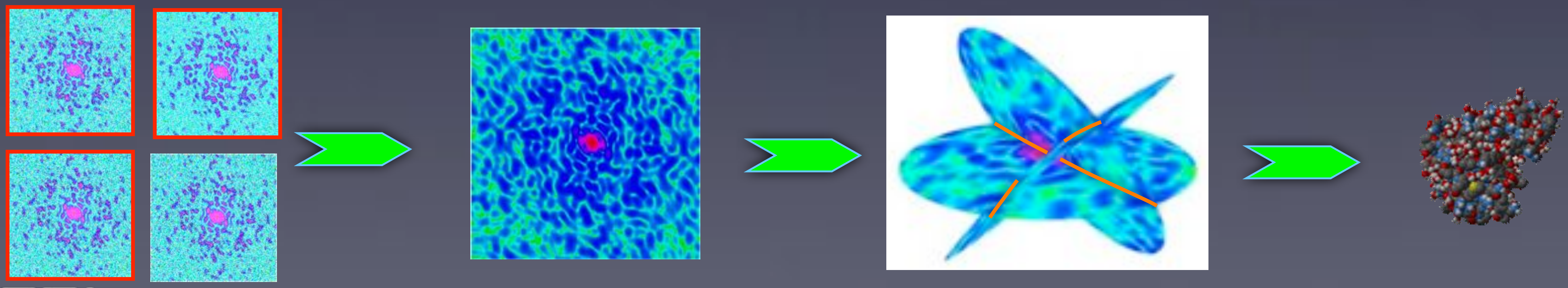
Particle injection

10 fs FEL pulse

One pulse per diffraction pattern

Diffraction pattern (low signal = noisy)

Combine 10^5-10^7 measurements



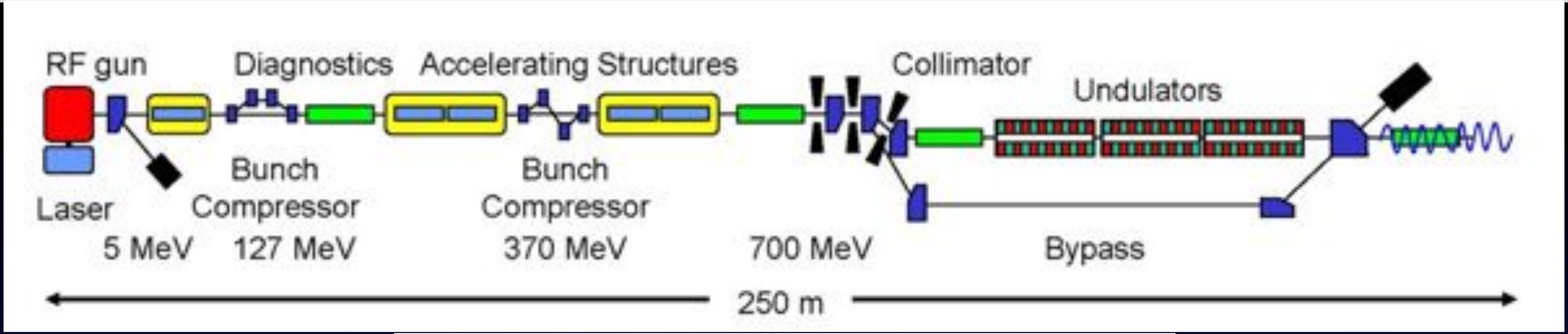
Classification

Averaging

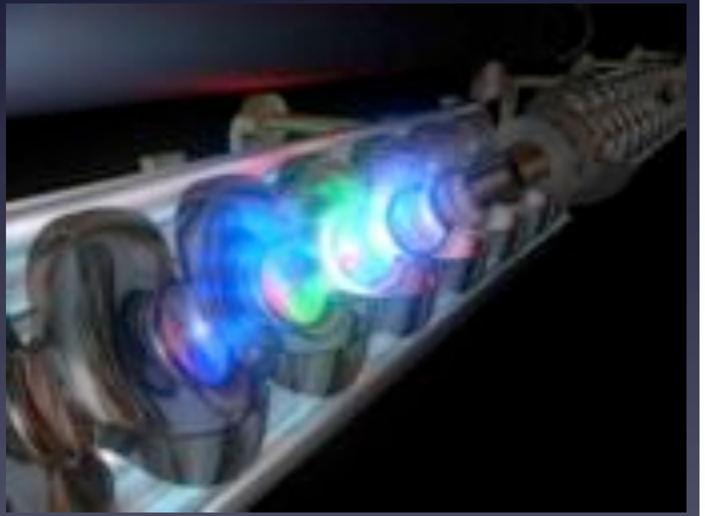
Orientation

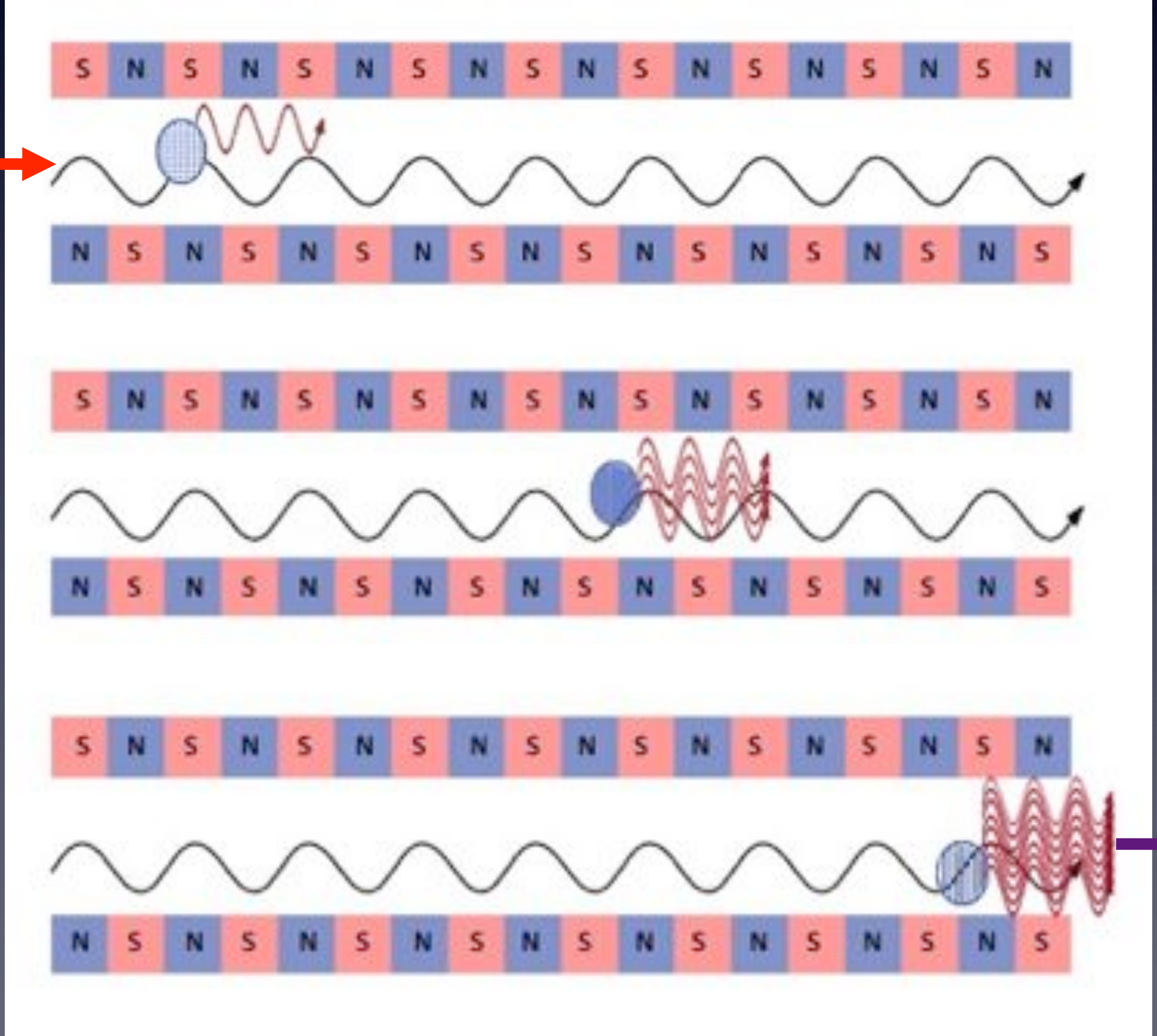
Reconstruction

Self Amplified Spontaneous Emission (SASE) produces intense, ultrafast, coherent X-ray pulses



Electron bunch
(from LINAC)



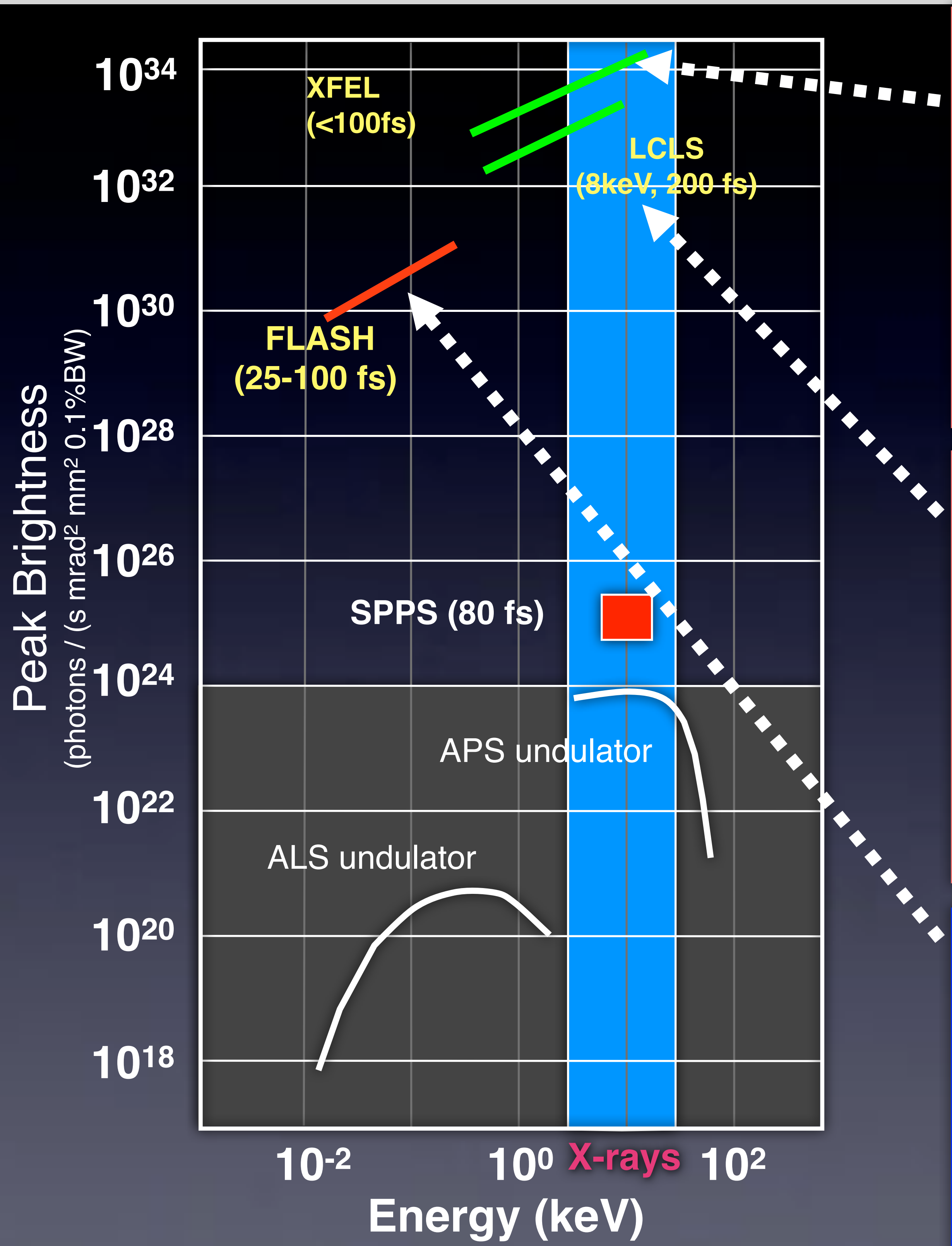


Graphics from:
vuv-fel.desy.de/
www-ssrl.slac.stanford.edu/lcls/

LCLS:
800 eV to 8 keV
λ from 15Å - 1.5Å
<100 fs pulses
~10^{12} - 10^{13} photons/pulse

X-ray pulses out

X-ray free electron lasers are a unique class of X-ray source



APS=Advanced Photon Source (ANL)
ALS=Advanced Light Source (LBNL)

operational 2015
- 1-8 keV
- 20-50 fs
- 10^{13} photons/pulse

European X-ray FEL,
DESY, Hamburg

operational
- 0.8-8 keV
- 200 fs
- 10^{12} photons/pulse

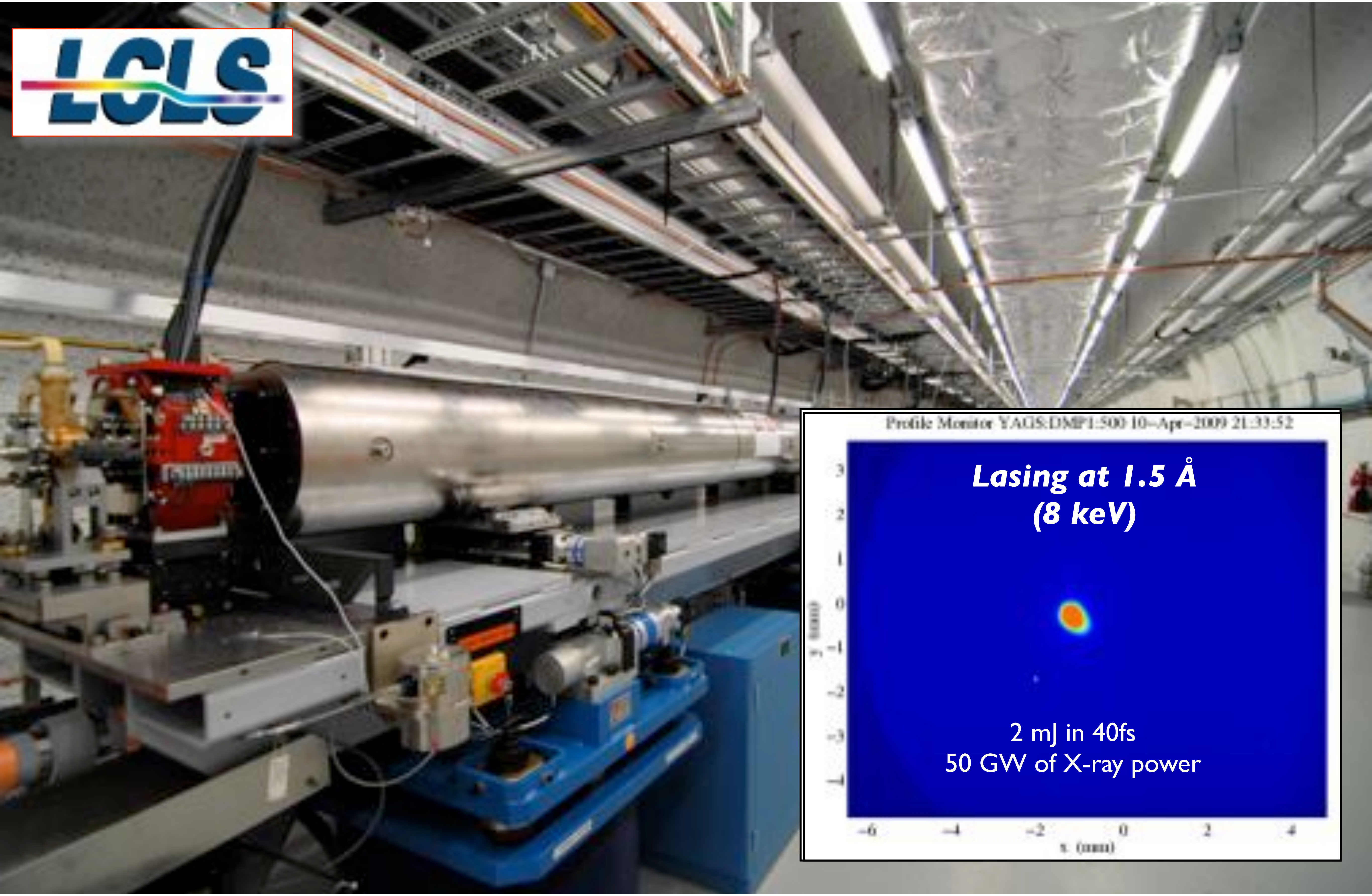
Linac Coherent Light Source,
SLAC, Stanford

operational
- 50-400 eV (7-50 nm)
- 25 fs
- 10^{12} photons/pulse

FLASH
DESY, Hamburg

The Linac Coherent Light Source lases at 0.15 nm wavelength

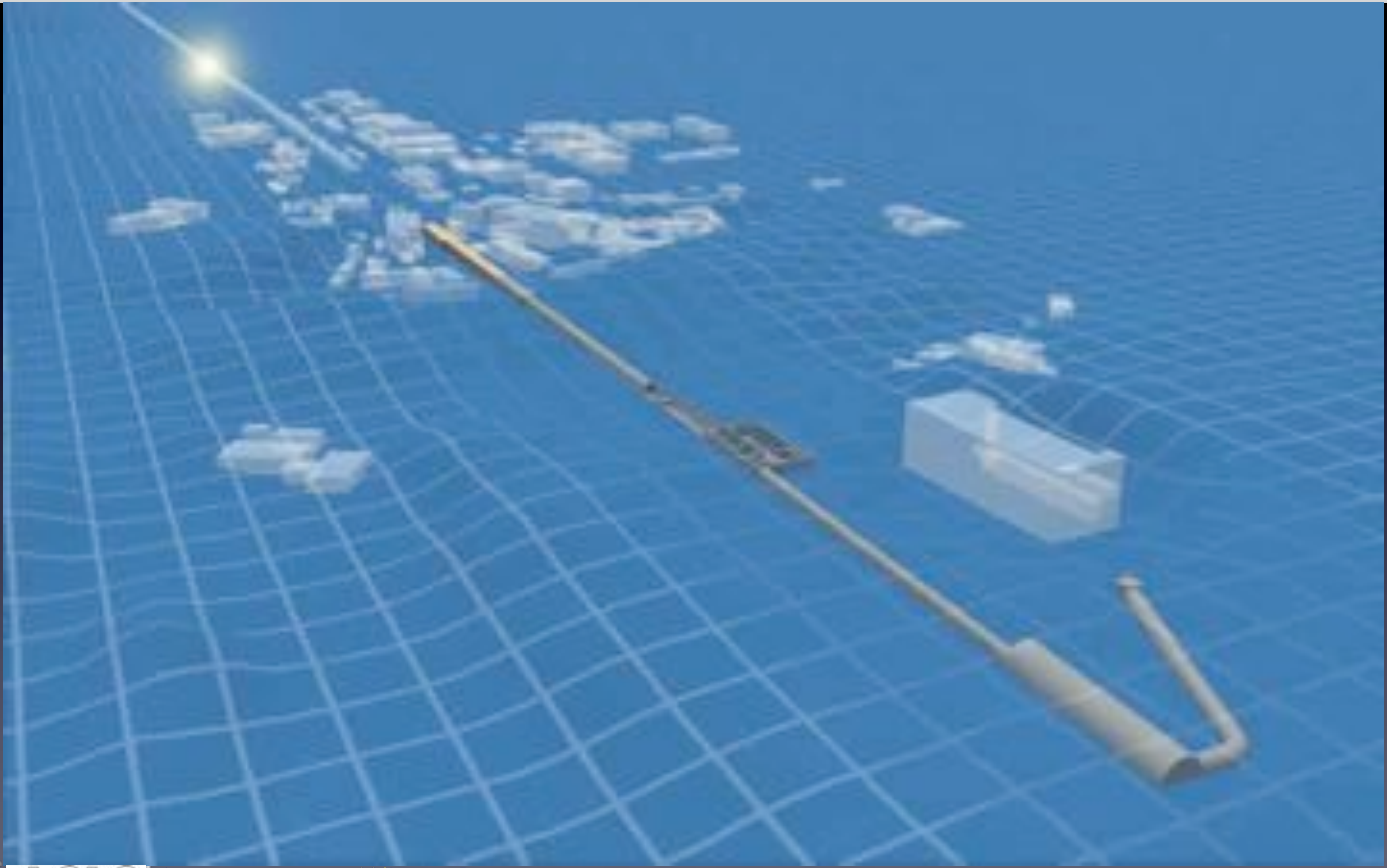
LCLS



Lasing at 1.5 Å
(8 keV)

2 mJ in 40fs
50 GW of X-ray power

Serial imaging at LCLS builds signal by collecting data from many copies of the same sample



Animation courtesy of Sébastien Boutet, CXI instrument scientist, SLAC

Serial imaging at X-ray free electron lasers poses many computational challenges

1. Data acquisition

- Imaging detectors create 8MB per frame (2k x 2k x 16 bit)
- Sometimes two detectors, plus as much data again in diagnostics
- Distributed data acquisition

10 Hz	(FLASH)
120 Hz	(LCLS)
27000 pps	(XFEL)

2. Data reduction and storage

- Data must be saved at a high data rate
- Currently save all data for offline analysis
- Robust online vetoing and frame rejection will becoine increasingly important

80 MB/sec (FLASH)
960 MB/sec (LCLS)
216,000 MB/sec (XFEL)

3. Data processing

- Typically 4,000,000 images per sample
- Data analysis must be automated

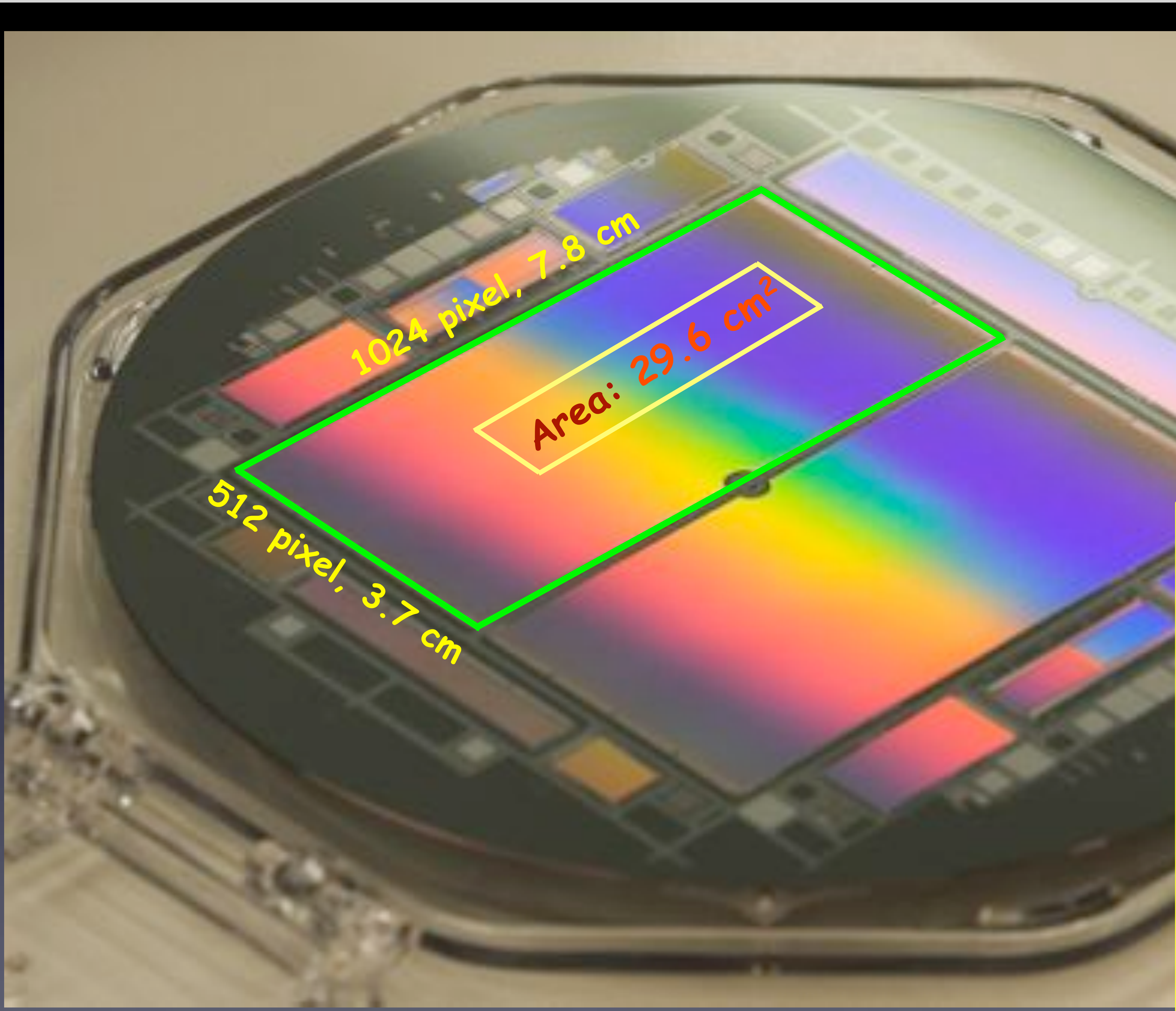
140 TB / experiment (LCLS)

4. Cultural challenges

- Photon scientists are used to analysing data by hand (hire more postdocs)
- Typically keep all data, throw away none, and want to take all data home
- No two experiments are entirely the same, a different experiment every week
- (Mostly) small research groups
- Short-term experiments, not 10-20 year projects with long-term management

CFEL SCIENCE

CCD with central hole enables direct detection at the LCLS pulse repetition rate of 120 frames per second



1024x1024 pixels

pixel size: 75 x 75 µm²

active area 60 cm²

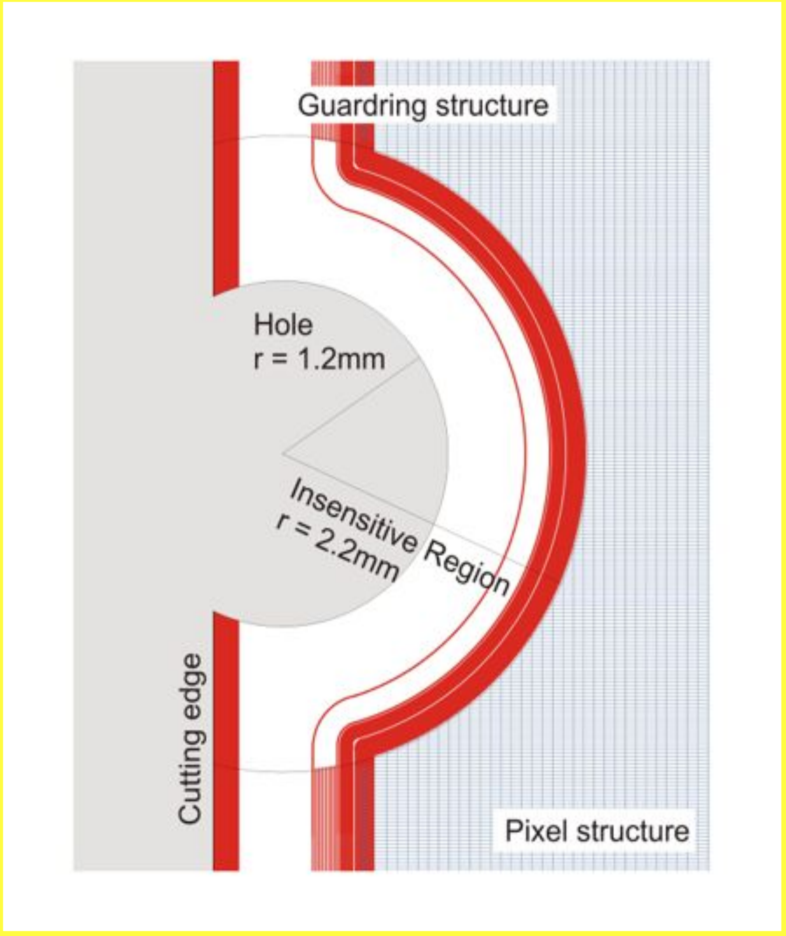
frame rate 125-900 Hz

single-photon resolution

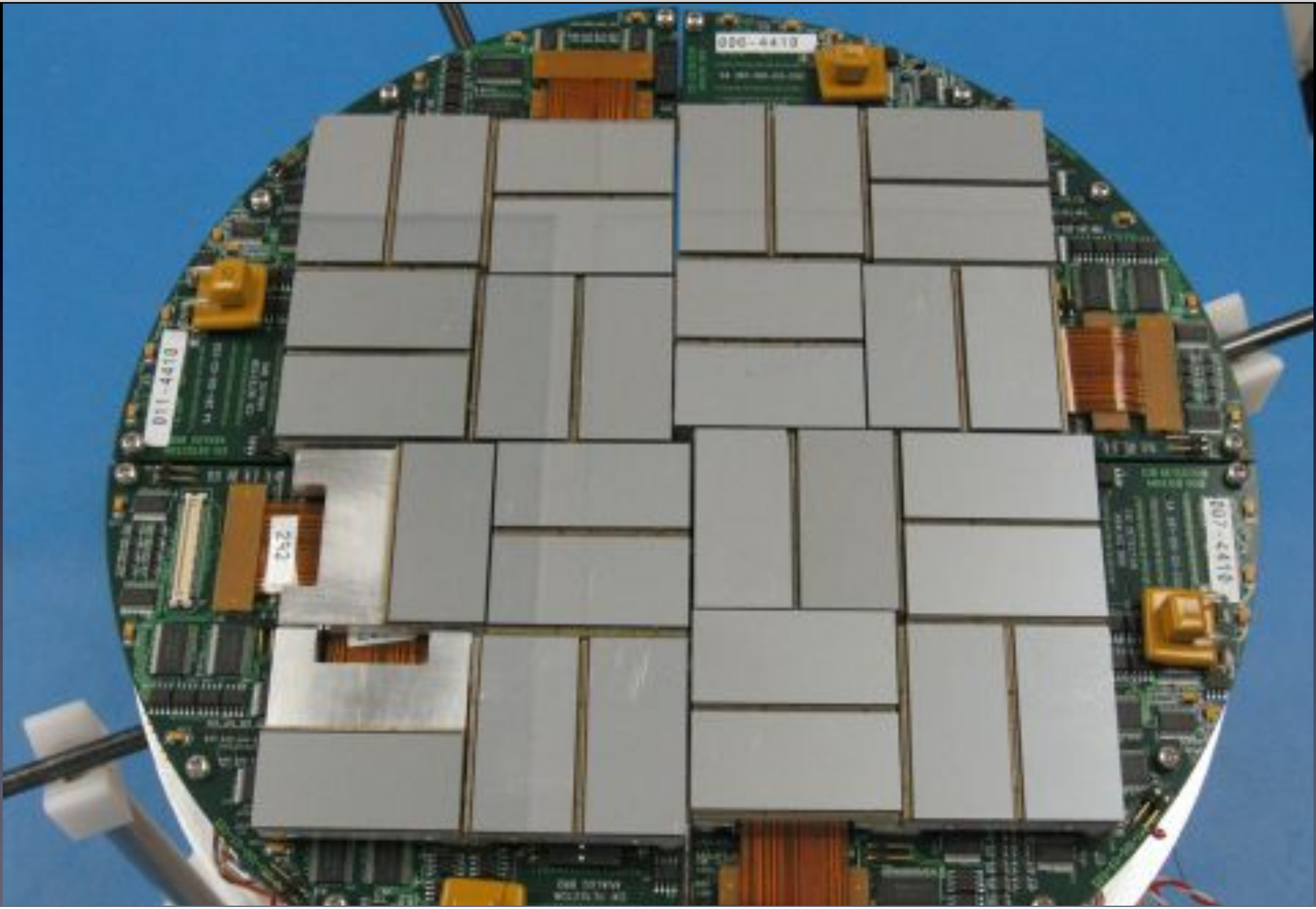
ΔE=50/80eV @ 800/2000eV

Q.E. ≥ 90 % from 0.4 to 10 keV

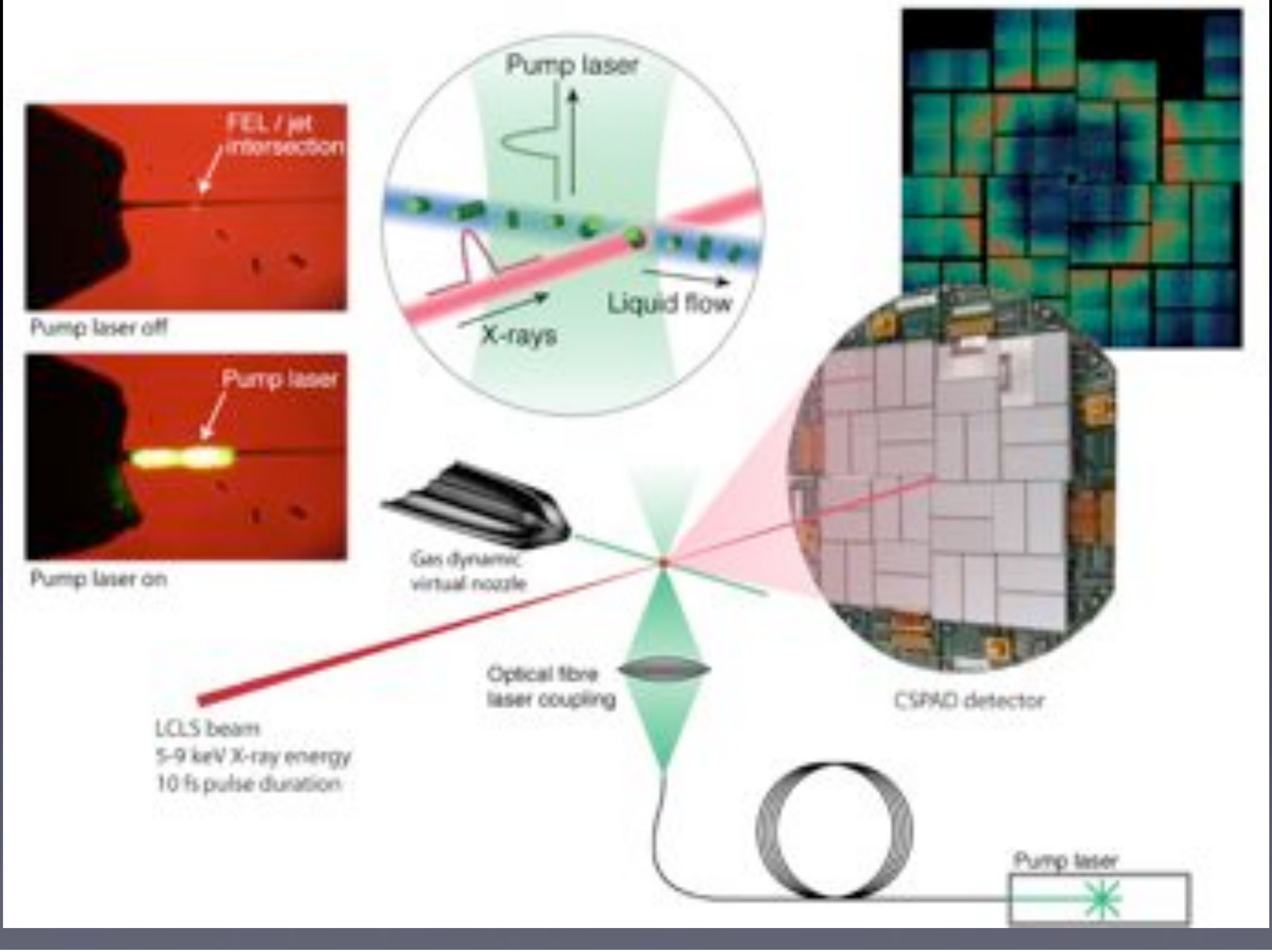
operating range 0.1 < E < 24 keV



The cspad pixel array hard X-ray detector has 2M pixels and runs continuously



We introduce hydrated nanocrystals into the LCLS beam using a flowing liquid jet



We measured 2Å resolution diffraction from an unsolved glyco-protein Cathepsin B using in-vivo crystallisation at LCLS

Glyco-proteins are extremely difficult to crystallize and hence solve by conventional methods

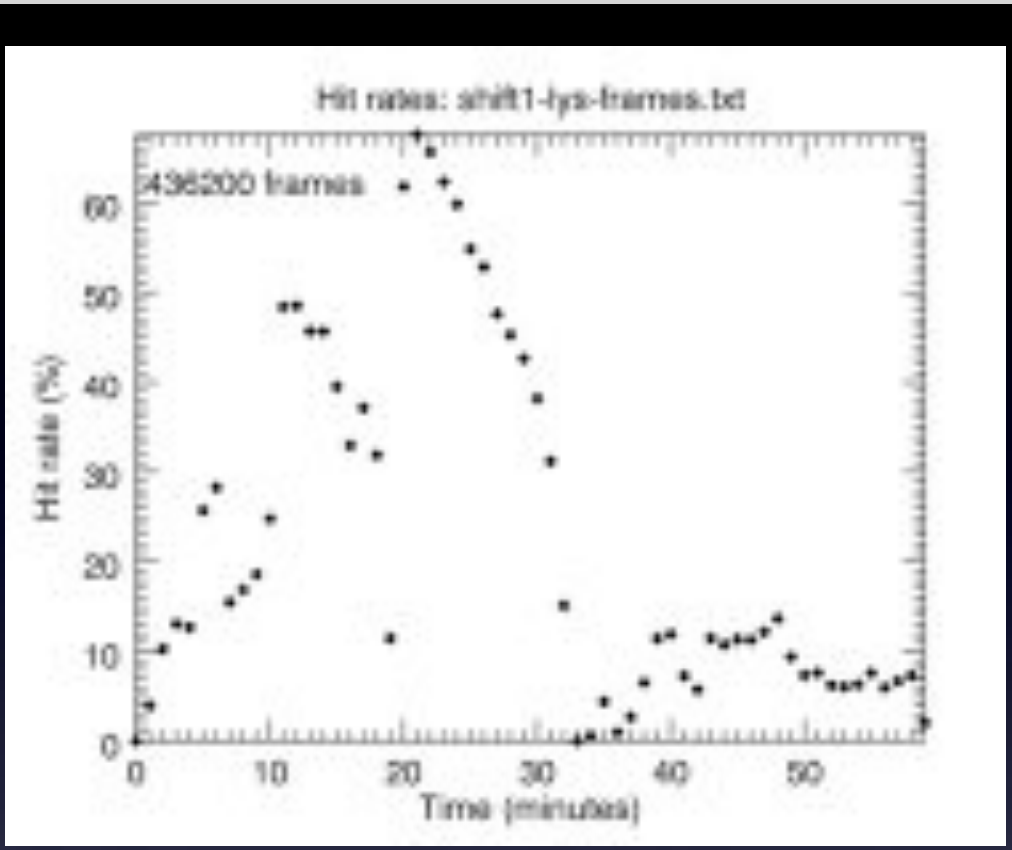
Redecke, Nass et al., 2013. Science, 339, pp.227–230.

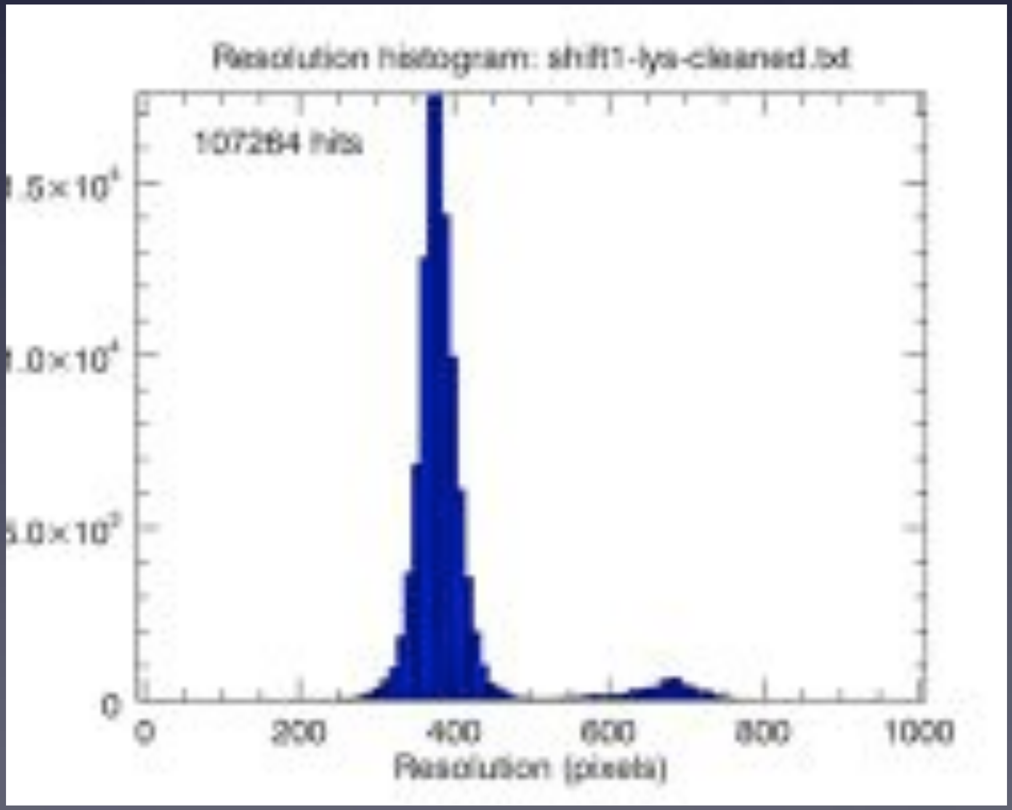
We generate statistics on data acquisition rates and data quality in near real time to guide decision making at the beamline

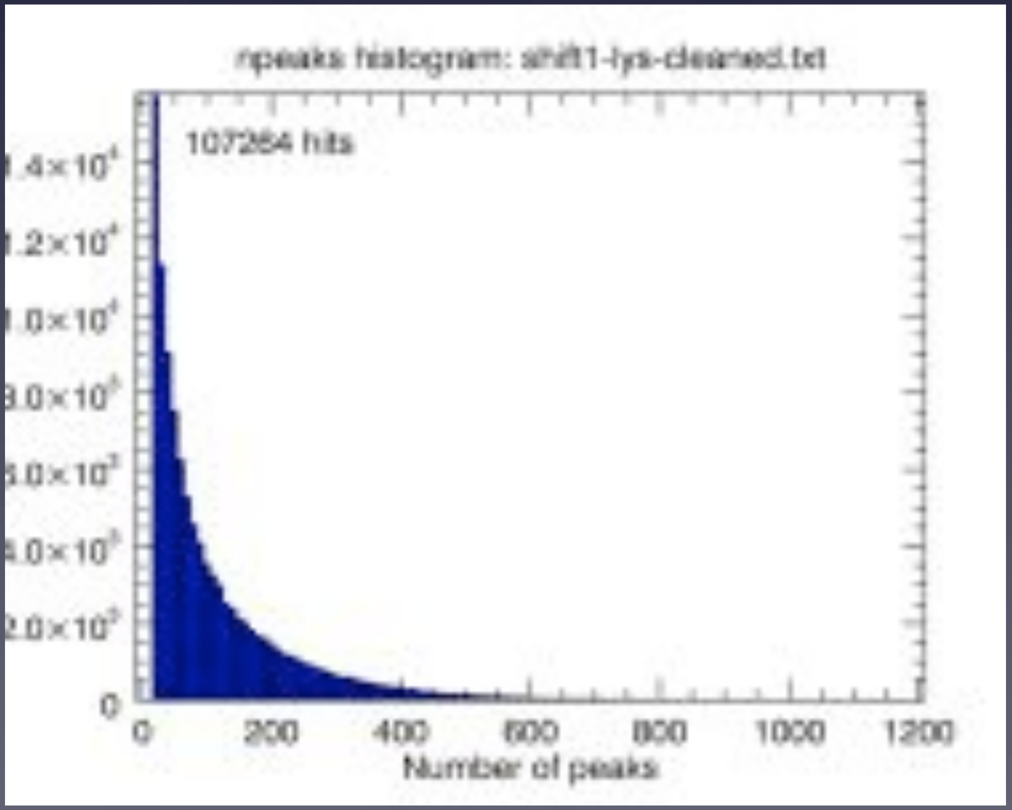
It is important to have near instant feedback on:

- Sample hit rates
- Average resolution of fames with data
- Number of peaks in each image

We can currently assess LCLS data at ~60 Hz (and can go faster)







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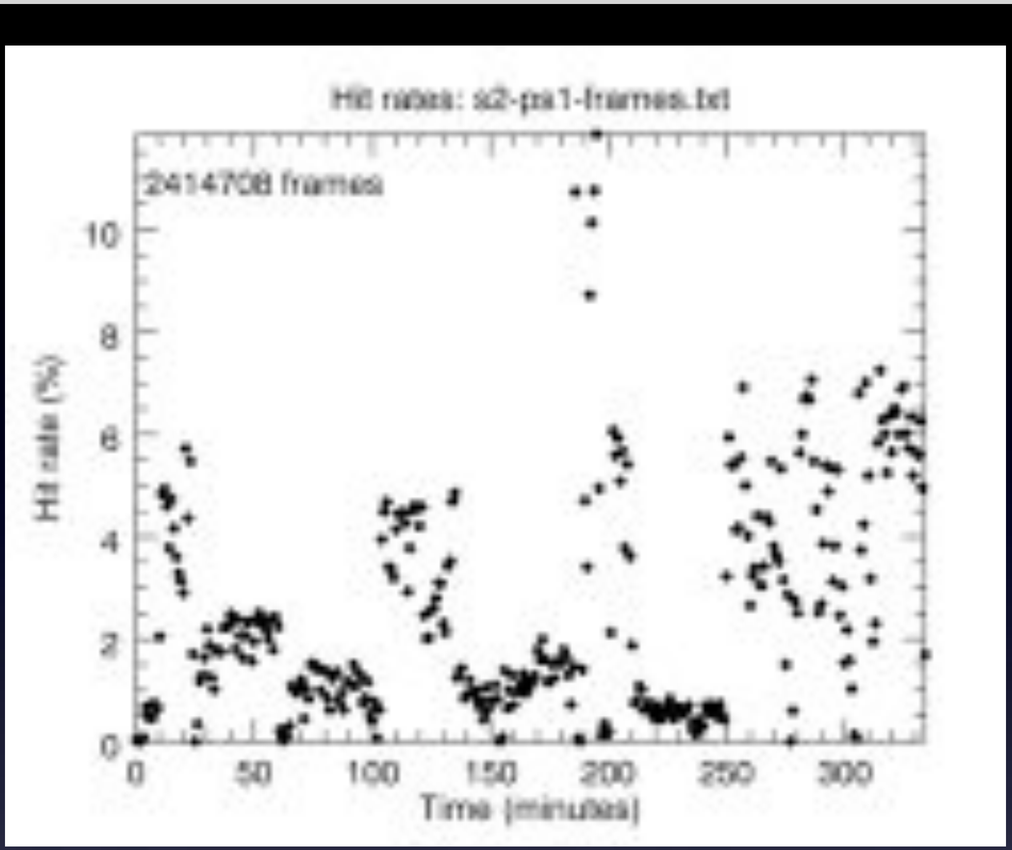
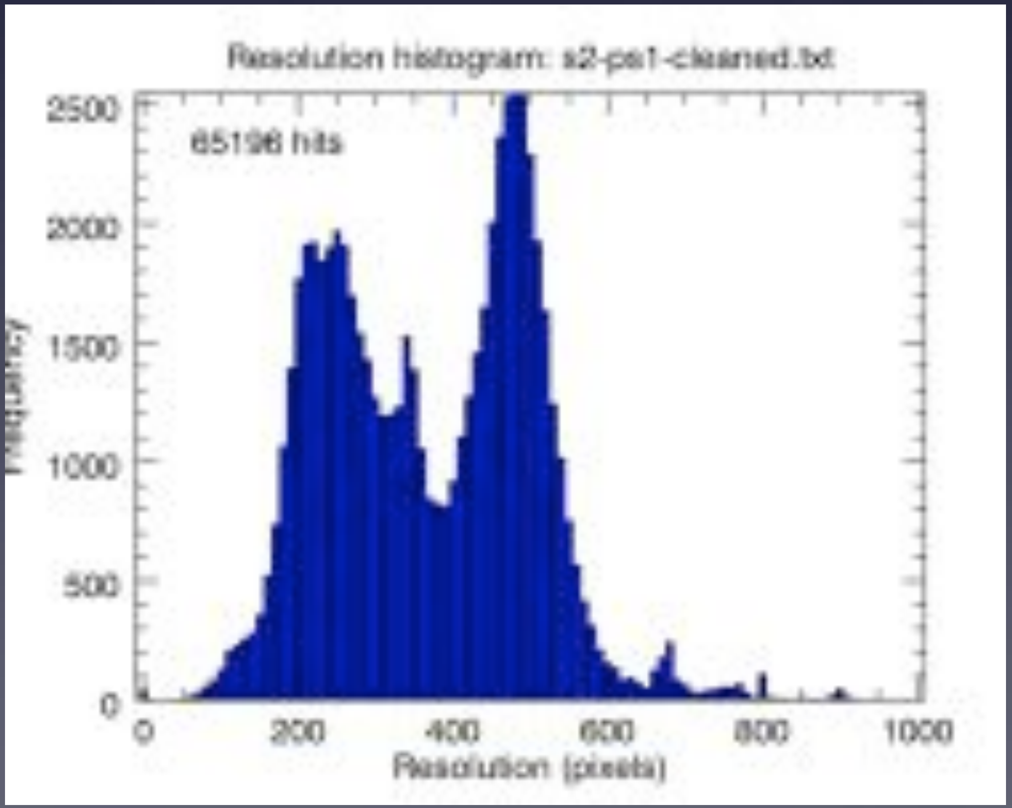
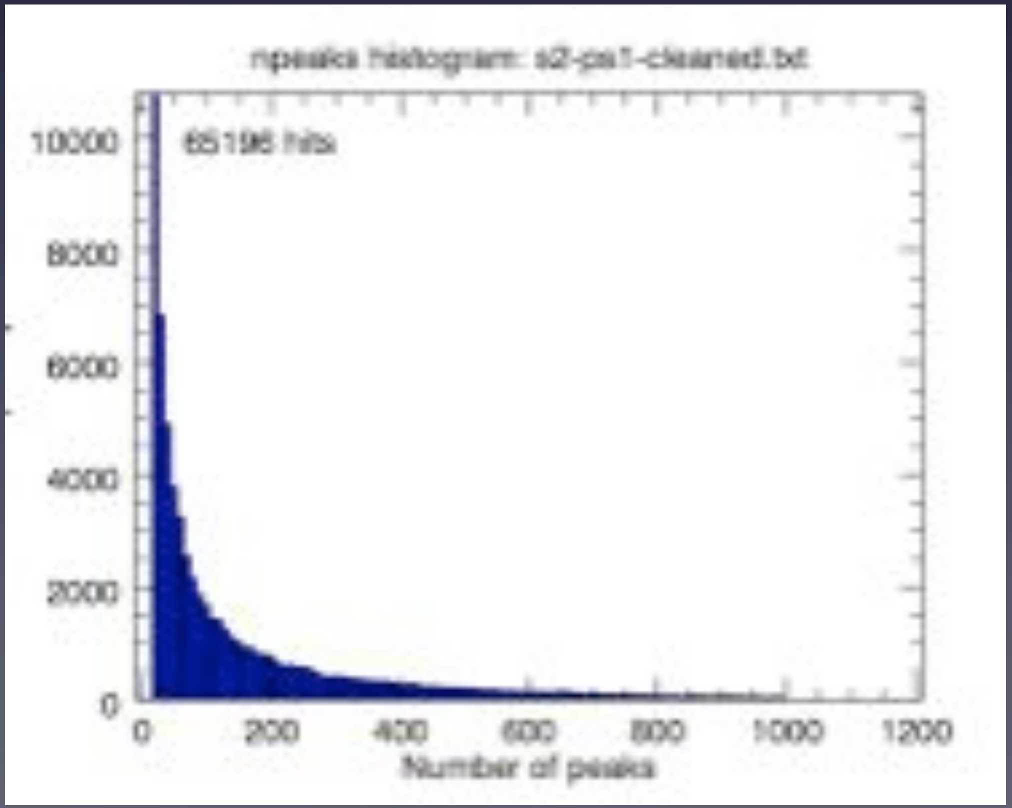
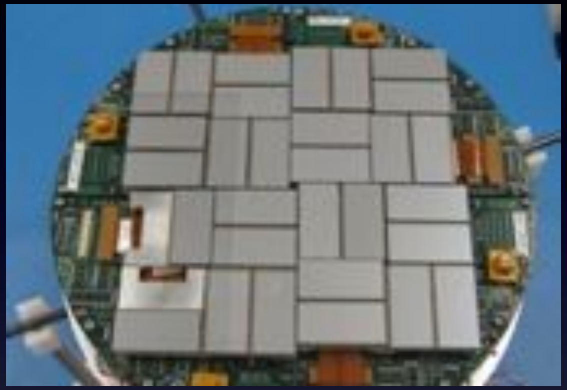






Our processing pipeline is an exercise in data volume reduction

Detector



120 Hz
4 MB/event
1.7 TB/hr
200TB/expt
(5 days)

→

Storage

> 20,000,000 frames

Store all data
(no corrections)

Cheetah →

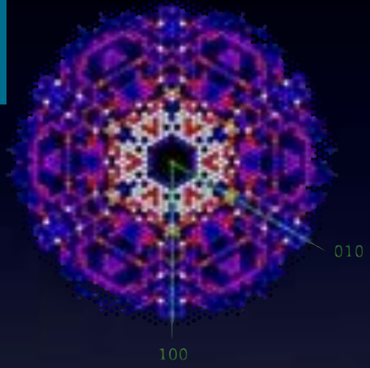
Offline reduction

< 1,000,000 frames

Retain only ‘hits’
(detector corrected)

CrystFEL →

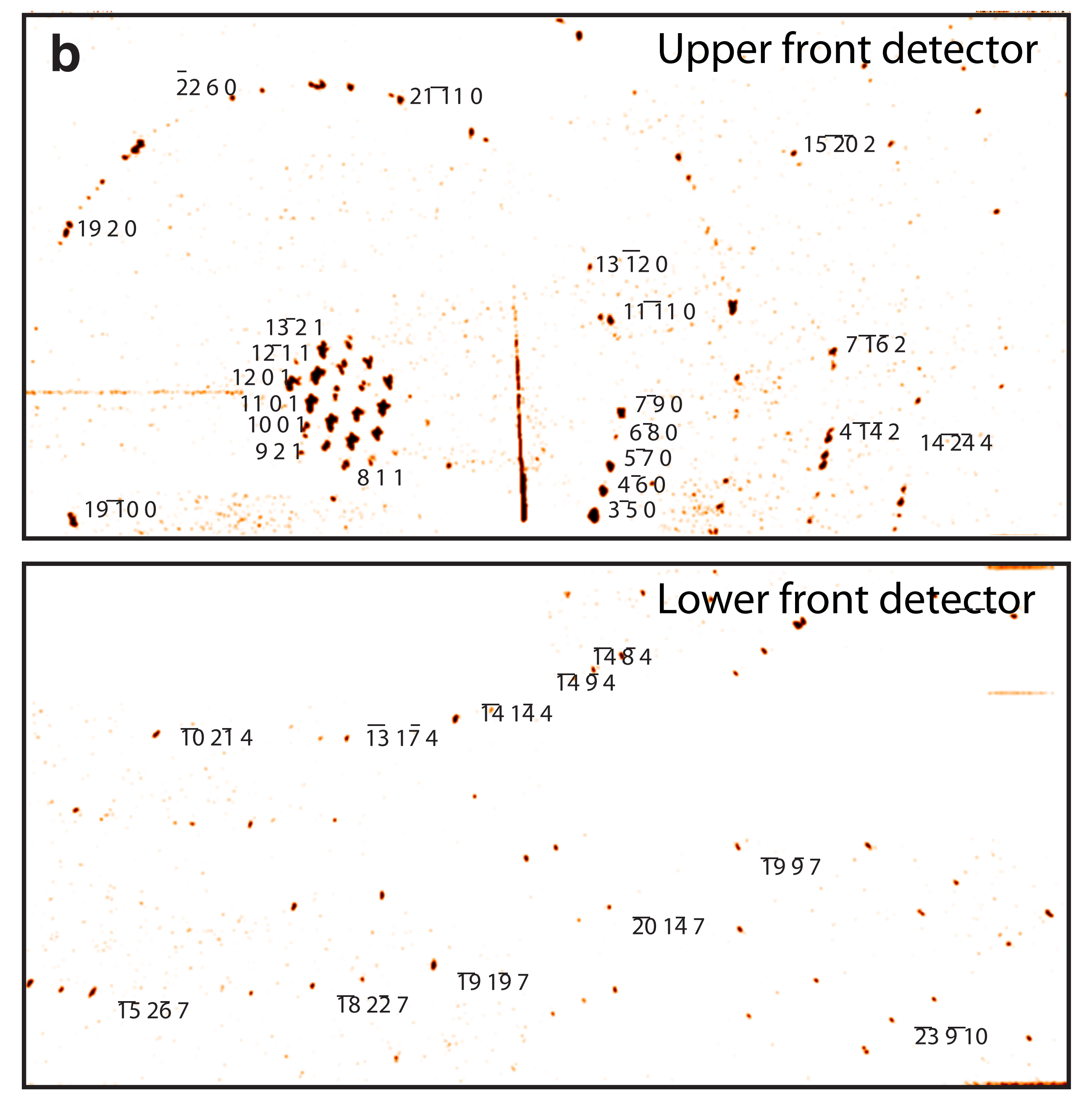
Analysis



<100,000 frames

Automated high volume image processing is essential
(eg: weeding useful data from useless data)

Nanocrystal diffraction patterns are sorted and indexed using software suites developed at CFEL (Cheetah and CrystFEL)

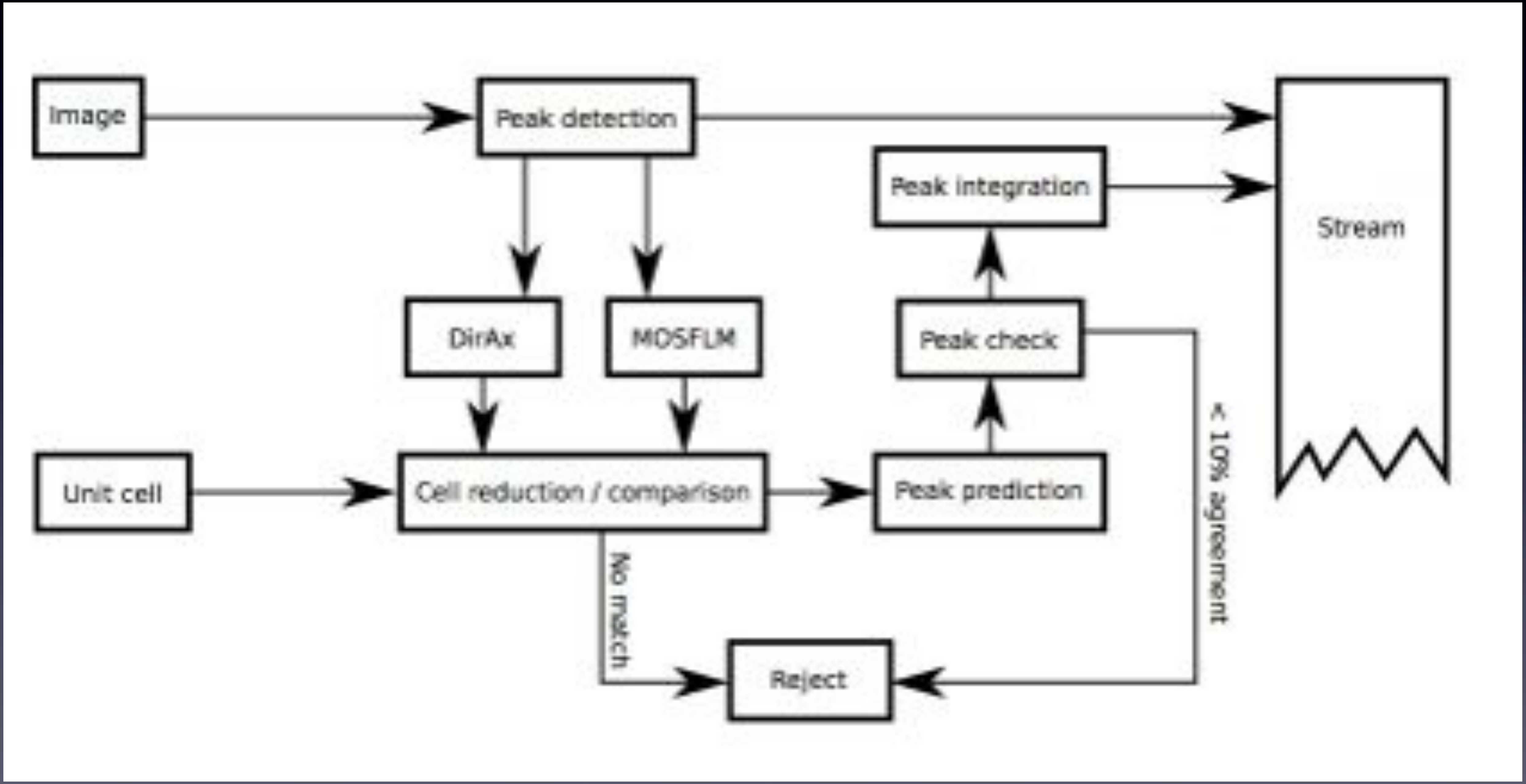


This is not conventional crystallography:

- Each frame is a still image (no time for oscillation)
- Each measurement is a new nanocrystal in a new orientation
- All reflections are partial and must be integrated over many frames.

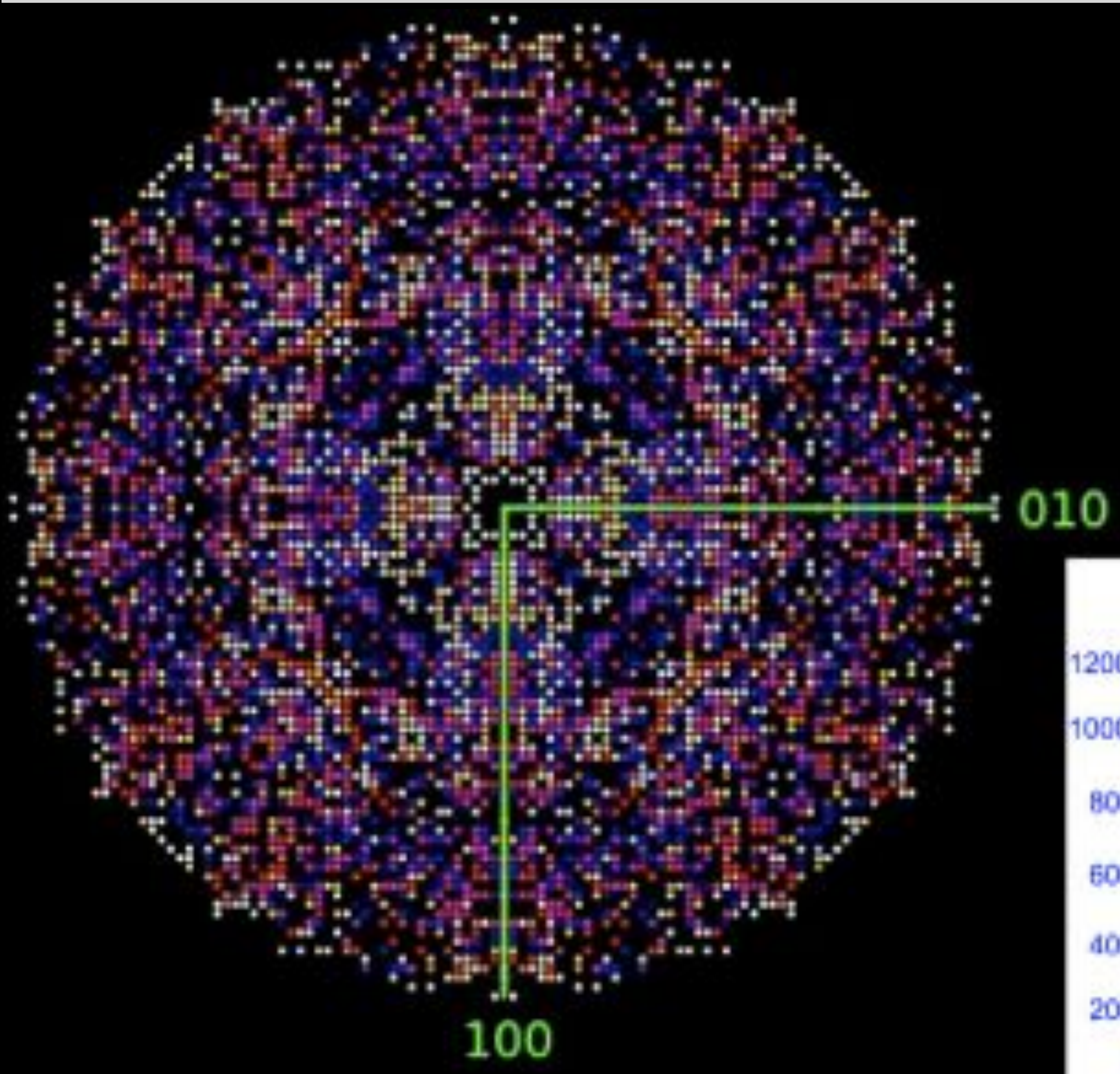
A modular approach to software design will smooth integration into the XFEL scientific computing master plan

Analysis tasks can be broken down into modules within the XFEL analysis framework

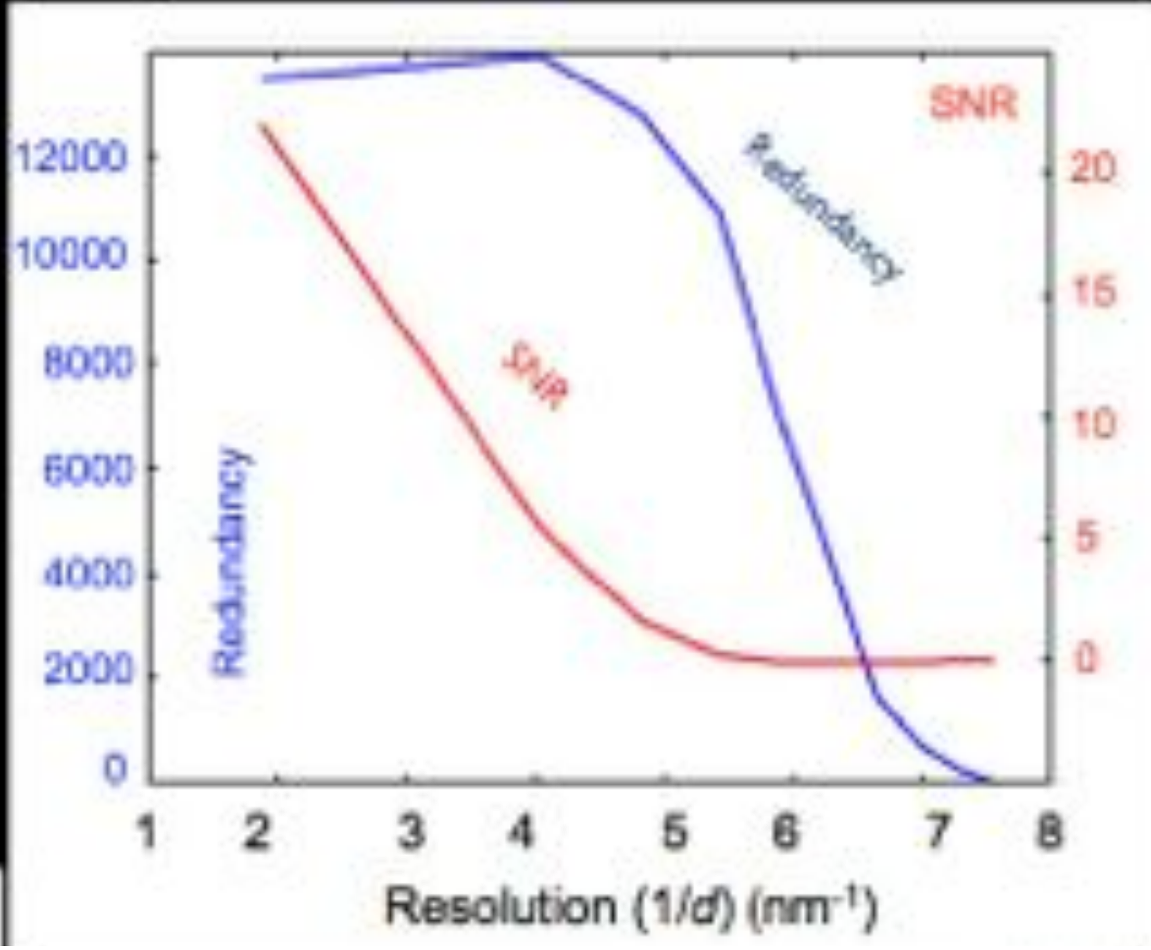


CFEL SCIENCE

We indexed over 150,000 individual diffraction patterns from Cathepsin B

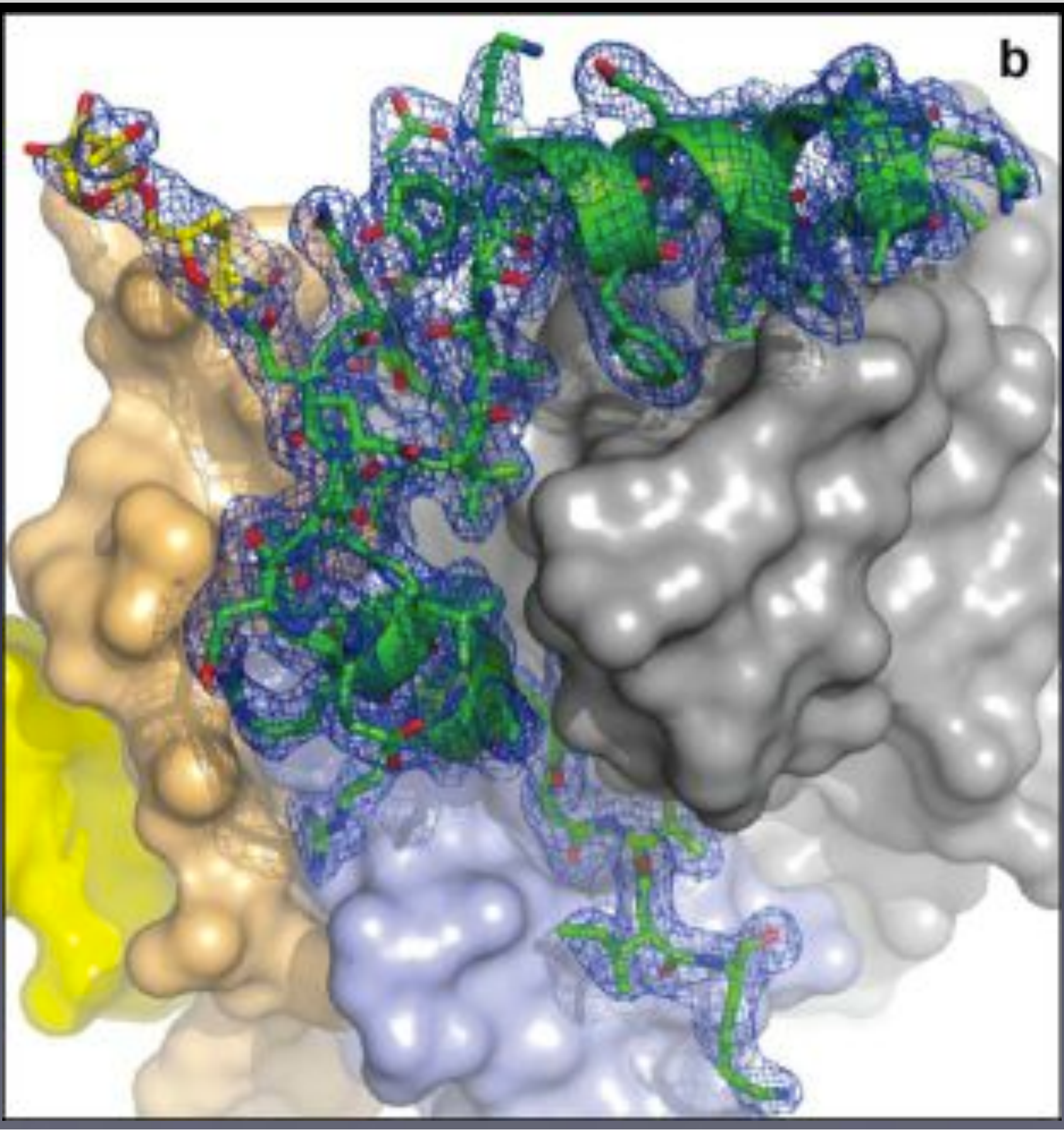


- 3,953,201 frames collected with 40 fs pulses
- 8 hours of data collection
- 357,555 "crystal hits" detected (9%)
- 156,565 indexed (44%)



Redecke, Nass et al., 2013. Science, 339, pp.227–230.

Refined structure 1.9 Å based on SFX data reveals structure of the natural pro-peptide binding

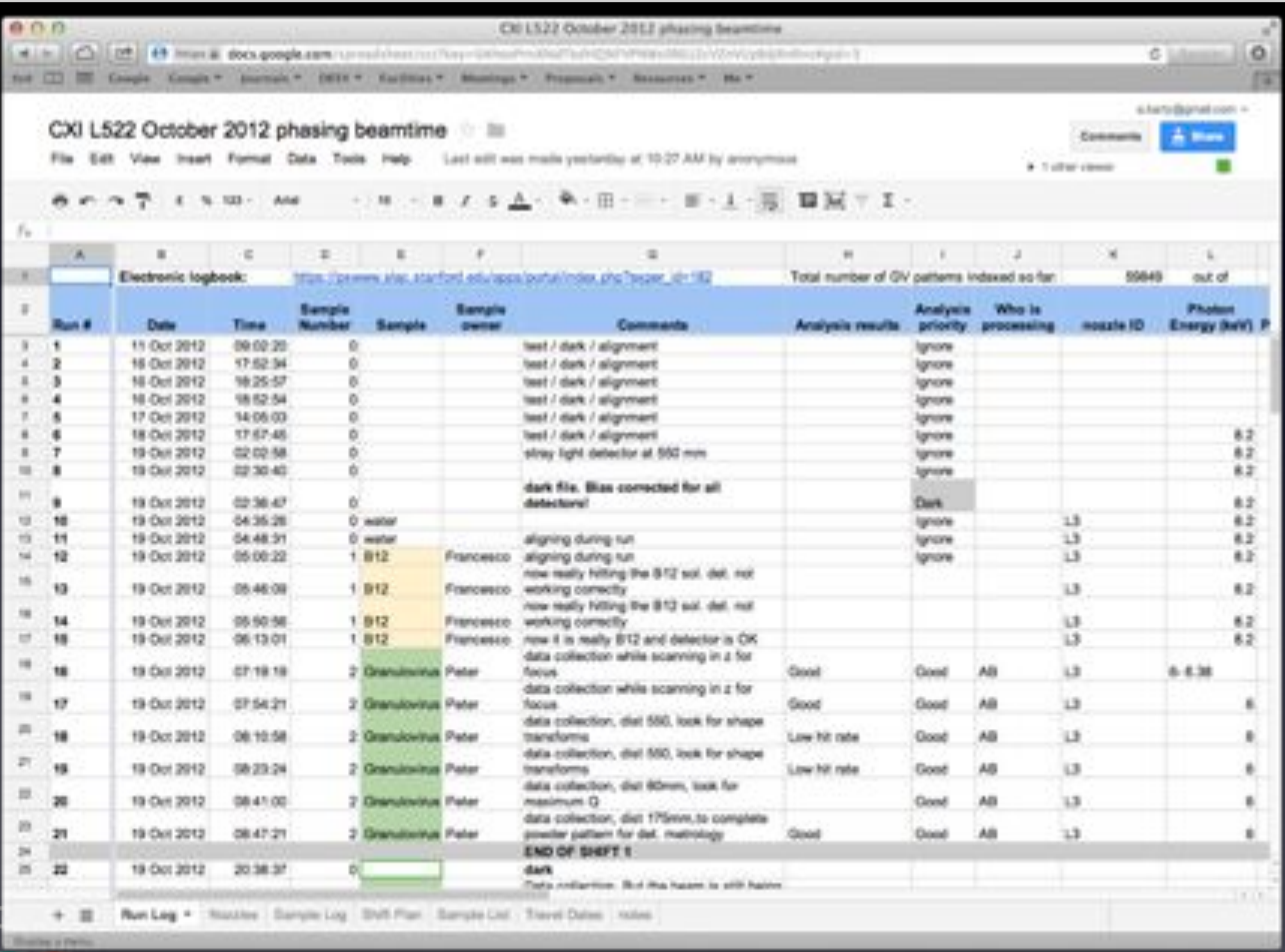


- 8 hours data collection
- 3,953,201 data frames collected (40 fs pulses, 9 keV X-rays)
- 357,555 crystal hits (9%)
- 156,565 indexed patterns (44%)
- 13,429 redundancy

Data collection	
Wavelength (Å)	1.32
X-ray focus FWHM (μm²)	6
Dose (MGy) per crystal	31
Space group	$P4_12_12$
Cell dimensions *a*, *b*, *c* (Å)	125.4, 125.4, 54.6
V_M (Å³/Da) / solvent content (%)	3.09 / 60.16
Number of collected patterns	3,953,201
Number of crystal hits (% of collected patterns)	357,555 (9)
Number of indexed patterns (% of hits)	156,565 (44)
Number of unique reflections	34,798
Resolution (Å)	20 – 1.9 (1.95 – 1.90)
Completeness (%)	99.6 (99.4)
I/σ (*I*)	9.26 (0.71)
R_{split}	0.152
Redundancy	13,429 (13,198)

Redecke, Nass et al., 2013. Science, 339, pp.227–230.

Cloud-based logging is an essential tool for data organisation



CXI L522 October 2012 phasing beamtime

Last edit was made yesterday at 10:27 AM by anonymous

Electronic logbook: https://pswww.slac.stanford.edu/apps/portal/index.php?exper_id=182

Total number of GV patterns indexed so far: 59849 out of

Run #	Date	Time	Sample Number	Sample	Sample owner	Comments	Analysis results	Analysis priority	Who is processing	nozzle ID	Photon Energy (keV)
1	11 Oct 2012	09:02:20	0			test / dark / alignment		Ignore			
2	16 Oct 2012	17:52:34	0			test / dark / alignment		Ignore			
3	16 Oct 2012	18:25:57	0			test / dark / alignment		Ignore			
4	16 Oct 2012	18:52:54	0			test / dark / alignment		Ignore			
5	17 Oct 2012	14:06:03	0			test / dark / alignment		Ignore			
6	18 Oct 2012	17:57:45	0			test / dark / alignment		Ignore			8.2
7	19 Oct 2012	02:02:58	0			stray light detector at 550 mm		Ignore			8.2
8	19 Oct 2012	02:30:40	0					Ignore			8.2
9	19 Oct 2012	02:38:47	0			**dark file. Bias corrected for all detectors!**		Dark			8.2
10	19 Oct 2012	04:35:28	0	water				Ignore		L3	8.2
11	19 Oct 2012	04:48:31	0	water		aligning during run		Ignore		L3	8.2
12	19 Oct 2012	05:00:22	1	B12	Francesco	aligning during run		Ignore		L3	8.2
13	19 Oct 2012	05:46:09	1	B12	Francesco	now really hitting the B12 sol. det. not working correctly				L3	8.2
14	19 Oct 2012	05:50:58	1	B12	Francesco	now really hitting the B12 sol. det. not working correctly				L3	8.2
15	19 Oct 2012	06:13:01	1	B12	Francesco	now it is really B12 and detector is OK				L3	8.2
16	19 Oct 2012	07:19:19	2	Granulovirus	Peter	data collection while scanning in z for focus	Good	Good	AB	L3	6- 6.38
17	19 Oct 2012	07:54:21	2	Granulovirus	Peter	data collection while scanning in z for focus	Good	Good	AB	L3	6
18	19 Oct 2012	08:10:58	2	Granulovirus	Peter	data collection, dist 550, look for shape transforms	Low hit rate	Good	AB	L3	6
19	19 Oct 2012	08:23:24	2	Granulovirus	Peter	data collection, dist 550, look for shape transforms	Low hit rate	Good	AB	L3	6
20	19 Oct 2012	08:41:00	2	Granulovirus	Peter	data collection, dist 80mm, look for maximum Q		Good	AB	L3	6
21	19 Oct 2012	08:47:21	2	Granulovirus	Peter	data collection, dist 175mm,to complete powder pattern for det. metrology	Good	Good	AB	L3	6
						END OF SHIFT 1					
22	19 Oct 2012	20:38:37	0			**dark**					

We copy data from SLAC to DESY over the web

Friday, November 2nd, 2012

October 2012 User of the Month: Dmitry Ozerov

I am pleased to announce that the user of the month for October 2012 is Dmitry Ozerov from DESY in Germany.

Dmitry has a background in particle physics research and is currently working as an IT data management specialist in the Scientific Data Management and Grid Computing team at DESY, Hamburg. The team manages 7.5 petabytes of disk and 4 petabytes of tape storage, and the batch facility for the scientists from the High Energy Physics and Photon Science.

Dmitry is helping scientists from the Center for Free-Electron Laser Science to transfer a large amount of data from the LCLS in Stanford, USA to his home institute in Hamburg, Germany. Dmitry moved a whooping 276 terabytes of data in less than a month! He achieved transfer rates as high as 450Mbps over the transatlantic link, with round trip time greater than 150 ms.

"Because of the large amount of data, the use of the transatlantic link, and the need

Recent Blog Posts

- January 2013 User of the Month: Ann Syrowski
- December 2012 User of the Month: Kurt LaButt
- Use Test Endpoints to Anticipate Your Data Transfer Rates
- Globus Online is a non-profit serving non-profits
- October 2012 User of the Month: Dmitry Ozerov

Blog Contributors

Borja Sotomayor (2)
Brigitte Raumann (1)
Bryce Allen (1)
Graham Jenkins (1)
Ian Foster (4)
Lee Liming (1)
Lisa Childers (1)
Paul Dave (7)
Peter Hadlaw (1)
Rajkumar Kettimuthu (14)
Ravi Madduri (1)
Stuart Martin (3)
Vas Vasiliadis (3)

Blog Archives

January 2013
December 2012
November 2012
October 2012
September 2012
August 2012

276 terabytes of data in less than a month

We currently process hundreds of TB of data each year using "off the shelf" hardware

One experiment at LCLS (120 Hz) can generate over 100TB of data per experiment.

Fast I/O access necessary for data screening

(600 disks per rack)

Martin Gasthuber, Pirmin Fix, DESY

Storage

Data Direct Networks SFA10000

60-bay HDD enclosures in 4U format

We have 2 racks totalling ~2PB:

600 x 2 TB HDDs + 600 x 3 TB HDDs

Already 60% full!

Scalable (??)

Computing

SGI Altix UV100

144 cores, 768 GB memory

Scales to 96 sockets (960 cores, 1920 threads)

Up to 12TB of shared memory

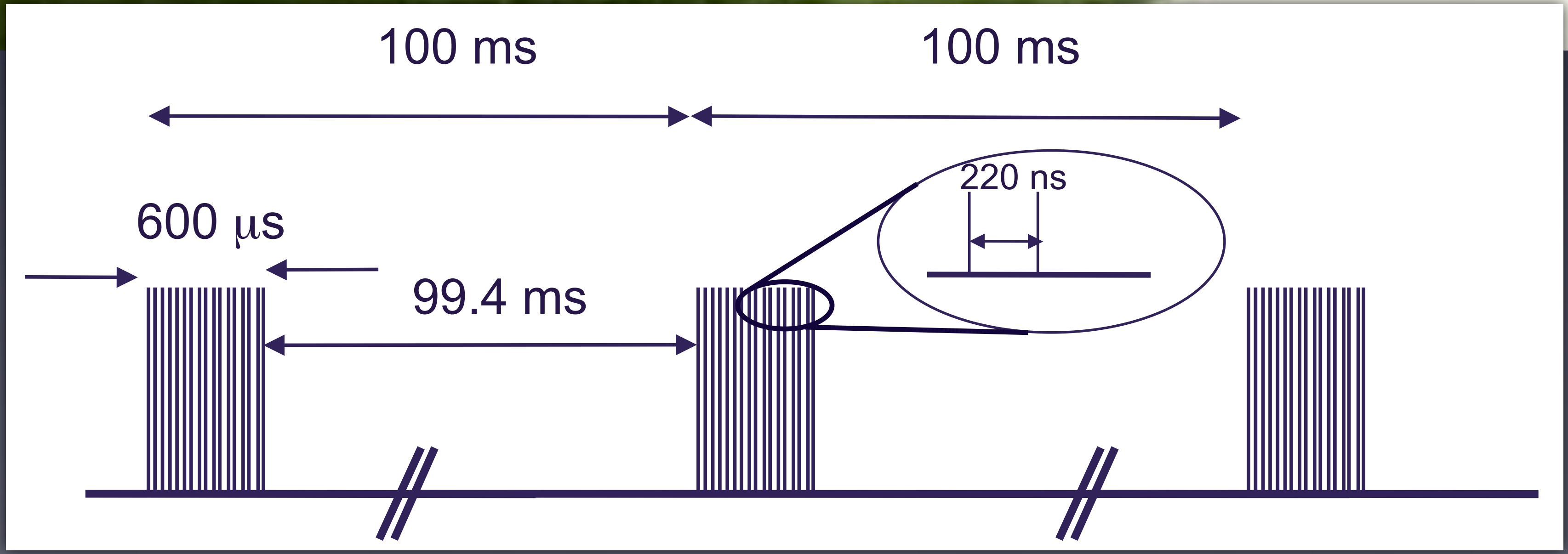
Altix UV 1000: 256 sockets (2560 cores), 16TB of shared memory,

The European XFEL project is in progress at DESY

http://xfel.desy.de/tdr/

The European XFEL microbunch structure can produce up to 26,000 pulses per second

200 frames @ 10 Hz, ~4 MB/image = 8 GB/sec, 28 TB/hr
26,000 pulses/sec, ~4 MB/image = 104 GB/sec, 374 TB/hr



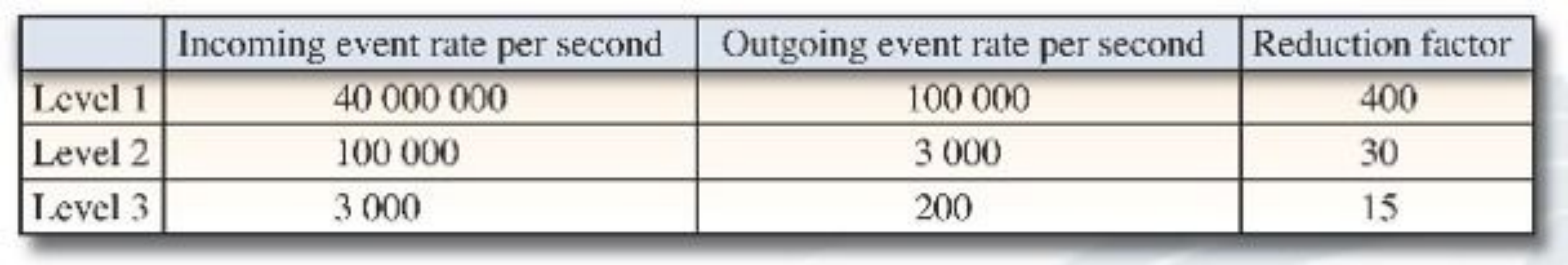
The ATLAS experiment at CERN has a comparable end data rate to the peak data rates anticipated for XFEL

Level 1 trigger (hardware)
Level 2 trigger (PC farm)
Event trigger (PC farm)

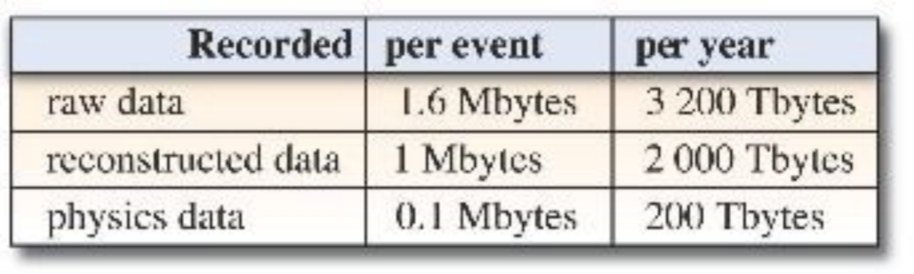
40 MHz
bunch crossing

→

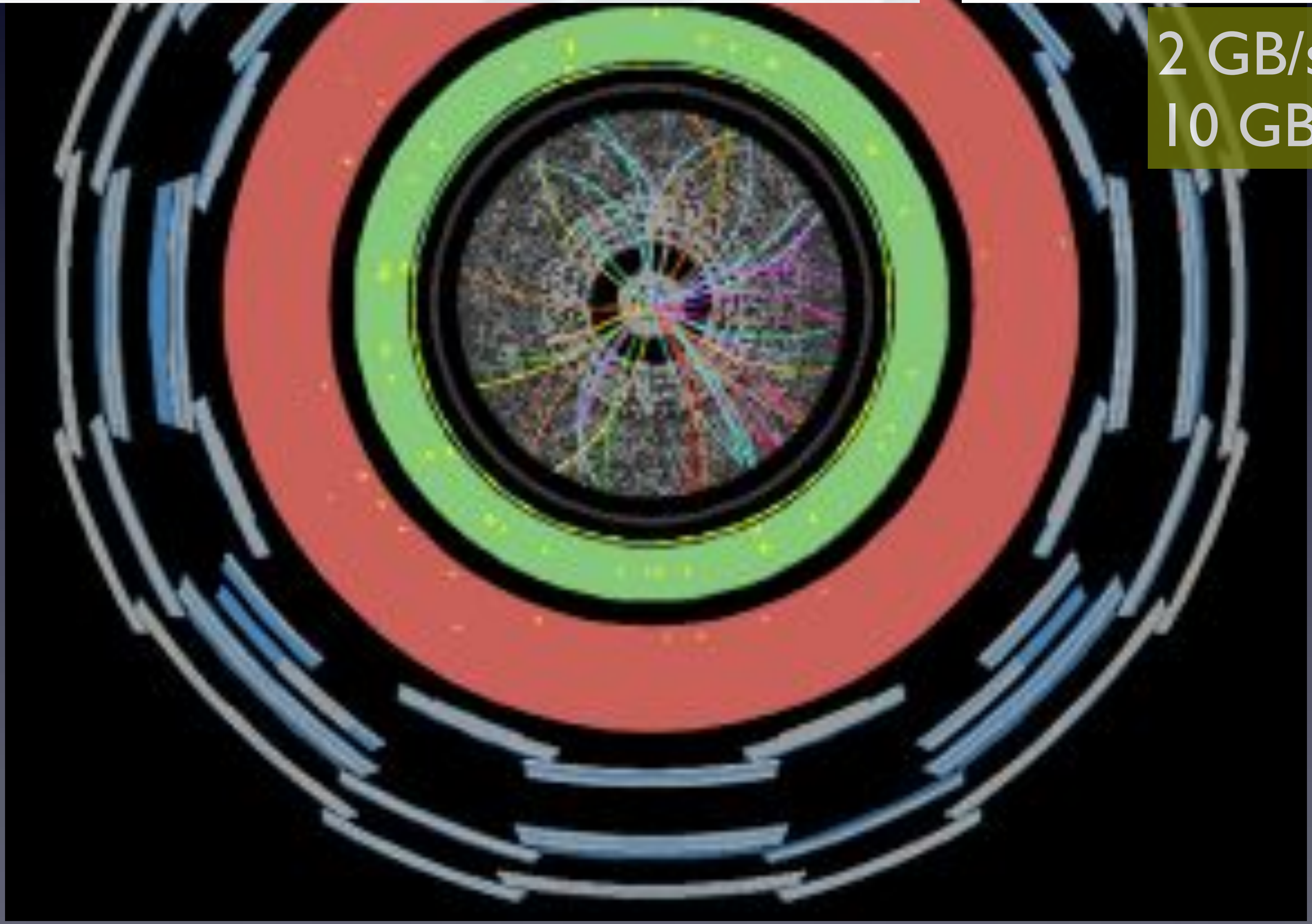
200 Hz
data rate



	Incoming event rate per second	Outgoing event rate per second	Reduction factor
Level 1	40 000 000	100 000	400
Level 2	100 000	3 000	30
Level 3	3 000	200	15

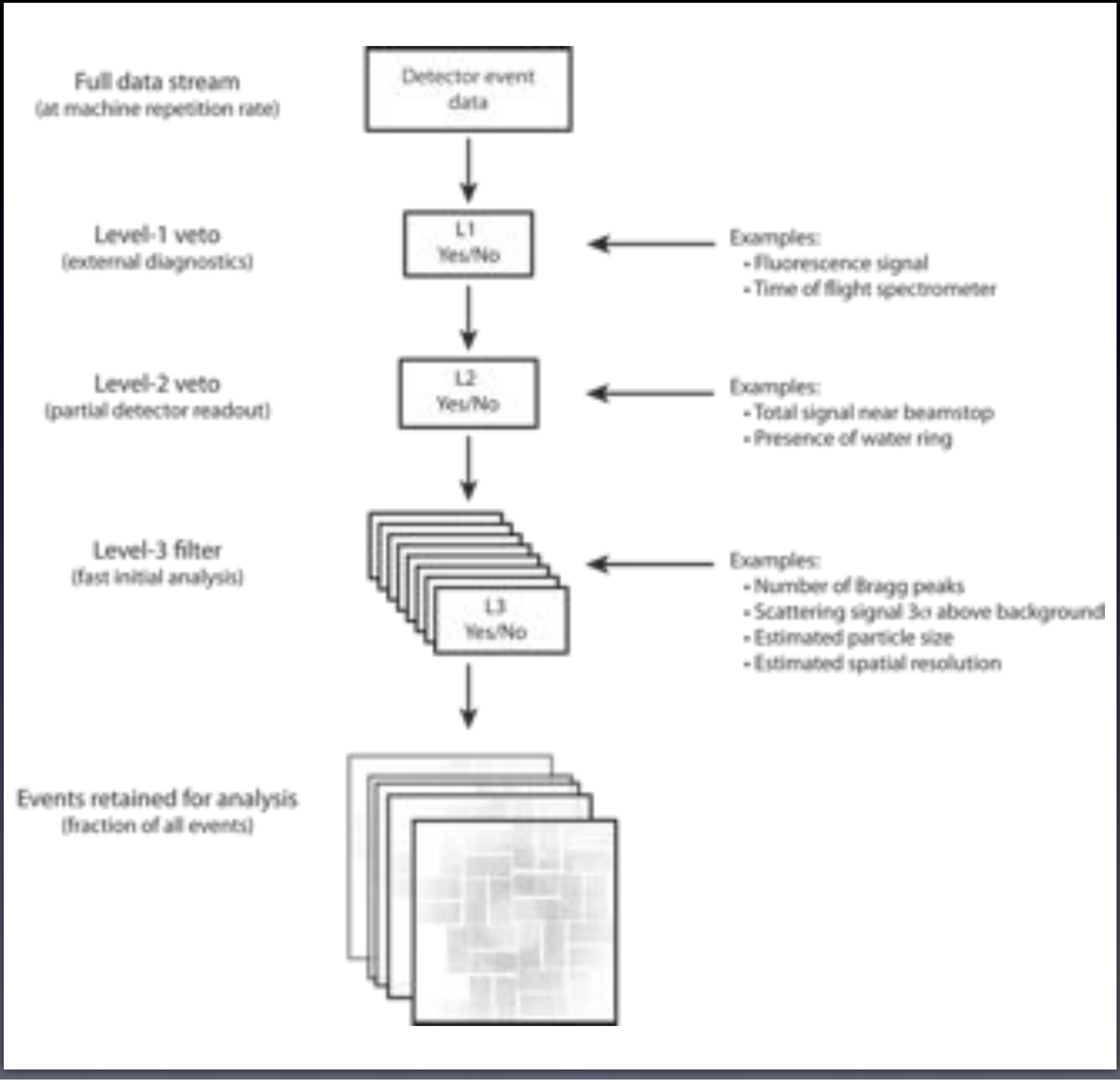


Recorded	per event	per year
raw data	1.6 Mbytes	3 200 Tbytes
reconstructed data	1 Mbytes	2 000 Tbytes
physics data	0.1 Mbytes	200 Tbytes



2 GB/sec (predicted)
10 GB/sec (actual peak)

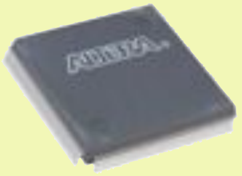
Online vetoing and rapid data reduction will be an important part of the XFEL data management pipeline



WP 1
(Rapid frame vetoing)

FEE
(Front End Equipment)

Develop and test options for fast frame veto before readout



FEI
(Front End Interface)

Develop and test options for rapid FPGA frame rejection after readout

WP 2
(Data reduction and screening)

PCL
(PC Layer)

Develop software for robust real-time frame rejection at PC layer

"Online"

Data cache
(Temporary storage)

Develop and implement software for data reduction and event filtering once data is saved to disk cache

WP 3
(Data analysis software)

WP 4
(Hardware)

"Offline"

Analysis
(Permanent storage)

Develop and refine software for the analysis of SPB data
Target single particles, nanocrystals and other typical samples.

Science output
(Users)

Implement and deploy software within the XFEL data analysis framework

The LCLS data retention policy retains all data for 6 months

Space	Size	Backup	Lifetime	Storage class	Comment
xtc	Unlimited	Tape archive	6 months	Short-term	Raw data
hdf5	Unlimited	Tape archive	6 months	Short-term	Data translated to HDF5
scratch	Unlimited	None	6 months	Short-term	Temporary data
xtc/hdf5	10TB	n/a	2 years	Medium-term	Selected XTC and HDF5 runs
ftc	10TB	None	2 years	Medium-term	Filtered, translated, compressed
res	1TB	Disk	2 years	Medium-term	Analysis results
User home	20GB	Disk + tape	Indefinite		User code
Tape archive	Unlimited	Two copies	10 years	Long-term	Raw data

Papers take ~2 years to publish:
6 months is very little time for deletion of raw data

Prediction: 10 PB user data storage will not be sufficient for XFEL

LCLS data stored on our CFEL server

LCLS 2009-2012
(3 years)

Data analysed:
1002 TB

Data taken home:
676 TB

Reduced data:
80 TB

XFEL = LCLS x10?
(120 Hz -> 1200 Hz)

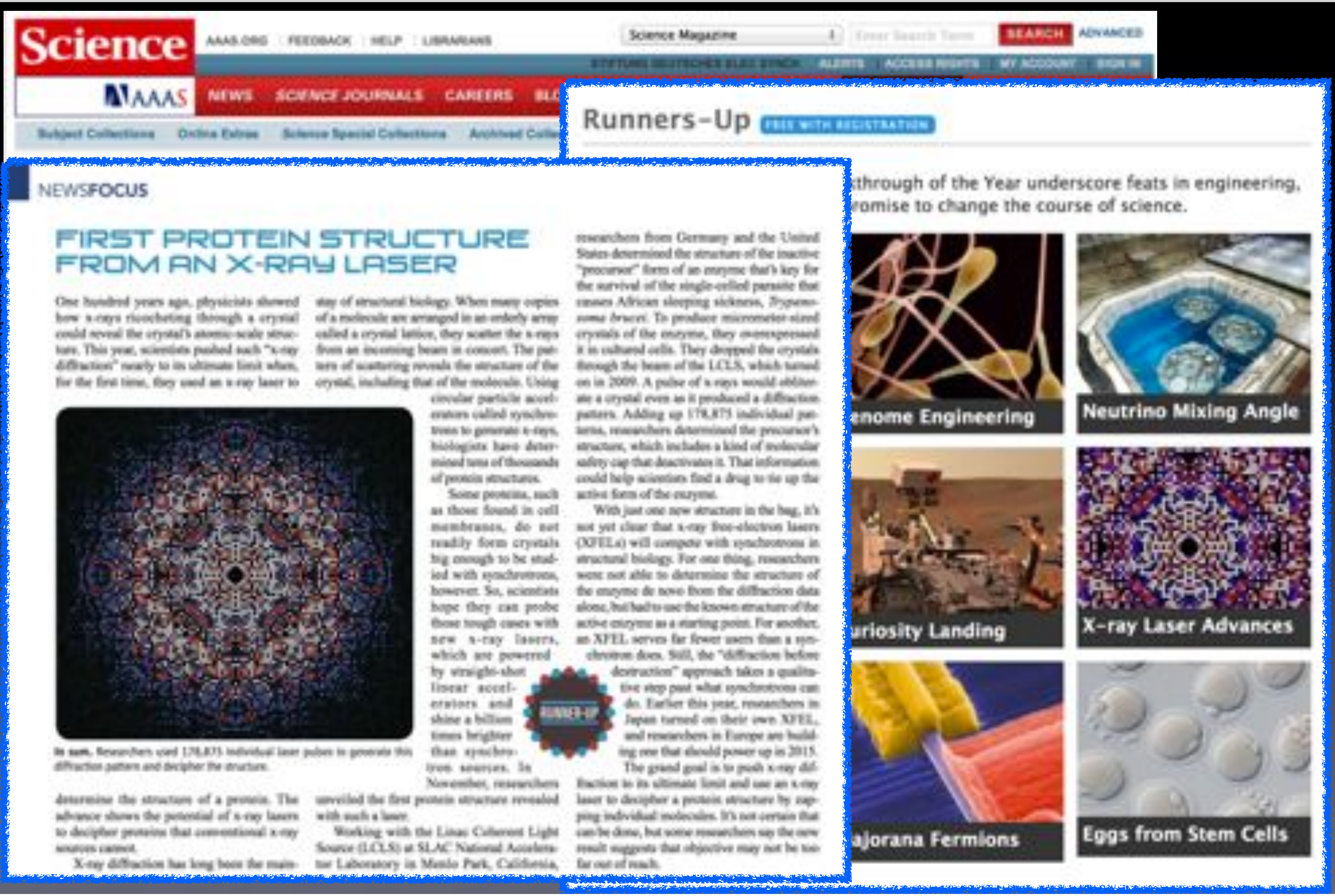
Data analysed:
10 PB

Data taken home:
6PB

Reduced data:
1 PB

* 120 Hz at LCLS becomes 27,000 Hz at XFEL
but AGIPD detector only handles ~2000 pulses/sec
10x is very rough, assuming shorter runs and that downtime wastes more pulses at XFEL than at LCLS

Science magazine nominated serial femtosecond crystallography as one of the top 10 technology breakthroughs of 2012



Runners-Up

through of the Year underscore feats in engineering,
romise to change the course of science.

NEWSFOCUS

FIRST PROTEIN STRUCTURE FROM AN X-RAY LASER

One hundred years ago, physicists showed how x-rays ricocheting through a crystal could reveal the crystal's atomic-scale structure. This year, scientists pushed such "x-ray diffraction" nearly to its ultimate limit when, for the first time, they used an x-ray laser to determine the structure of a protein. The advance shows the potential of x-ray lasers to decipher proteins that conventional x-ray sources cannot.

X-ray diffraction has long been the mainstay of structural biology. When many copies of a molecule are arranged in an orderly array called a crystal lattice, they scatter the x-rays from an incoming beam in concert. The pattern of scattering reveals the structure of the crystal, including that of the molecule. Using circular particle accelerators called synchrotrons to generate x-rays, biologists have determined tens of thousands of protein structures.

Some proteins, such as those found in cell membranes, do not readily form crystals big enough to be studied with synchrotrons, however. So, scientists hope they can probe those tough cases with new x-ray lasers, which are powered by straight-shot linear accelerators and shine a billion times brighter than synchrotron sources. In November, researchers unveiled the first protein structure revealed with such a laser.

Working with the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory in Menlo Park, California, researchers from Germany and the United States determined the structure of the inactive "precursor" form of an enzyme that's key for the survival of the single-celled parasite that causes African sleeping sickness, *Trypanosoma brucei*. To produce micrometer-sized crystals of the enzyme, they overexpressed it in cultured cells. They dropped the crystals through the beam of the LCLS, which turned on in 2009. A pulse of x-rays would obliterate a crystal even as it produced a diffraction pattern. Adding up 178,875 individual patterns, researchers determined the precursor's structure, which includes a kind of molecular safety cap that deactivates it. That information could help scientists find a drug to tie up the active form of the enzyme.

With just one new structure in the bag, it's not yet clear that x-ray free-electron lasers (XFELs) will compete with synchrotrons in structural biology. For one thing, researchers were not able to determine the structure of the enzyme de novo from the diffraction data alone, but had to use the known structure of the active enzyme as a starting point. For another, an XFEL serves far fewer users than a synchrotron does. Still, the "diffraction before destruction" approach takes a qualitative step past what synchrotrons can do. Earlier this year, researchers in Japan turned on their own XFEL, and researchers in Europe are building one that should power up in 2015.

The grand goal is to push x-ray diffraction to its ultimate limit and use an x-ray laser to decipher a protein structure by zapping individual molecules. It's not certain that can be done, but some researchers say the new result suggests that objective may not be too far out of reach.

In sum. Researchers used 178,875 individual laser pulses to generate this diffraction pattern and decipher the structure.

The days of photon scientists taking data home are numbered

At the European XFEL:

26,000 pulses/sec, ~4 MB/image = 104 GB/sec, 374 TB/hr

200 frames @ 10 Hz, ~4 MB/image = 8 GB/sec, 28 TB/hr

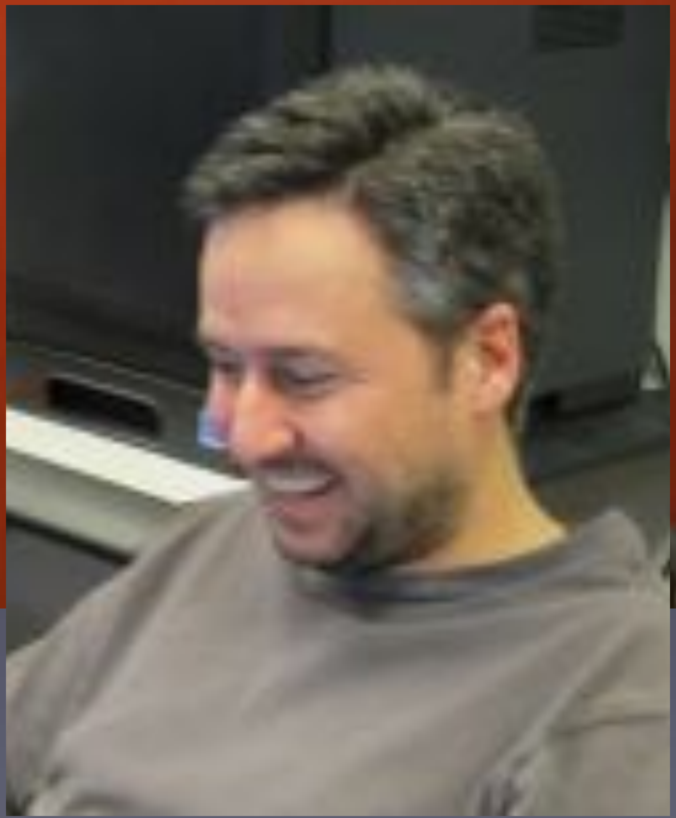
Experiments and analyses are carried out as a large collaboration

CFEL-DESY	H. Chapman, A. Barty, M. Liang, T. White, D. Deponte, S. Stern, A. Martin, C. Caleman, K. Beyerlein, R. Kirian, K. Nass, F. Stellato, F. Wang, H. Fleckenstein, L. Gumprecht, L. Galli, S. Bajt, M. Barthelmess, R. Bean, O. Yefamov
Arizona State Uni.	J. Spence, P. Fromme, U. Weierstall, B. Doak, N. Zatsepin, X. Wang, I. Grotjohann, R. Fromme
MPG CFEL ASG	I. Schlichting, R. Shoeman, L. Lomb, S. Kassemeyer, S. Bari, T. Barends, J. Steinbrener, D. Rolles, S. Epp, A. Rudenko, L. Strüder, R. Hartmann, L. Foucar, N. Kimmel, P. Holl, J. Ullrich
SLAC-LCLS	S. Boutet, G. Williams, M. Messerschmidt, M. Seibert, J. Kryzwinski, W. White, R. Coffee, C. Kenney, R. Herbst, J. Pines, P. Hart, J. Morse, P. Emma, J. Frisch, J. Galayda *and many others*
SLAC-PULSE	M. Bogan, D. Starodub, R. Sierra, C. Hampton, D. Loh
Uppsala University	J. Hajdu, Nic Timneanu, J. Andreasson, M. Seibert, F. Maia, M. Svenda, T. Ekeberg, J. Andreasson, A. Rocker, O. Jonsson, D. Westphal
European XFEL	A. Mancuso, A. Aquila, J. Schulz
LLNL	M. Frank, M. Hunter, S. Hau-Riege
LBNL	J. Holton
Gotheburg	R. Neutze, L. Johansson, D. Arnlund
U. Hamburg	L. Redecke, C. Betzel
U. Tübingen	M. Duszenko, R.Koopman, K. Cupelli

The hard X-ray coherent imaging instrument at LCLS became available in 2011

Marvin Seibert

Garth Williams



Sébastien Boutet

Marc Messerschmidt