The Turn on of LCLS: The X-Ray Free Electron Laser at SLAC

Persis S. Drell
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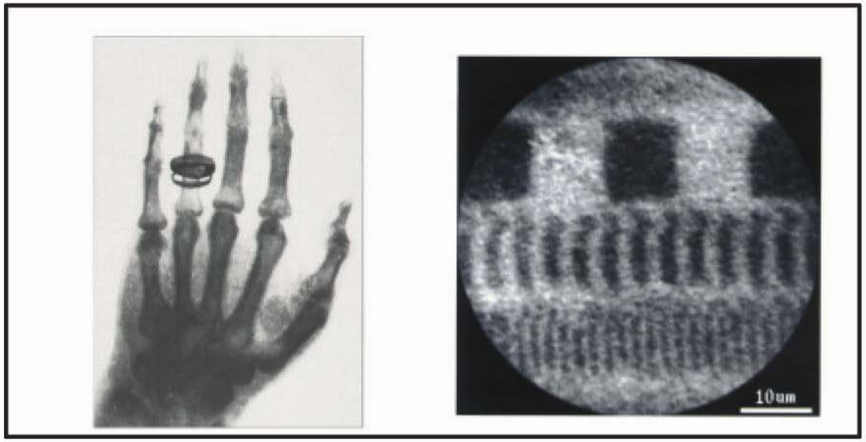
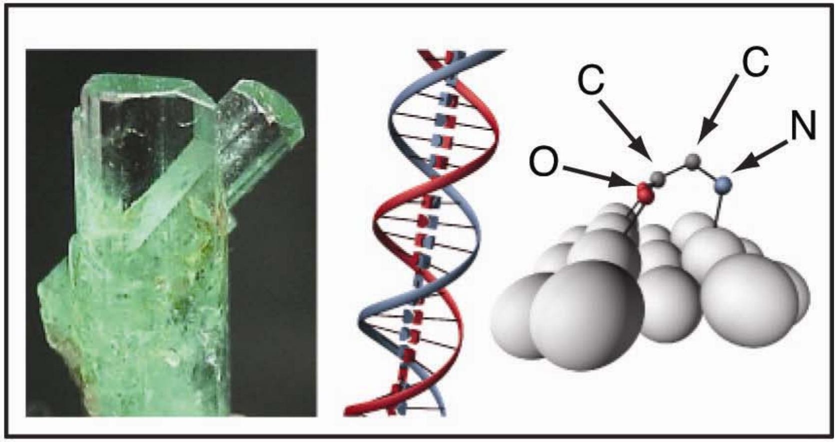
What are X-rays Good For ?

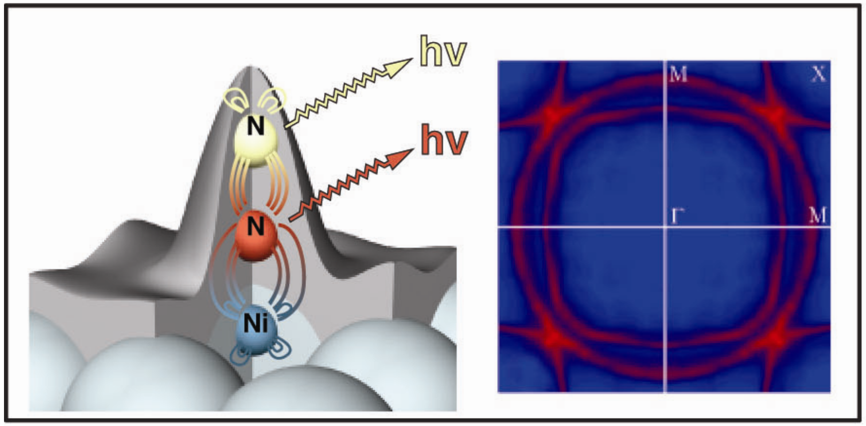
Seeing the invisible



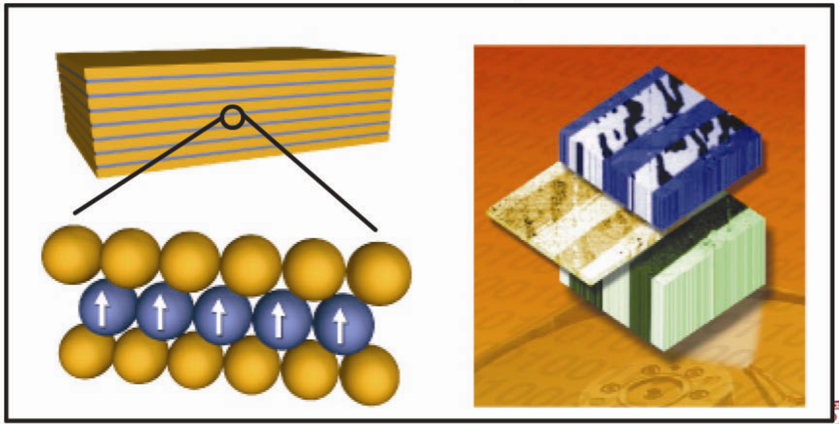
Where are the atoms?



Where are the electrons?



Where are the spins?



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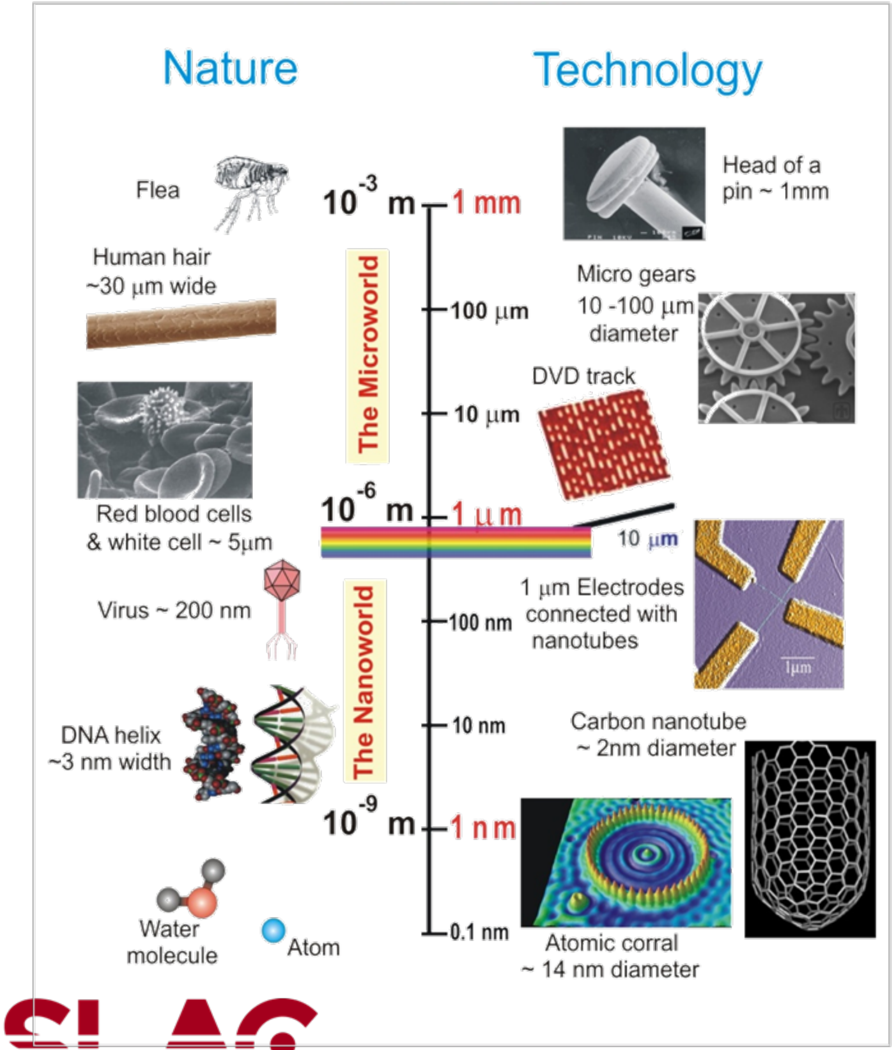
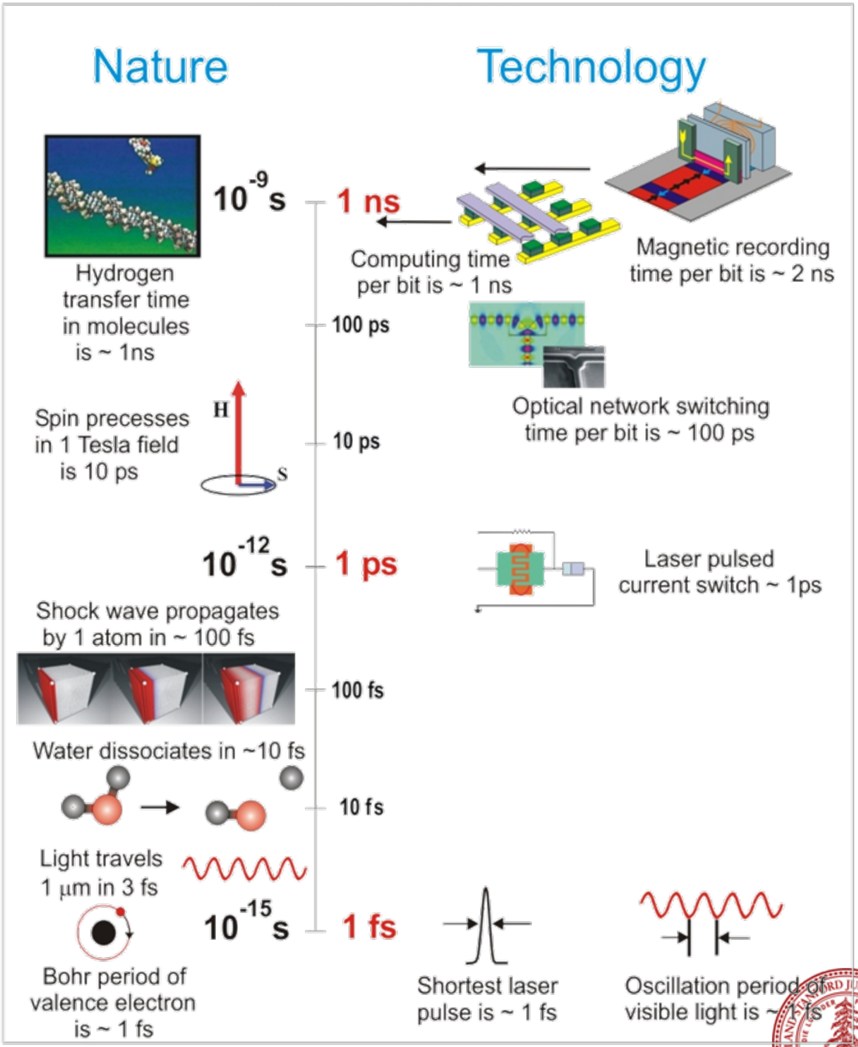
Static “Structure” Combined with Dynamic “Function”

Ultra-Small

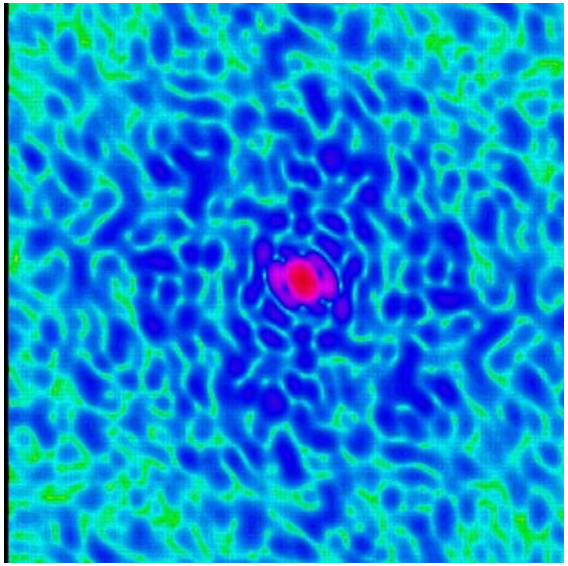


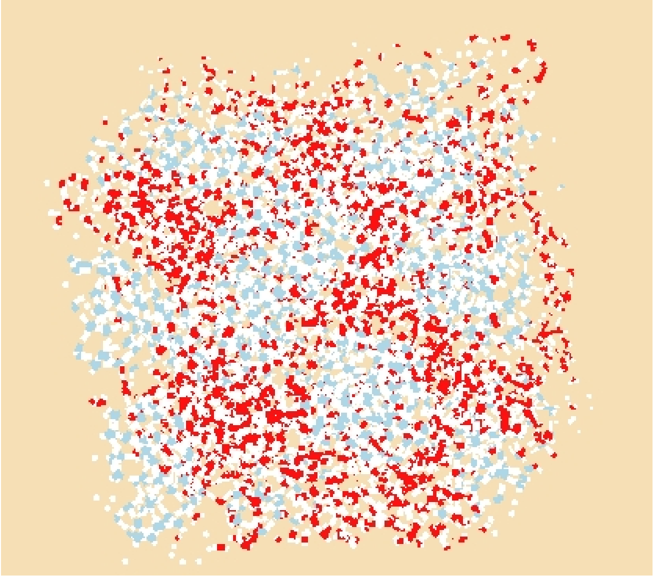
Ultra-Fast



What We Can Do With An ‘Ultra-Fast, Ultra-Bright’ X-ray Source

- Make movies of the chemistry in action
- Study the structure and time-resolved function of single molecules e.g. proteins
- Do 3D imaging and dynamical studies of the bio-world
- Solve the (transient) structure of water and other liquids
- Characterize the transient states of matter created by radiation, pressure, fields, etc.





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A New Generation of X-ray Sources

- Goal is atomic resolution in energy, space and time
- Current focus is on dynamics
  - Goal is femtosecond or better resolution
- Technical Options
  - Energy Recovery Linacs (ERLs)
    - In R&D at Cornell and other places
  - Free Electron Lasers (FELs)
    - First X-ray FEL has just come into operation

Talk Outline

- X-ray FEL basics
  - How does a SASE FEL work?
  - Parameters of the SLAC LCLS
- LCLS Construction and Early Performance
- Early Experiments at LCLS
- Looking Forward

FEL Basics

An FEL is Not Your Ordinary LASER

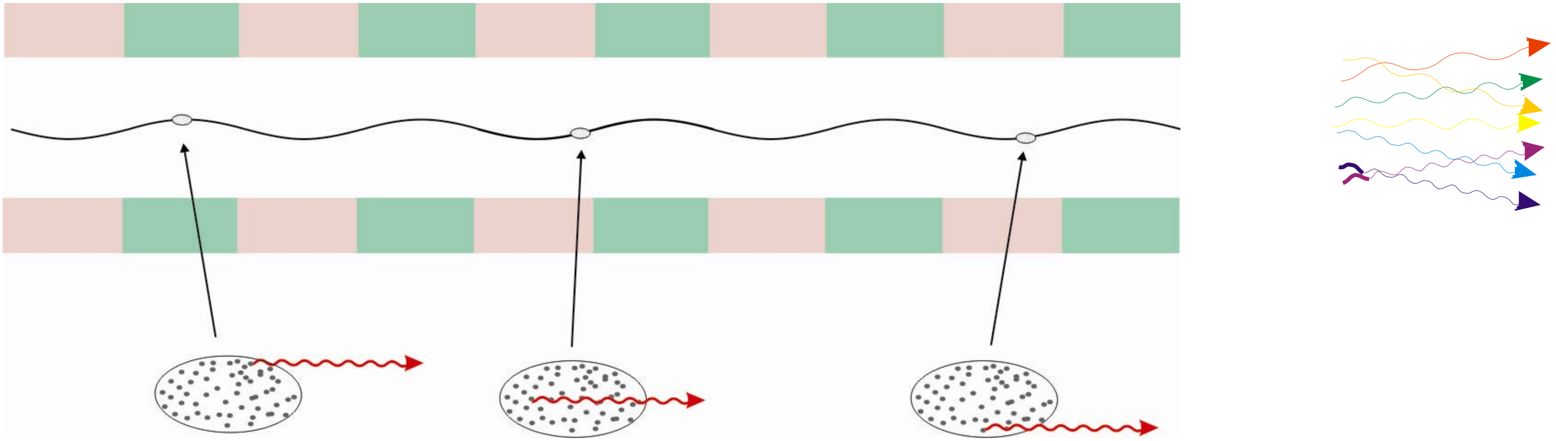
- Process of generation of radiation is different that conventional laser*

- Radiation product: Intense, coherent radiation output definitely LASER like
  - Complete tunability because electrons are free from atoms

***Light amplification by stimulated emission of radiation**

Synchrotron Radiation from Undulator in Storage Ring

- Electron bunch is “stored” in ring and used over and over

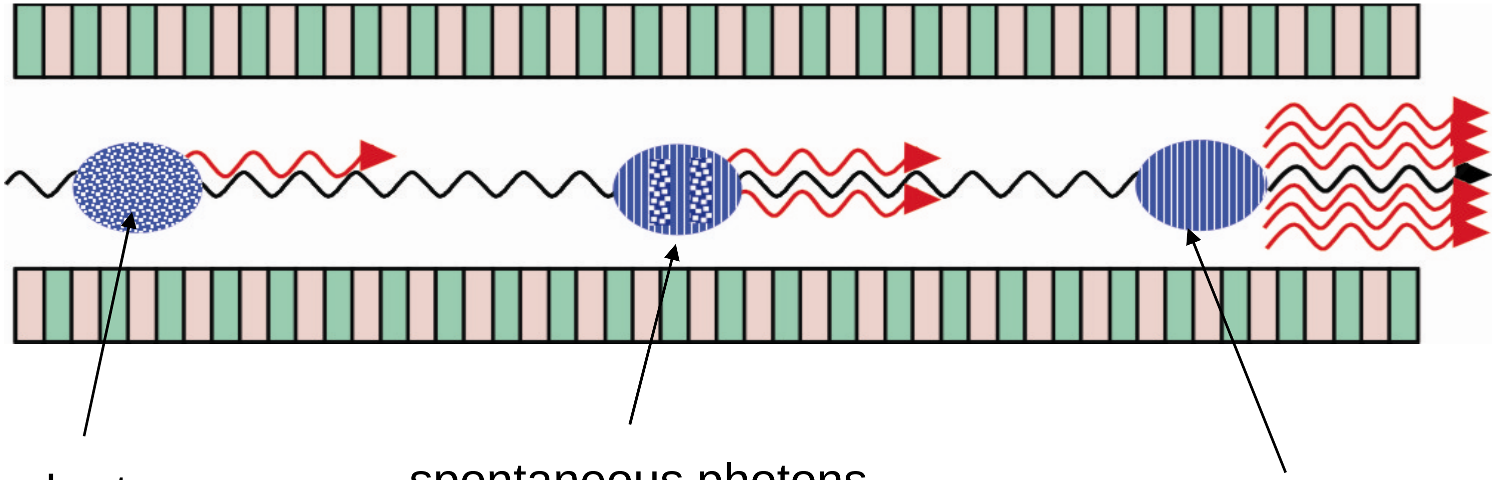


electron bunch
~ 1cm long

- Each bunch contains $N_e \sim 10^9$ electrons
  - electrons emit spontaneously and photons are not coherent

Concept of a Free Electron X-ray Laser

- Replace storage ring by a linear accelerator
  allows compression of electron bunch – use once, then throw away
- Send electron bunch through a very long undulator



very short
bunch length
(μm)

spontaneous photons
from back of bunch
create order

ordered electrons
radiate coherently

Electron Beam is Key to FEL Success

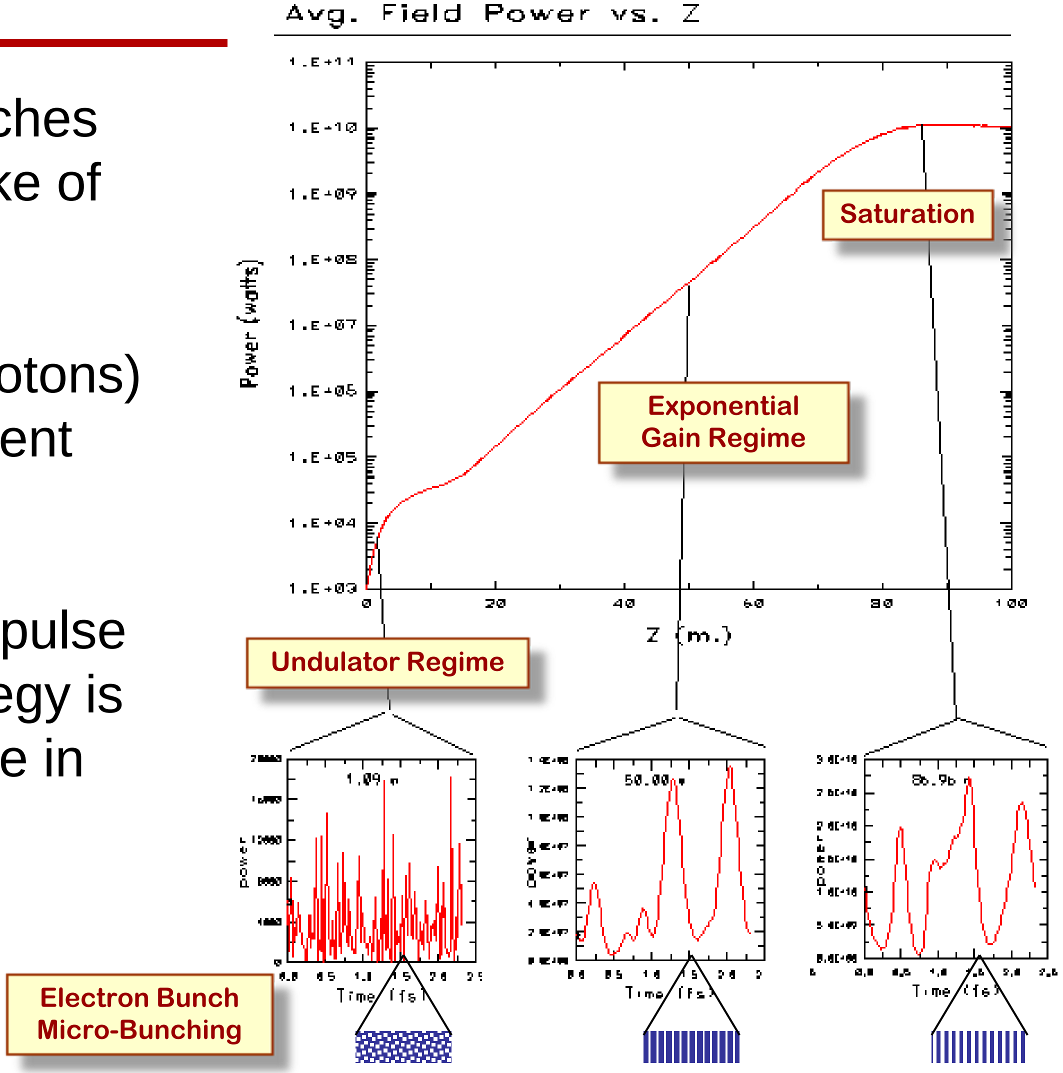
- FEL requires extremely bright e- beam
  - – High Peak Current
  - – Low emittance (6-D phase space volume)
  - – Performance depends exponentially on e- beam quality
- For LCLS
  - – 3kA e^- beam
    - 6×10^9 e^- in ~30μm sphere

Linac Coherent Light Source (LCLS)

- Output of ~1000 microbunches results in ~1fs coherent spike of radiation

- Typical FEL pulse (10^{12} photons) made of few hundred coherent spikes

- Where coherence or short pulse length is critical, initial strategy is to isolate one coherent spike in the FEL pulse
    - Ultimately → seeding



Free-Electron Lasers

- 1977- First operation of a free-electron laser at Stanford University
  - – Deacon, et al. PRL v. 38, no.16, pp. 892-894
- Today
  - – 22 free-electron lasers operating worldwide
  - – 19 FELs proposed or in construction
- Before LCLS turn on, shortest wavelength FEL was FLASH @ DESY
  - – 6.5 nm -- 50 nm
- Compare
  - – 0.15nm – 1.5 nm design goal for LCLS

Design Parameters for LCLS

FEL Fundamental	**1.5**	**15**	**A**
Electron Beam Energy	14.3	14.5	GeV
Normalized RMS Slice Emittance	1.2	1.2	µm
Peak Current	3.4	3.4	kA
Bunch/Pulse Length	<230	<230	fs
Saturation Length	87	25	m
FEL Fundamental Saturation Power @ exit	8	17	GW
FEL Photons per Pulse	1	29	10^{12}
Peak Brightness @ Undulator Exit	0,8	0.06	10^{33}*
Transverse Coherence	Full	Full	
RMS Projected x-ray bandwidth	0.13	0.47	%

* photons/sec/mm^2/mrad^2/0.1%-BW

LCLS Construction and Early Performance

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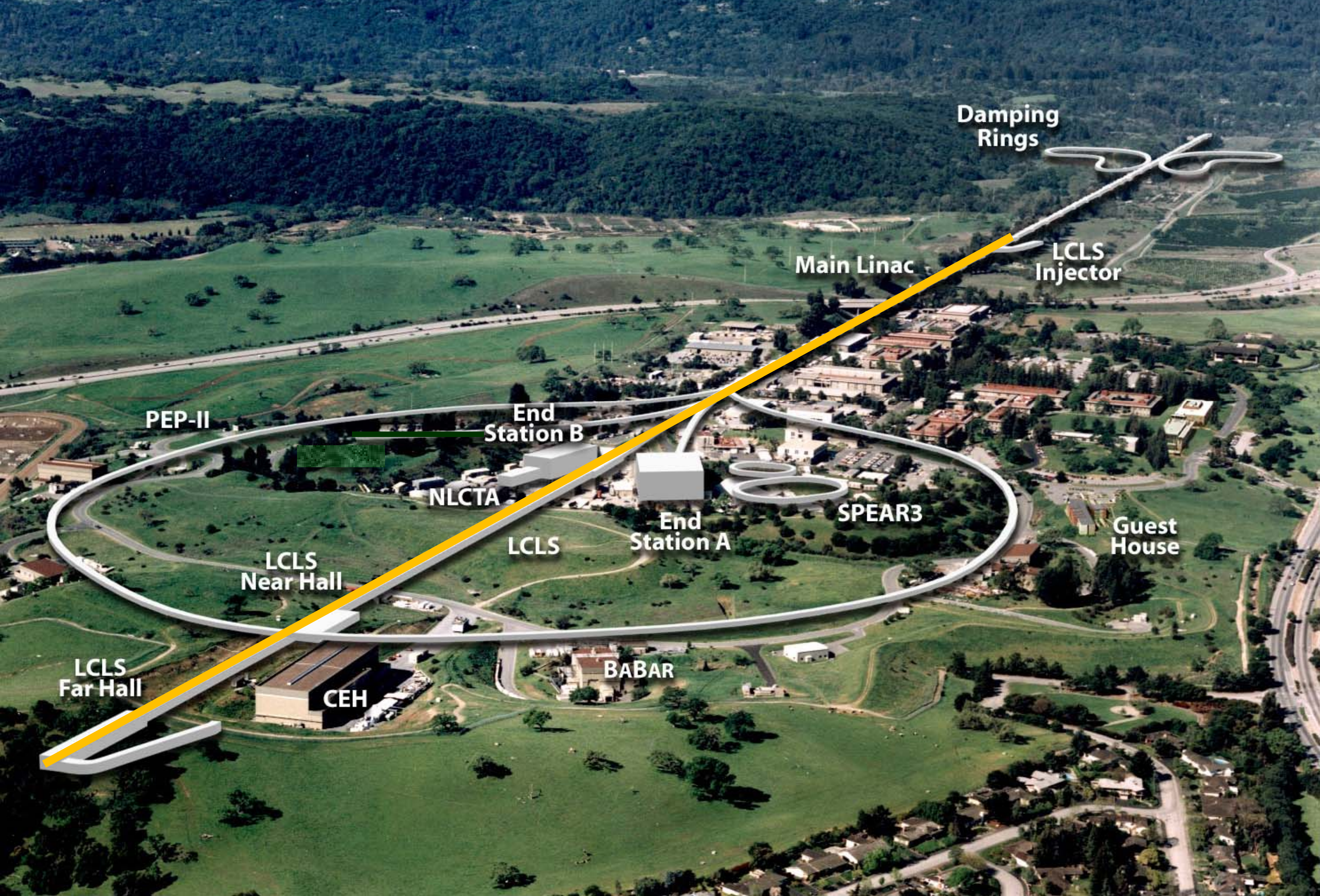

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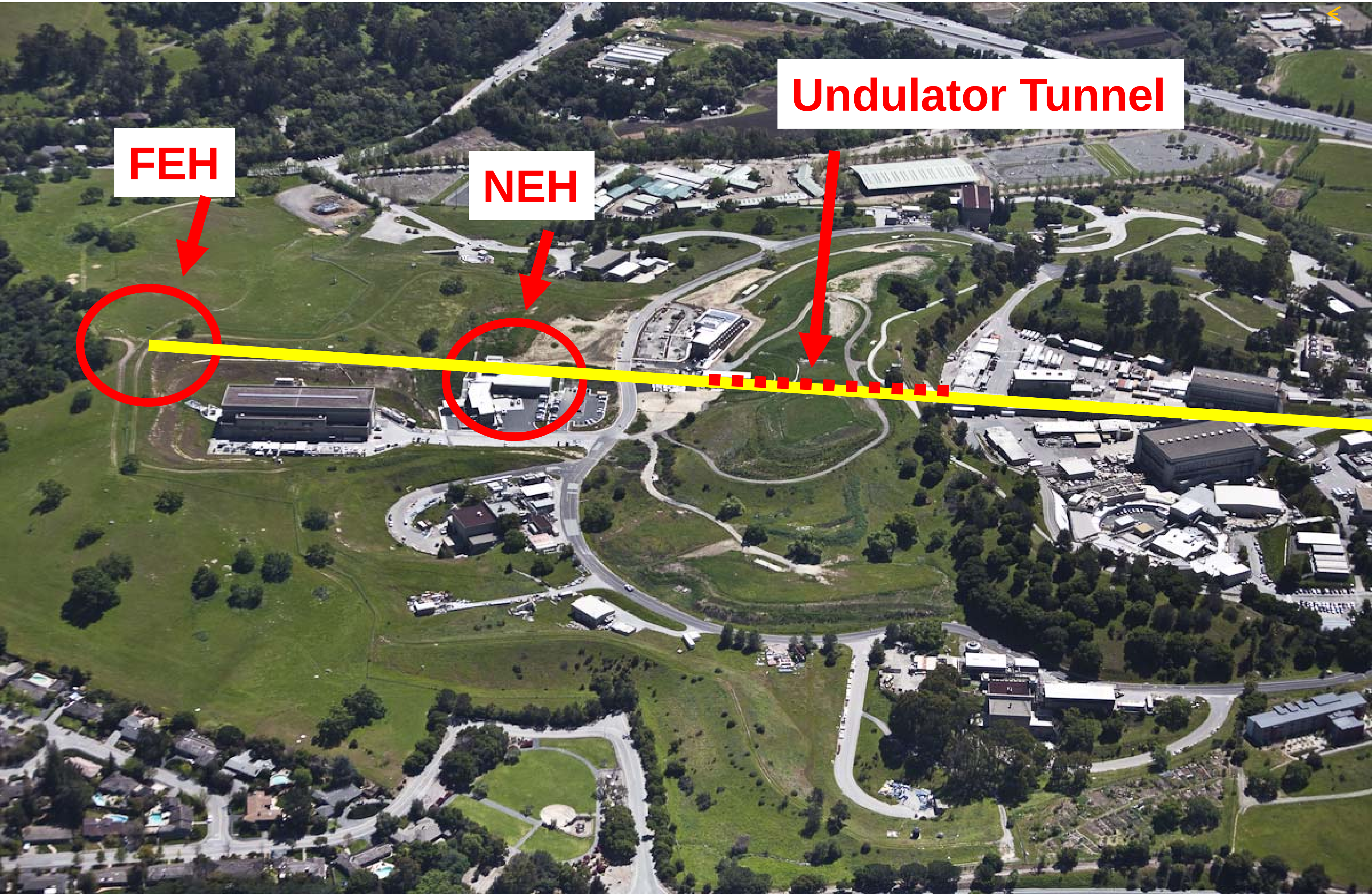
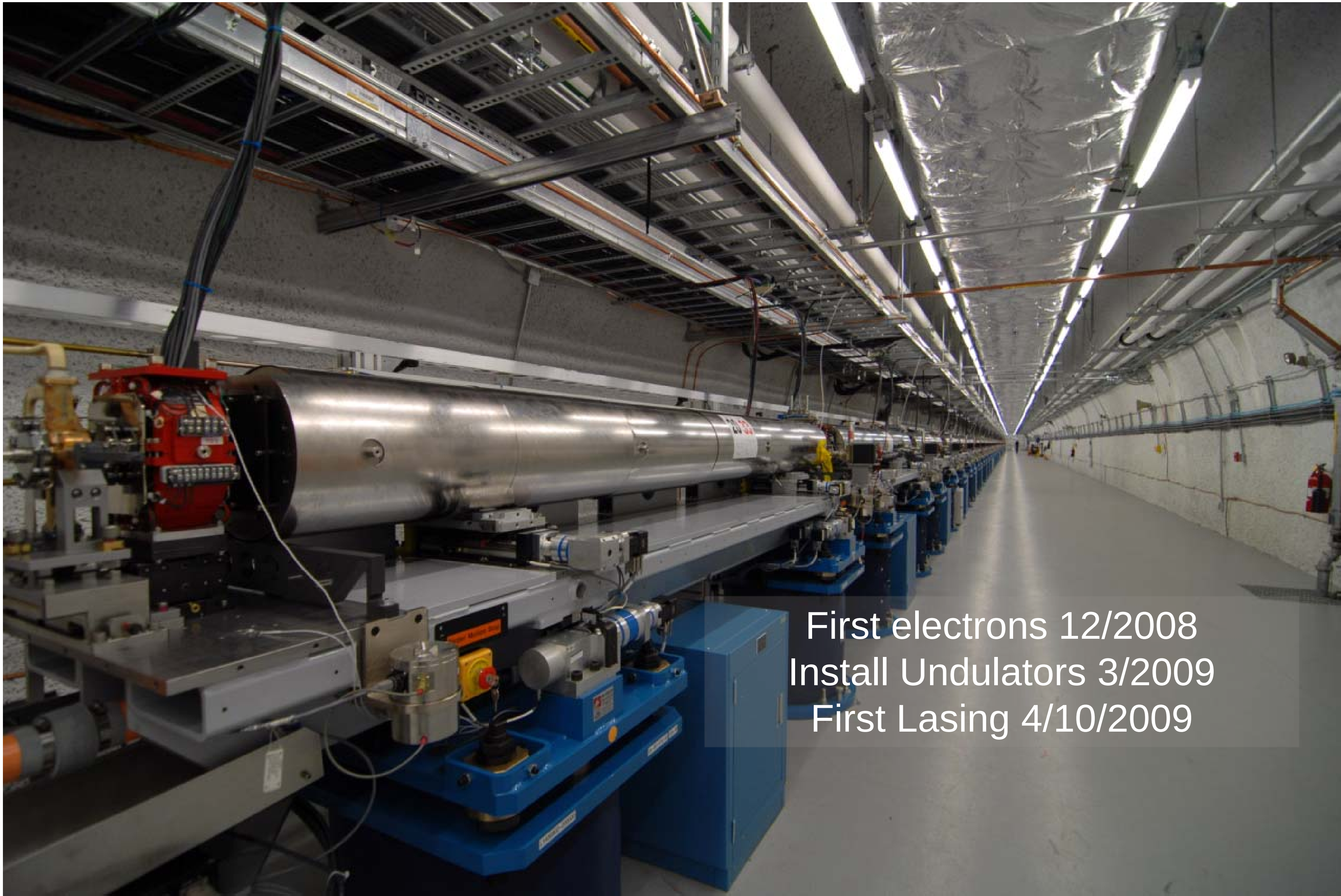
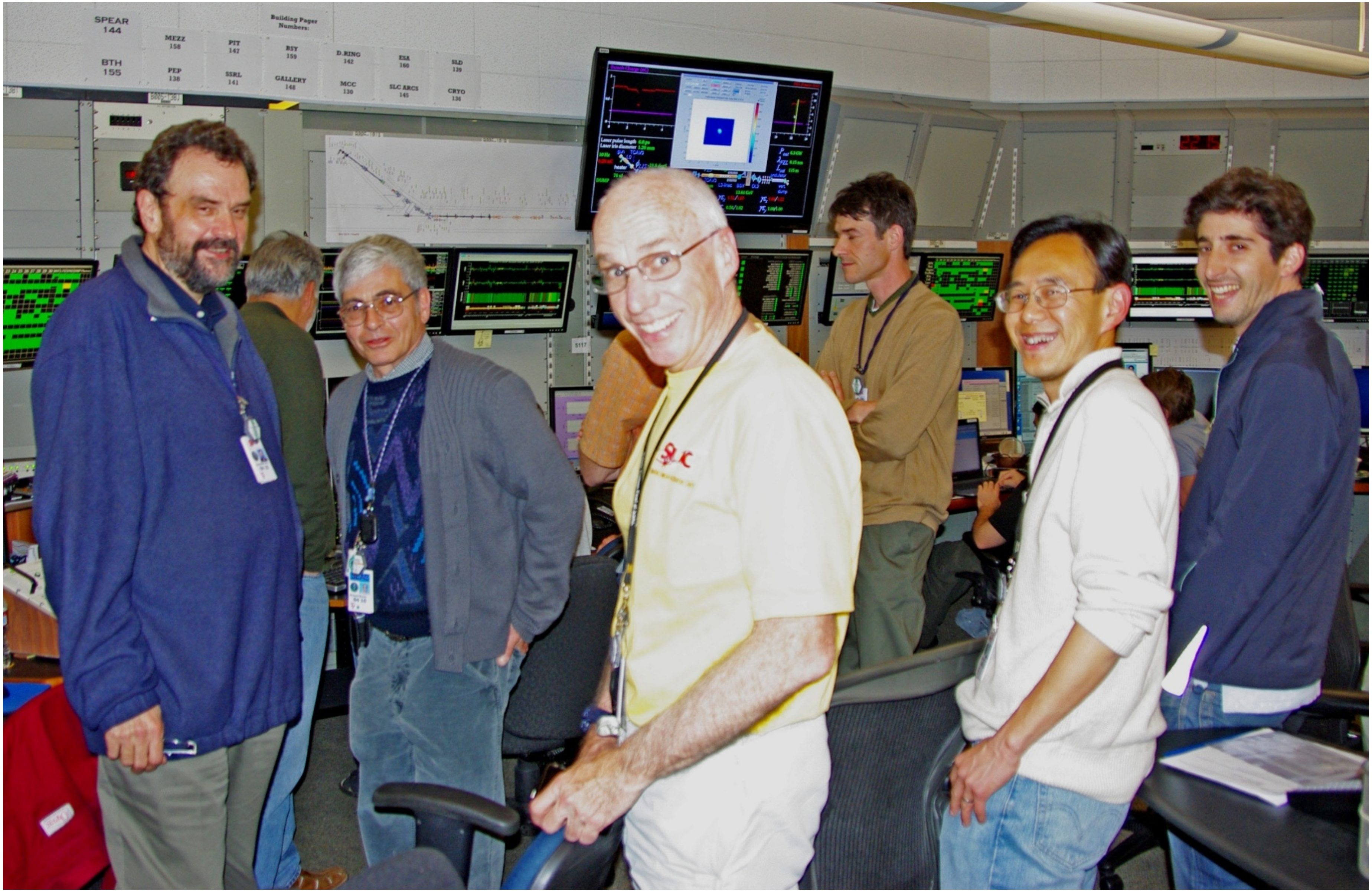


LCLS Undulator Hall: 132 meters

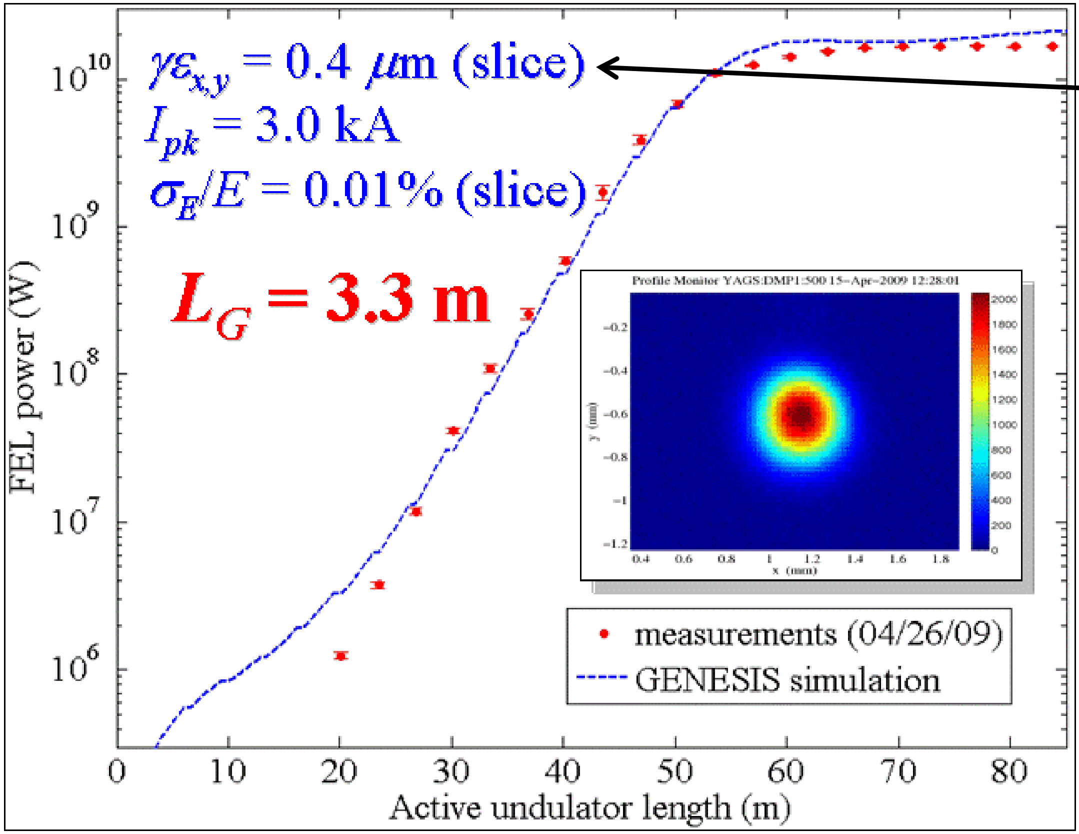


First electrons 12/2008
Install Undulators 3/2009
First Lasing 4/10/2009

April 10, 2009– The Lasing Campaign



First Performance Exceeds Expectation



Design: 1.2μm

- Typical x-ray beam energy **> 1 mJ** or **> 10^{12}** photons per pulse
- Typical x-ray pulse duration at 300pC charge **~ 100 fs** (FWHM).
- X-ray pulse duration at 20 pC charge < **10 fs**
- Saturation at 65 m (anticipated 87 m)

LCLS Performance

	Baseline performance	**Current performance**
Photon energy range	830 to 8300 eV	**480 to 10,000 eV**
FEL pulse length	230 fs	**5 - 500 fs**
FEL pulse energy	up to 2 mJ	**up to 4 mJ**

- 120 fs pump probe synchronization has been achieved
- Further improvements are underway

Early Experiments with LCLS: Early results and future dreams

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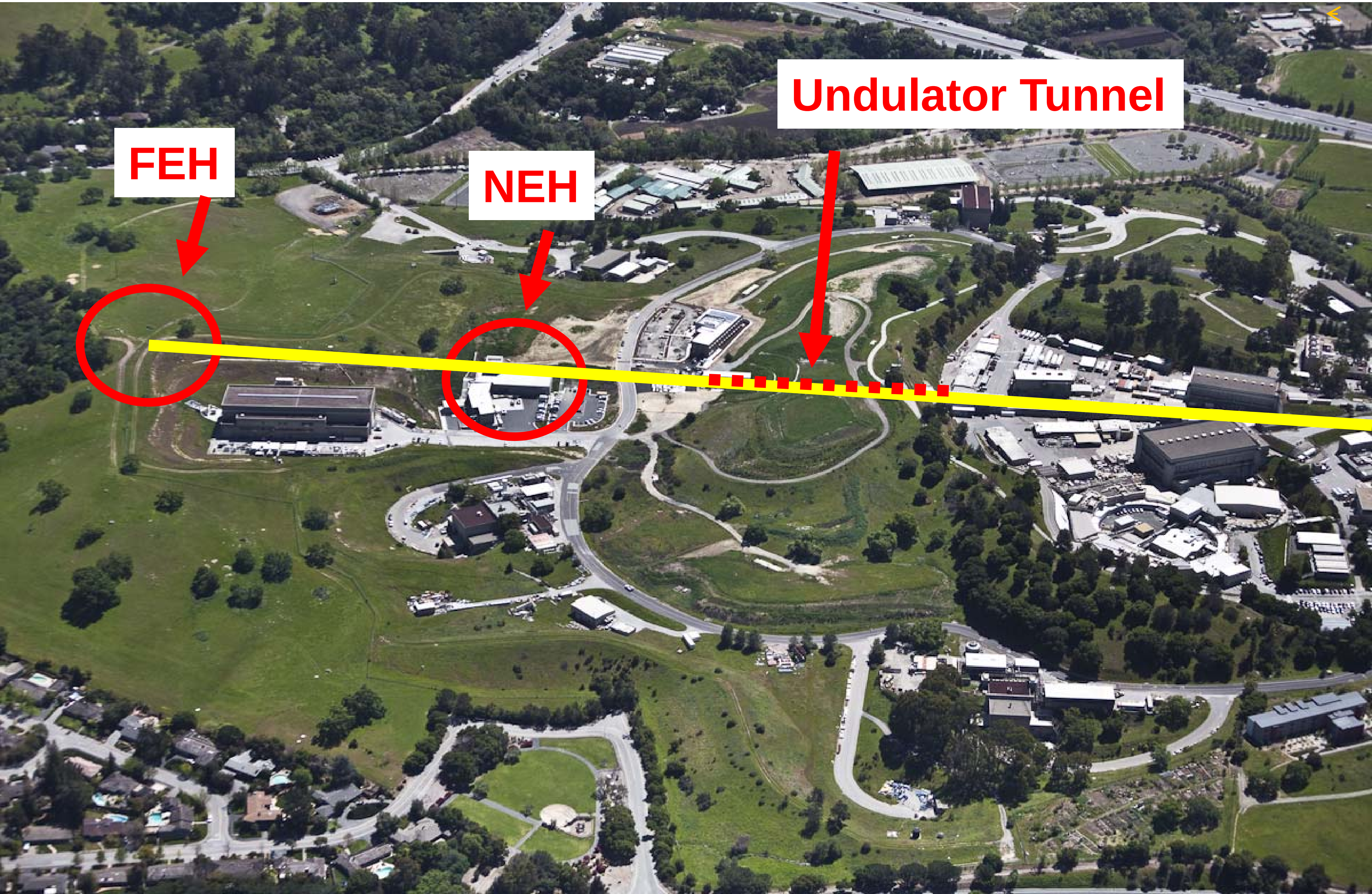
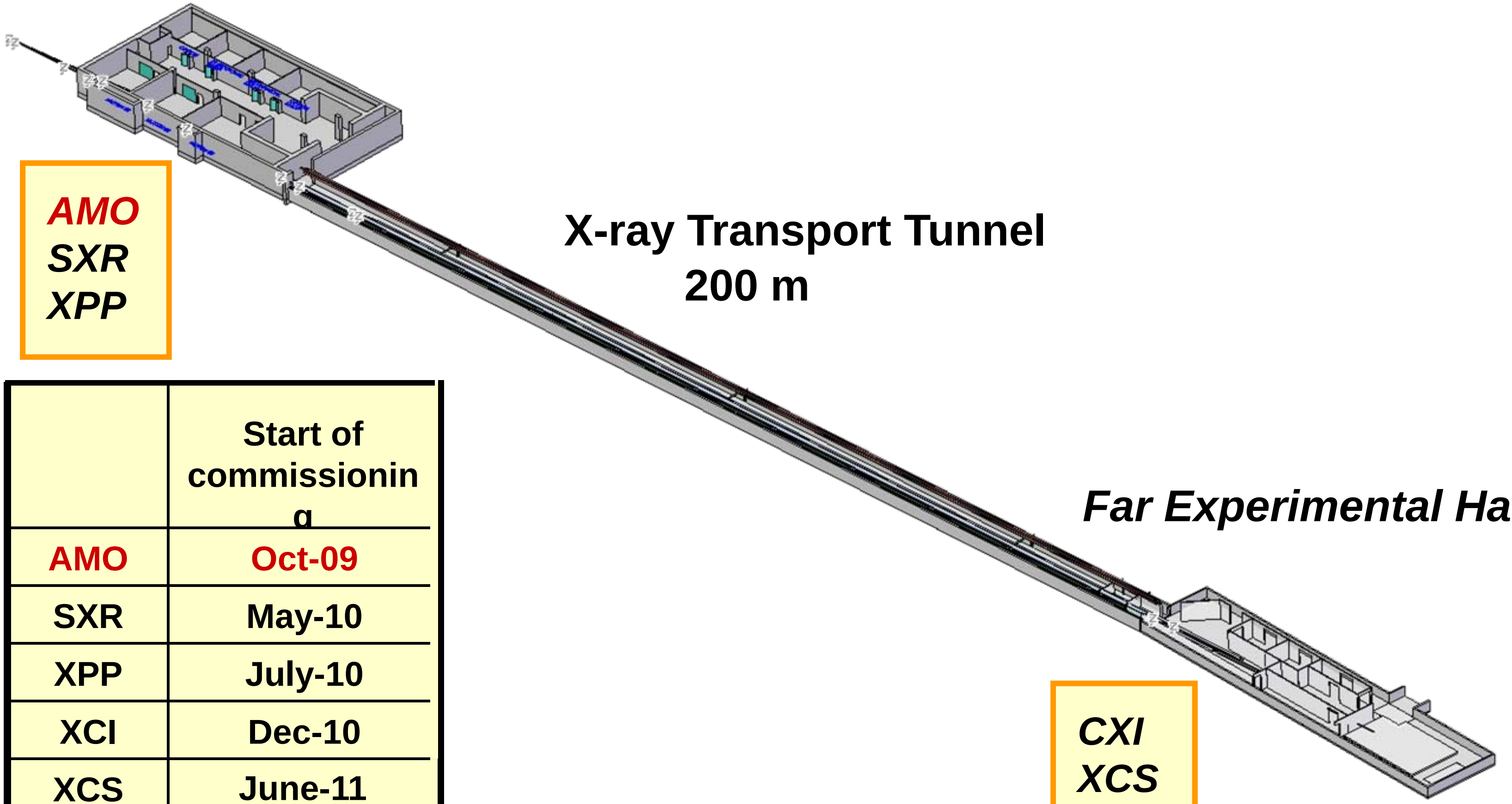


LCLS Experimental Halls

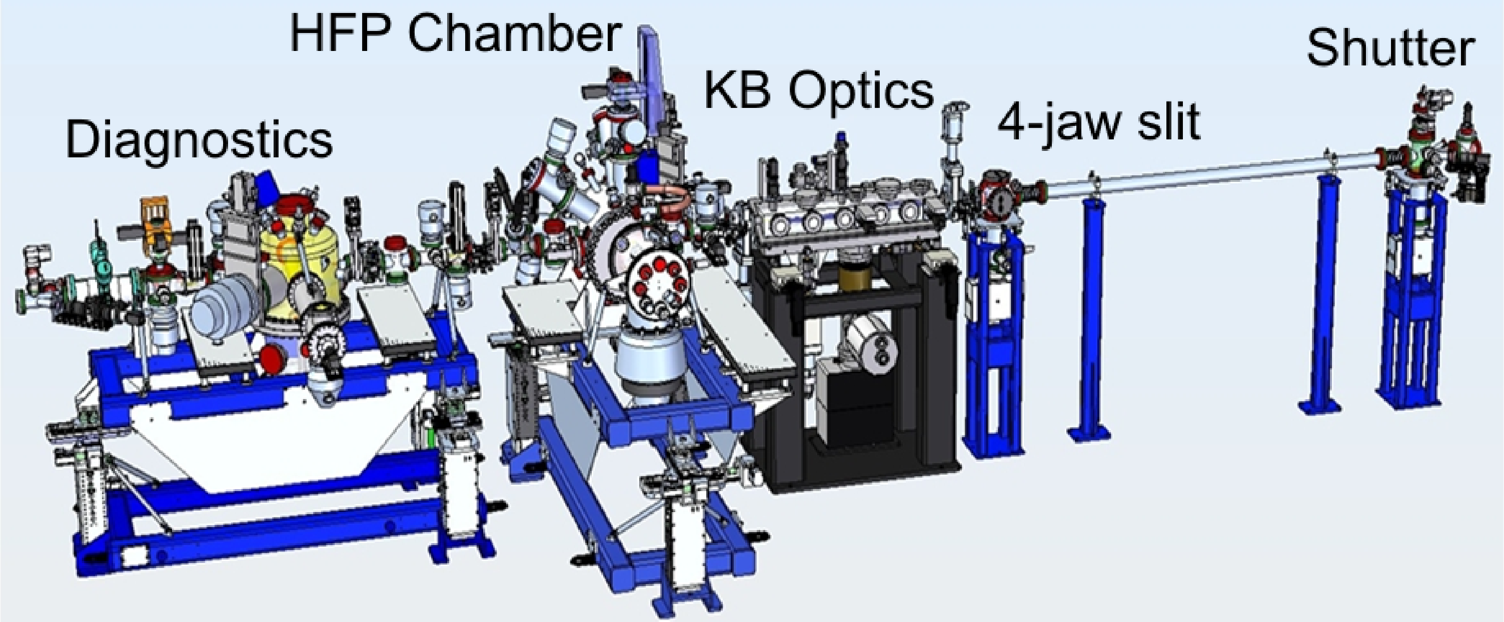
only first of six stations used so far

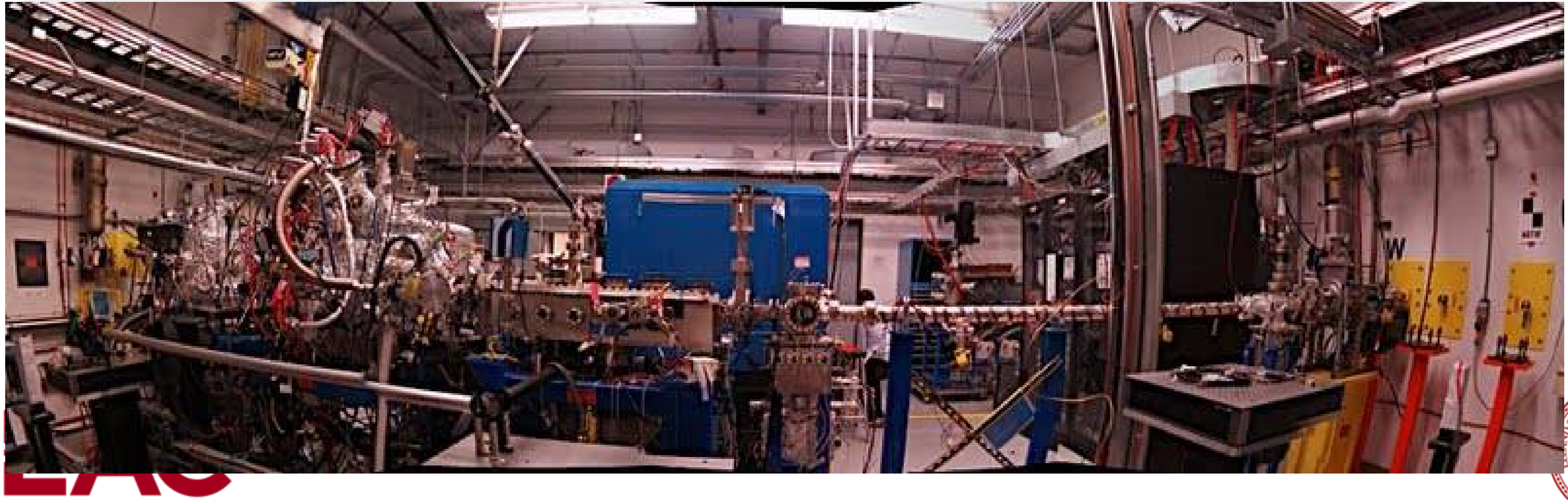


	Start of commissioning
AMO	Oct-09
SXR	May-10
XPP	July-10
XCI	Dec-10
XCS	June-11
MEC	2012

Tentative instrument operation scheme

Atomic Molecular Optical (AMO) Instrument





AMO Control Room

LCLS 2-Year Science Strategy

- First round of experiments are largely proof of principle
- Currently beam time is awarded to maximize number of user groups and diversity of experiments (no program proposals)
- Plan is to follow this scheme for another year until all stations are operating and new fields are tested
- In 2012 start to identify and invest in science areas where LCLS will have critical impact
- Start to schedule more strategically, identify program proposals

What have we learned so far?

- Multi-Photon processes within atoms and molecules have been observed → Provides new spectroscopic signatures

- Concept of `probe-before-destroy′ works → Opens the door for imaging of nanocrystals and nanostructures

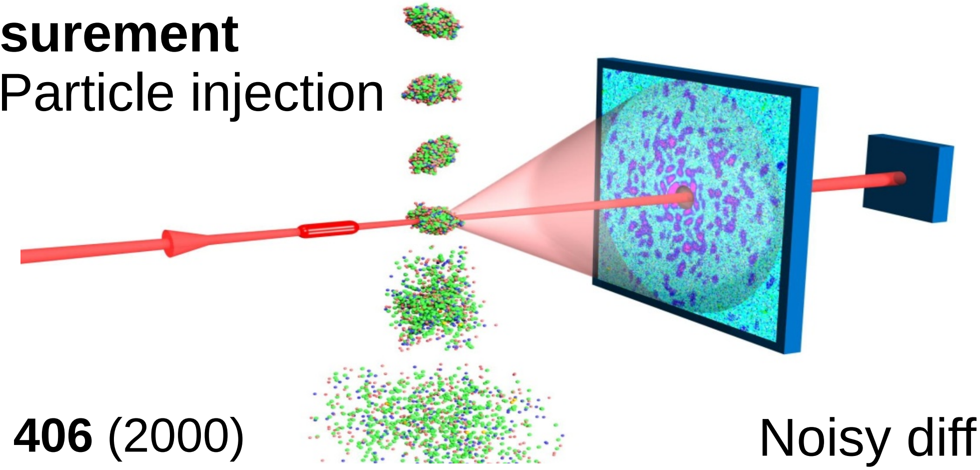
- Concept of single shot imaging of individual viruses & cells works but major improvements are needed to have an impact → 3D imaging of the bio-world

- Soft x-ray single shot spectroscopy and imaging of solids & surfaces is possible. Despite large cross sections, ultra-short pulses can beat electronic “damage” (i.e. changes in valence configurations, densities)

- **The fact that LCLS has performed much better than the baseline parameters (pulse length, energy range) already proves to be critical for many experiments!**

X-ray Free-Electron Lasers May Enable Atomic-Resolution Imaging of Biological Macromolecules

One pulse, one measurement



Particle injection

XFEL pulse

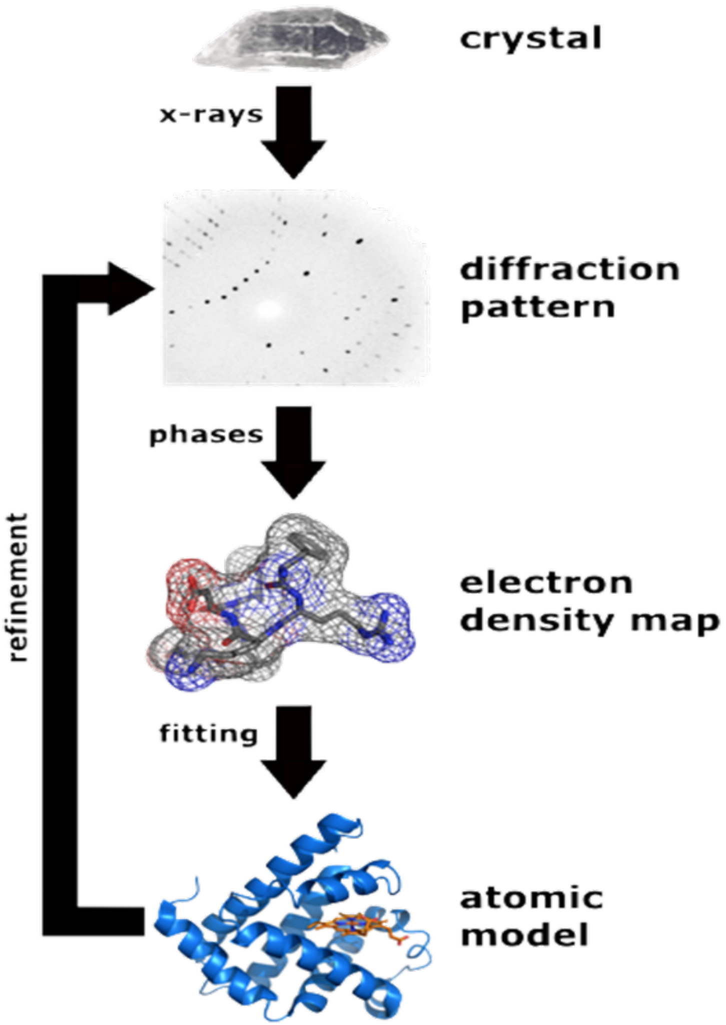
R. Neutze et al, Nature **406** (2000)

Noisy diffraction pattern

- What happens to molecules or particles irradiated by intense FEL pulses?
- Can we hope to obtain the atomic positions?
- How does achievable resolution depend on
    - pulse fluence?
    - molecule or particle size?
- Can we measure ultrafast dynamics in time and space domains, and observe reactions, reaction intermediates, and products?

Probe Before Destroy:
Femtosecond Nanocrystalography

Crystallography Achieves Atomic Resolution But Requires Crystals



- Radiation damage is spread out over 10^{10} identical unit cells
- Diffraction from unit cells adds up coherently to form strong Bragg peaks
- > 60,000 structures solved (in protein data bank), but ~15,000 distinct structures
- The bottleneck is in growing crystals of large enough size to diffract well for a tolerable X-ray dose (<50 MGy)
- The larger the unit cell volume, the greater the required dose

Femtosecond X-ray protein nanocrystallography   Nature 09750

Henry N. Chapman[1,2], Petra Fromme[3], Anton Barty[1], Thomas A. White[1], Richard A. Kirian[4], Andrew Aquila[1], Mark S. Hunter[3], Joachim Schulz[1], Daniel P. DePonte[1], Uwe Weierstall[4], R. Bruce Doak[4], Filipe R. N. C. Maia[5], Andrew V. Martin[1], Ilme Schlichting[6,7], Lukas Lomb[7], Nicola Coppola[1], Robert L. Shoeman[7], Sascha W. Epp[6,8], Robert Hartmann[9], Daniel Rolles[6,7], Artem Rudenko[6,8], Lutz Foucar[6,7], Nils Kimmel[10], Georg Weidenspointner[11,10], Peter Holl[9], Mengning Liang[1], Miriam Barthelmess[12], Carl Caleman[1], Sébastien Boutet[13], Michael J. Bogan[14], Jacek Krzywinski[13], Christoph Bostedt[13], Saša Bajt[12], Lars Gumprecht[1], Benedikt Rudek[6,8], Benjamin Erk[6,8], Carlo Schmidt[6,8], André Hömke[6,8], Christian Reich[9], Daniel Pietschner[10], Lothar Strüder[6,10], Günter Hauser[10], Hubert Gorke[15], Joachim Ullrich[6,8], Sven Herrmann[10], Gerhard Schaller[10], Florian Schopper[10], Heike Soltau[9], Kai-Uwe Kühnel[8], Marc Messerschmidt[13], John D. Bozek[13], Stefan P. Hau-Riege[16], Matthias Frank[16], Christina Y. Hampton[14], Raymond G. Sierra[14], Dmitri Starodub[14], Garth J. Williams[13], Janos Hajdu[5], Nicusor Timneanu[5], M. Marvin Seibert[5], Jakob Andreasson[5], Andrea Rocker[5], Olof Jönsson[5], Martin Svenda[5], Stephan Stern[1], Karol Nass[2], Robert Andritschke[10], Claus-Dieter Schröter[8], Faton Krasniqi[6,7], Mario Bott[7], Kevin E. Schmidt[4], Xiaoyu Wang[4], Ingo Grotjohann[3], James M. Holton[17], Thomas R. M. Barends[7], Richard Neutze[18], Stefano Marchesini[17], Raimund Fromme[3], Sebastian Schorb[19], Daniela Rupp[19], Marcus Adolph[19], Tais Gorkhover[19], Inger Andersson[20], Helmut Hirsemann[12], Guillaume Potdevin[12], Heinz Graafsma[12], Björn Nilsson[12] & John C. H. Spence[4]

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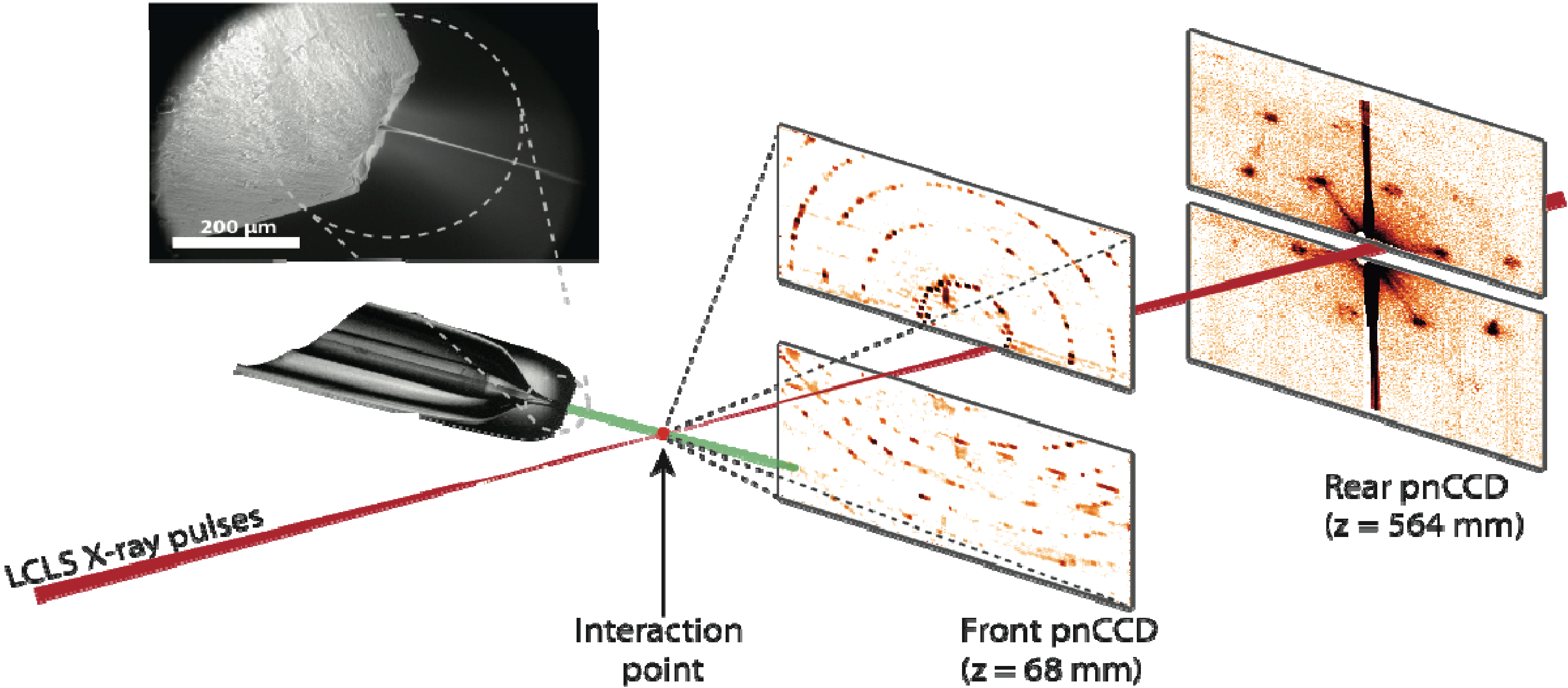
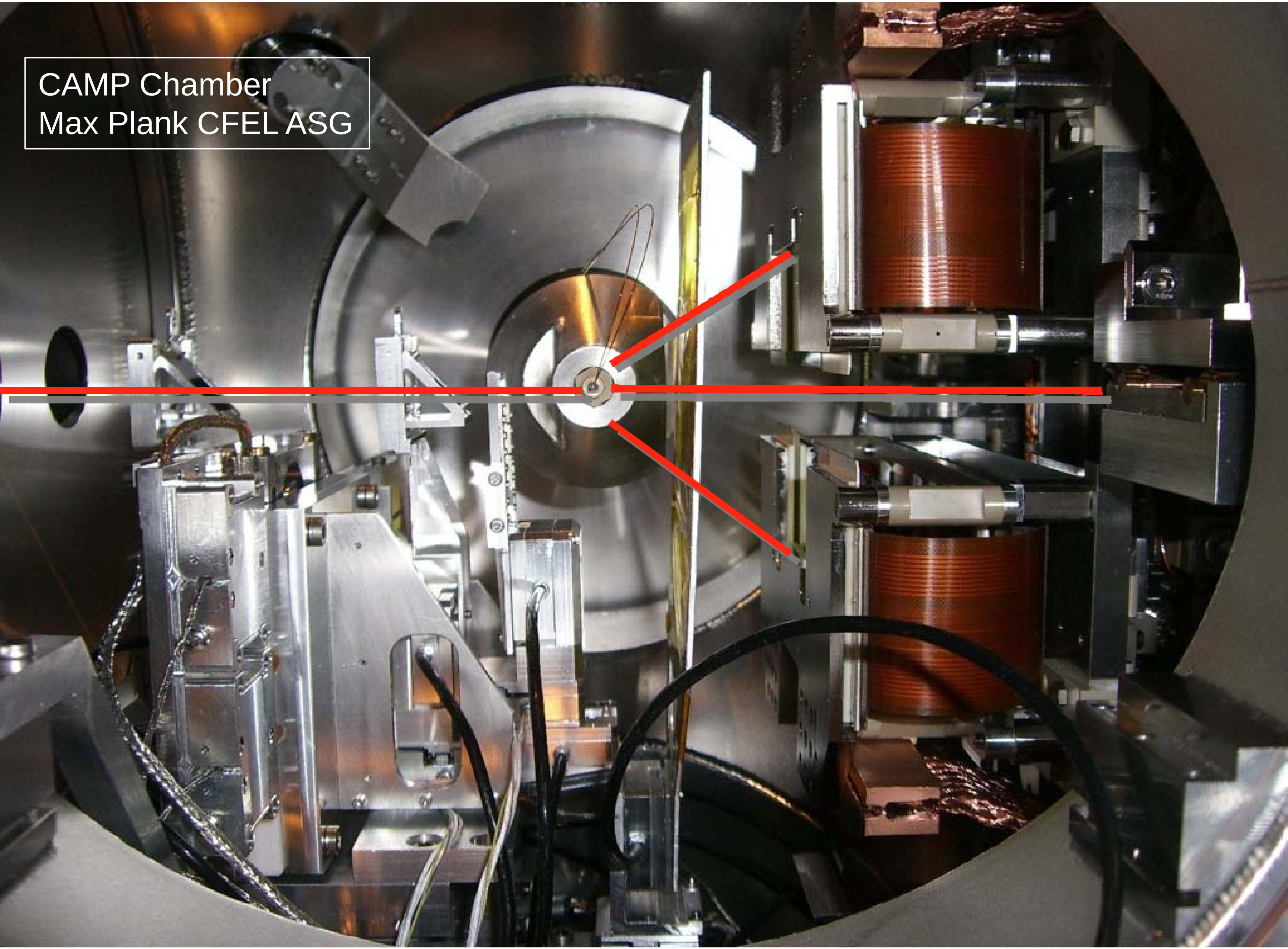
Nanocrystallography carried out in a flowing water microjet

- Single pulse diffraction from Photosystem 1 nanocrystals at LCLS
- *E* = 1.8 keV
- <10, 60, 200 fs pulse

- 2 mJ pulse energy
- patterns collected at 30 Hz
- hit rate >50%
- 5 Tb data in one night!

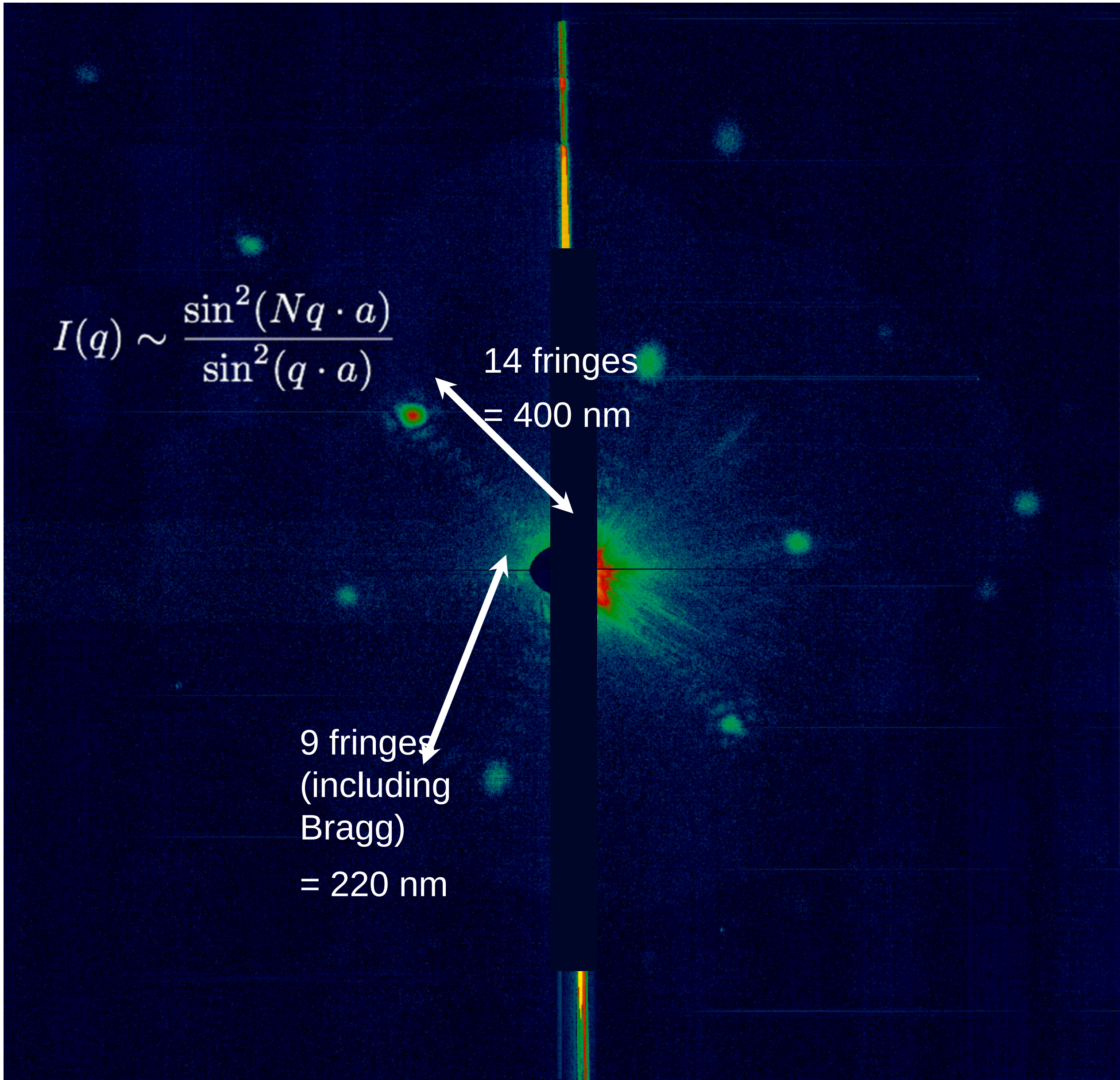




CAMP Chamber
Max Plank CFEL ASG

Small Angle Diffraction (Far Detector)

- Coherence of beam is evident
- Crystals are sub micron size



$$I(q) \sim \frac{\sin^2(Nq \cdot a)}{\sin^2(q \cdot a)}$$

14 fringes

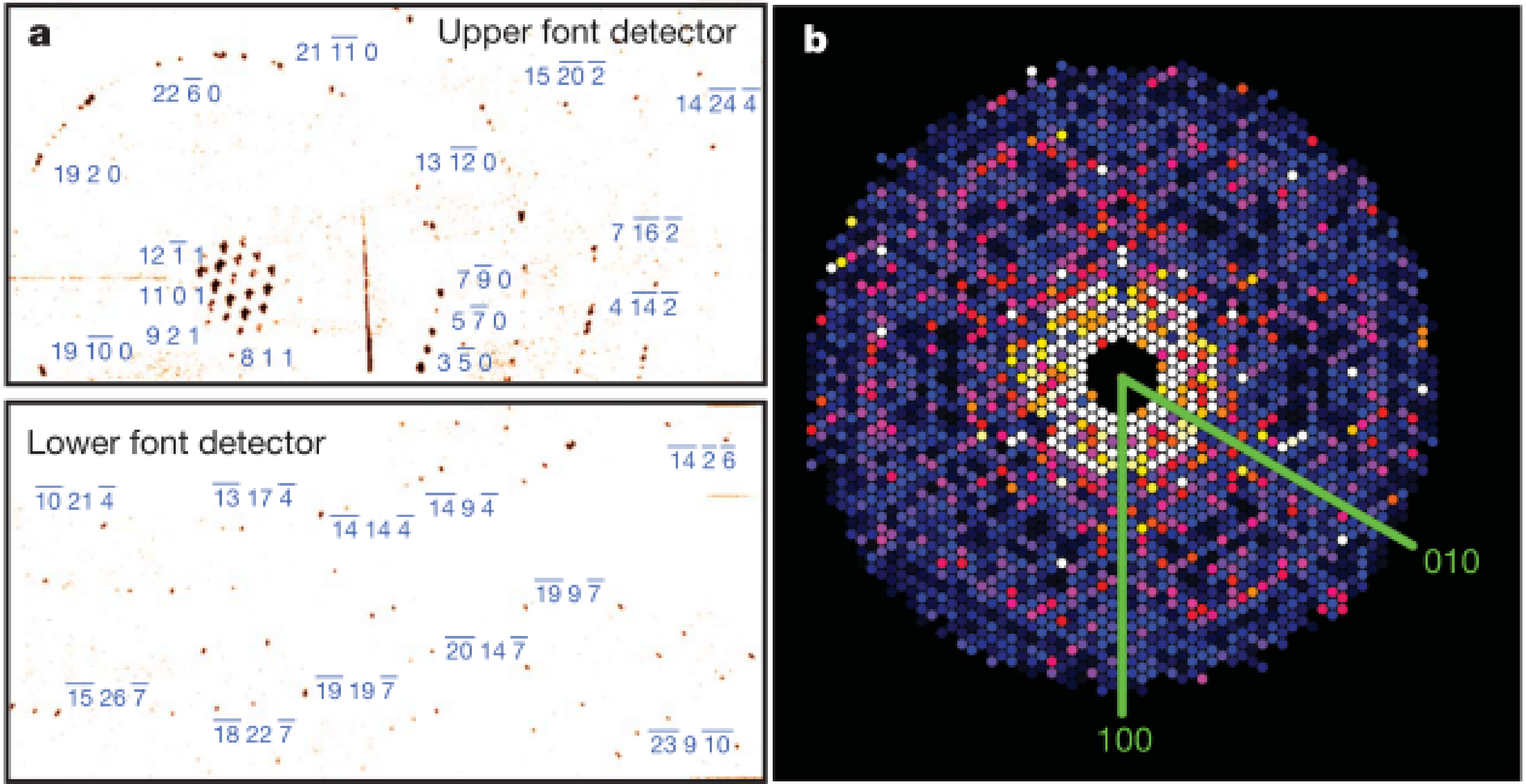
= 400 nm

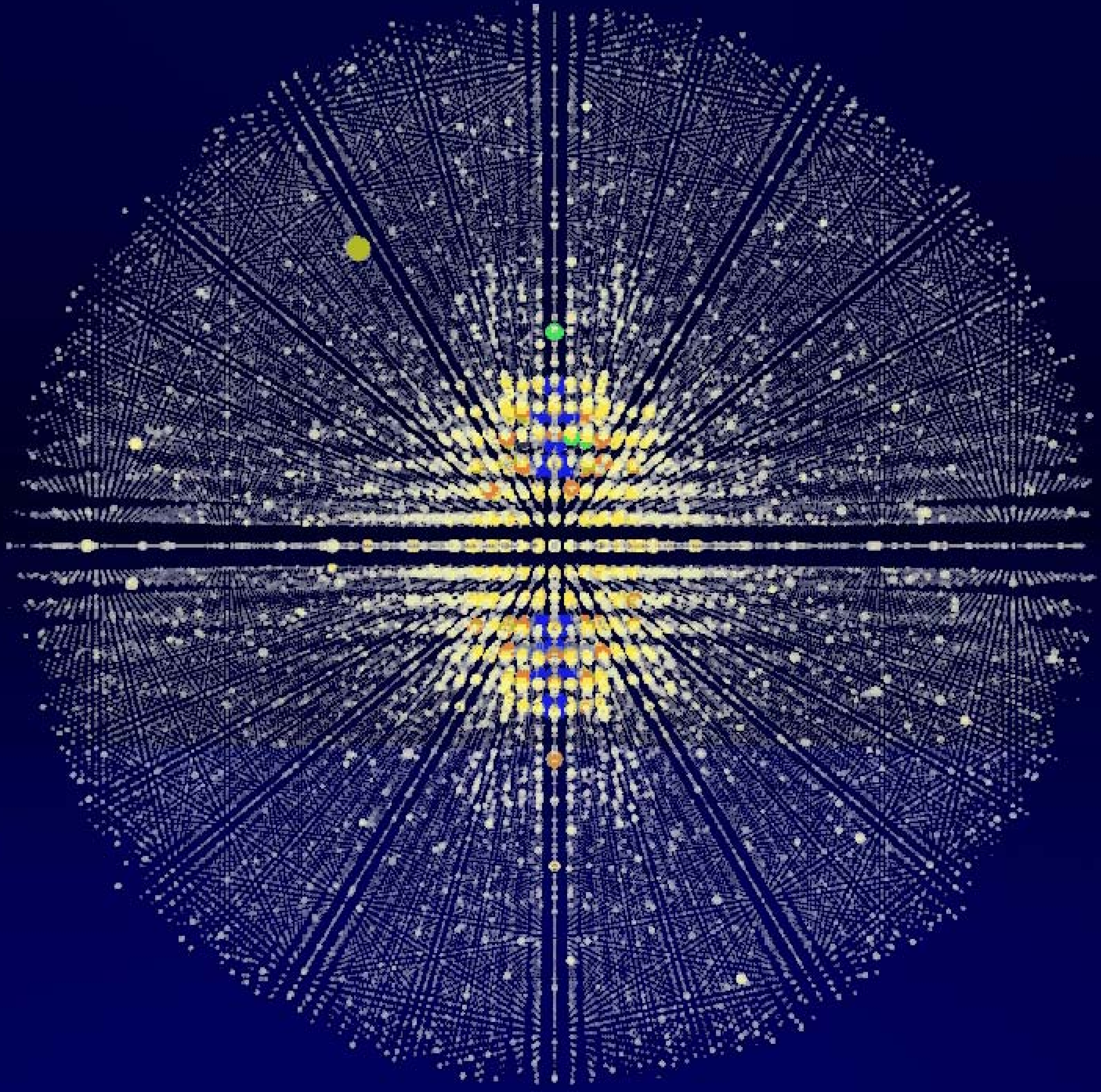
9 fringes (including Bragg)

= 220 nm

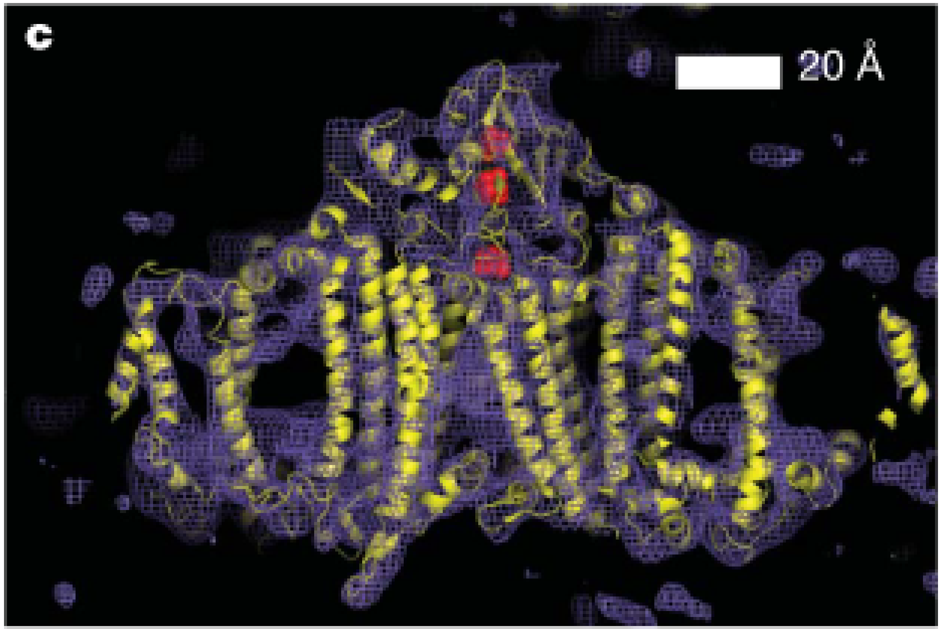
Wide Angle Diffraction (Near Detector)

- Structure determination of large macromolecules requires indexing each pattern
- For PS1, have merged indexed patterns into a 3D diffraction pattern
- ***8.5Å resolution with 1.8 keV photons; experiments at shorter wavelength (9 keV) underway***

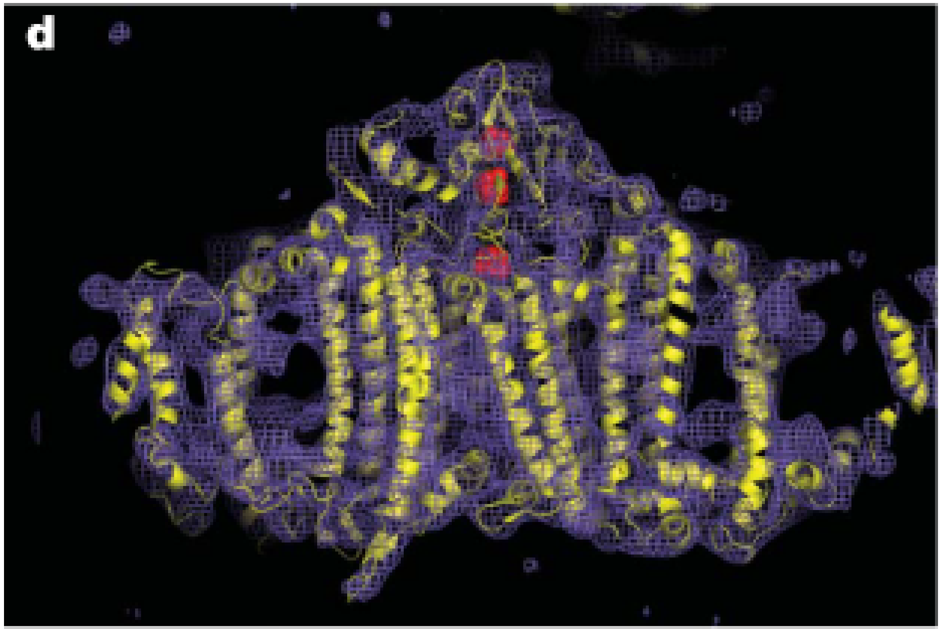




Electron Density Map for PS I

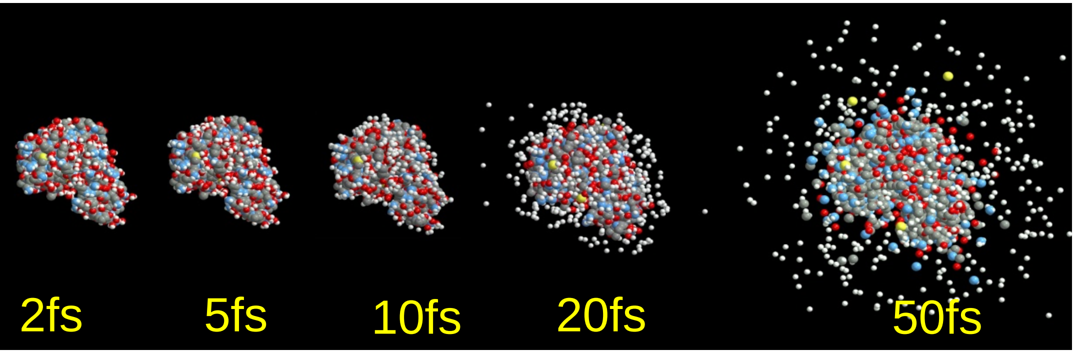


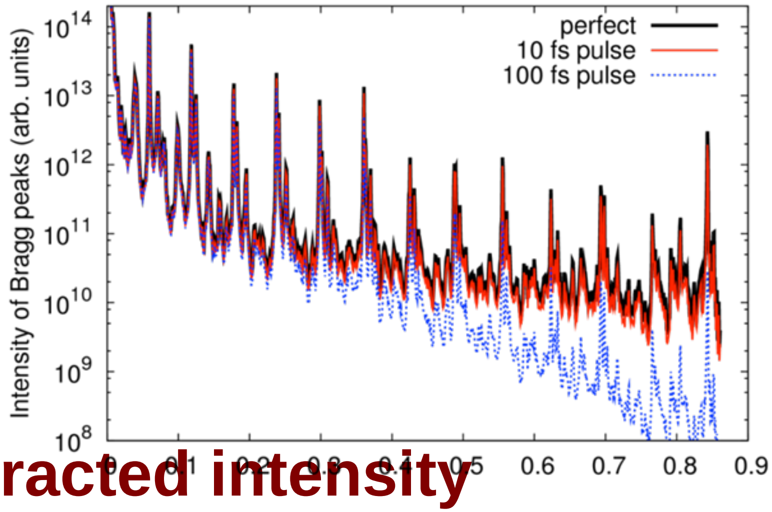
Calculated from 70fs LCLS data



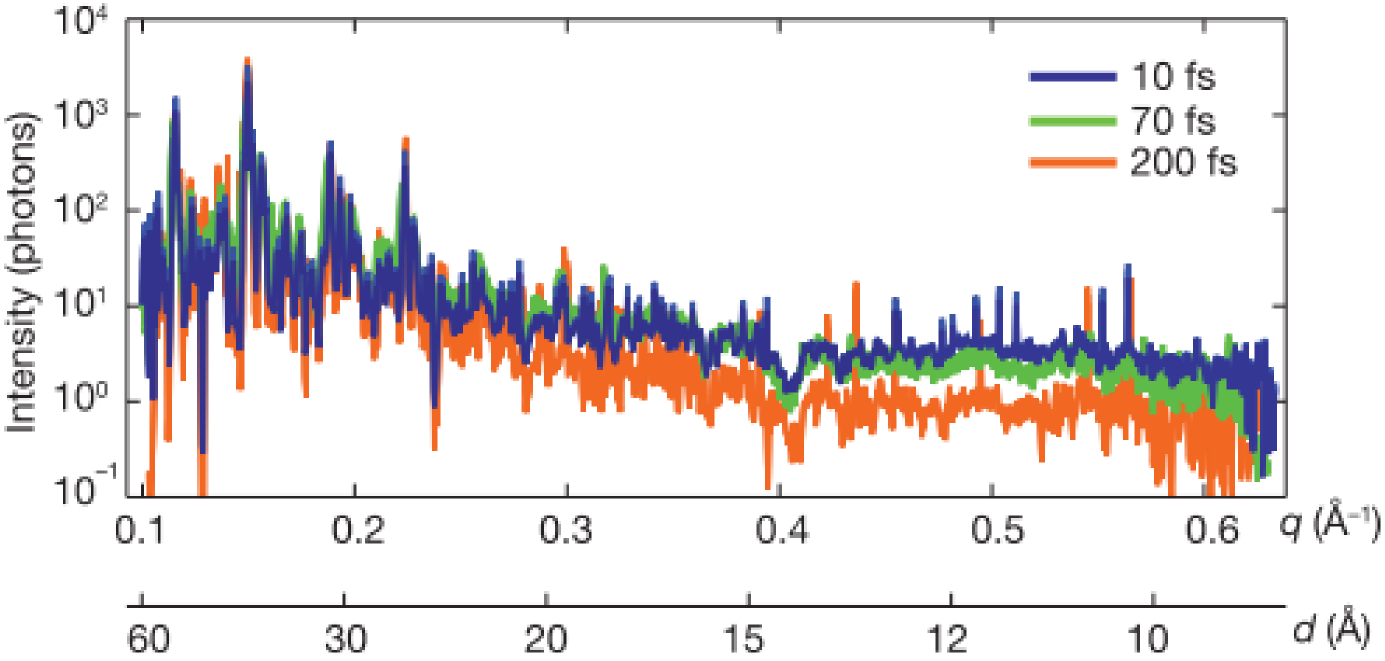
Conventional synchrotron data truncated to 8.5 A resolution

Preliminary analysis shows degradation of the sample at longer pulse durations





Photosystem I radial average of diffracted intensity



Conclusions from Nanocrystal Imaging Experiments

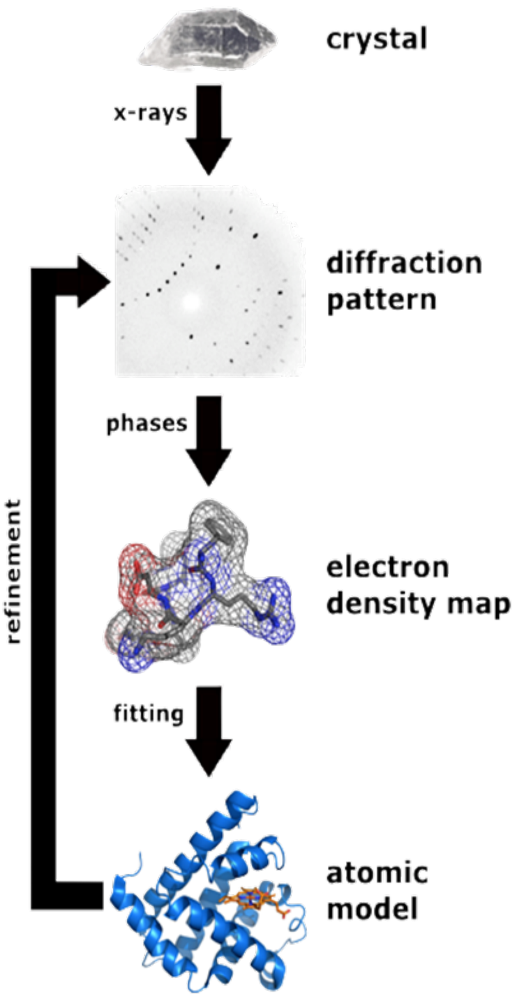
- Femtosecond nanocrystallography opens up a new route for small or radiation sensitive single-crystal structure determination

- High-quality diffraction patterns can be collected at the pulse rate of the LCLS

- **“Diffraction before destruction” concept validated to sub-nanometer resolution**

- Nanocrystallography is immediately extendible to femtosecond time-resolved measurements of photoinduced dynamics

- We are seeing the first ‘killer ap’ for LCLS



Single shot imaging of individual viruses & cells

Single mimivirus particles intercepted and imaged with an X-ray laser Nature 09748

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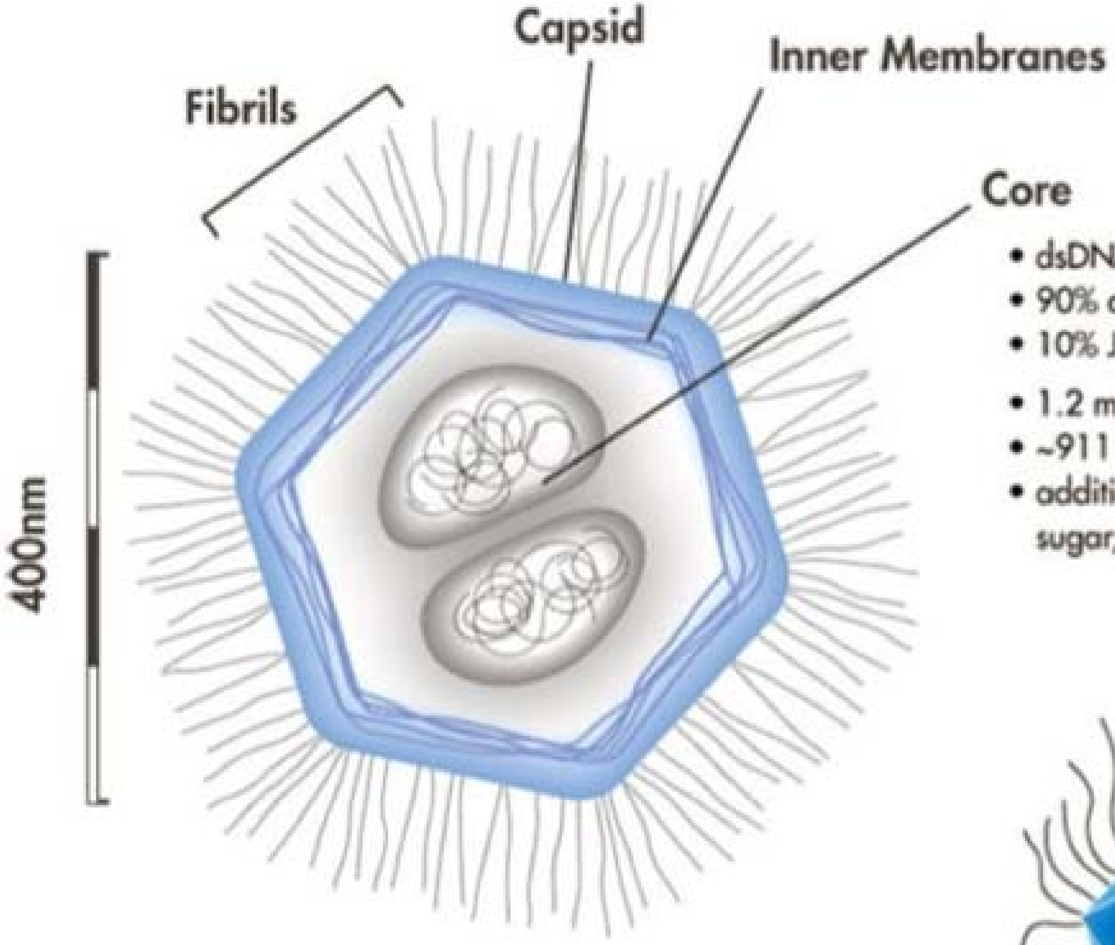
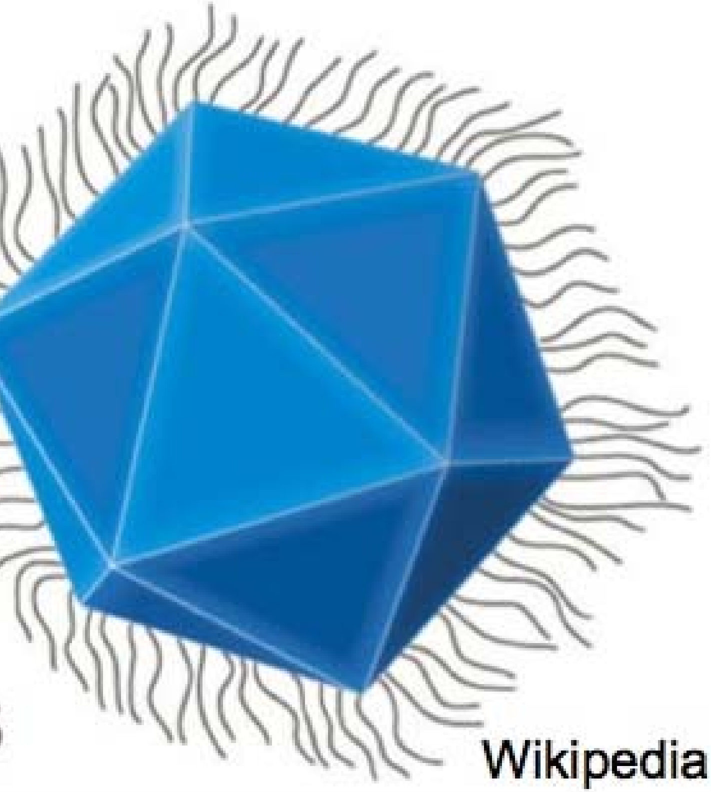


- dsDNA virus
- 90% coding capacity
- 10% Junk DNA
- 1.2 million base pairs
- ~911 protein coding genes
- additional genes (inc. aminoacyl tRNA synthetases; sugar, lipid, and amino acid metabolism)

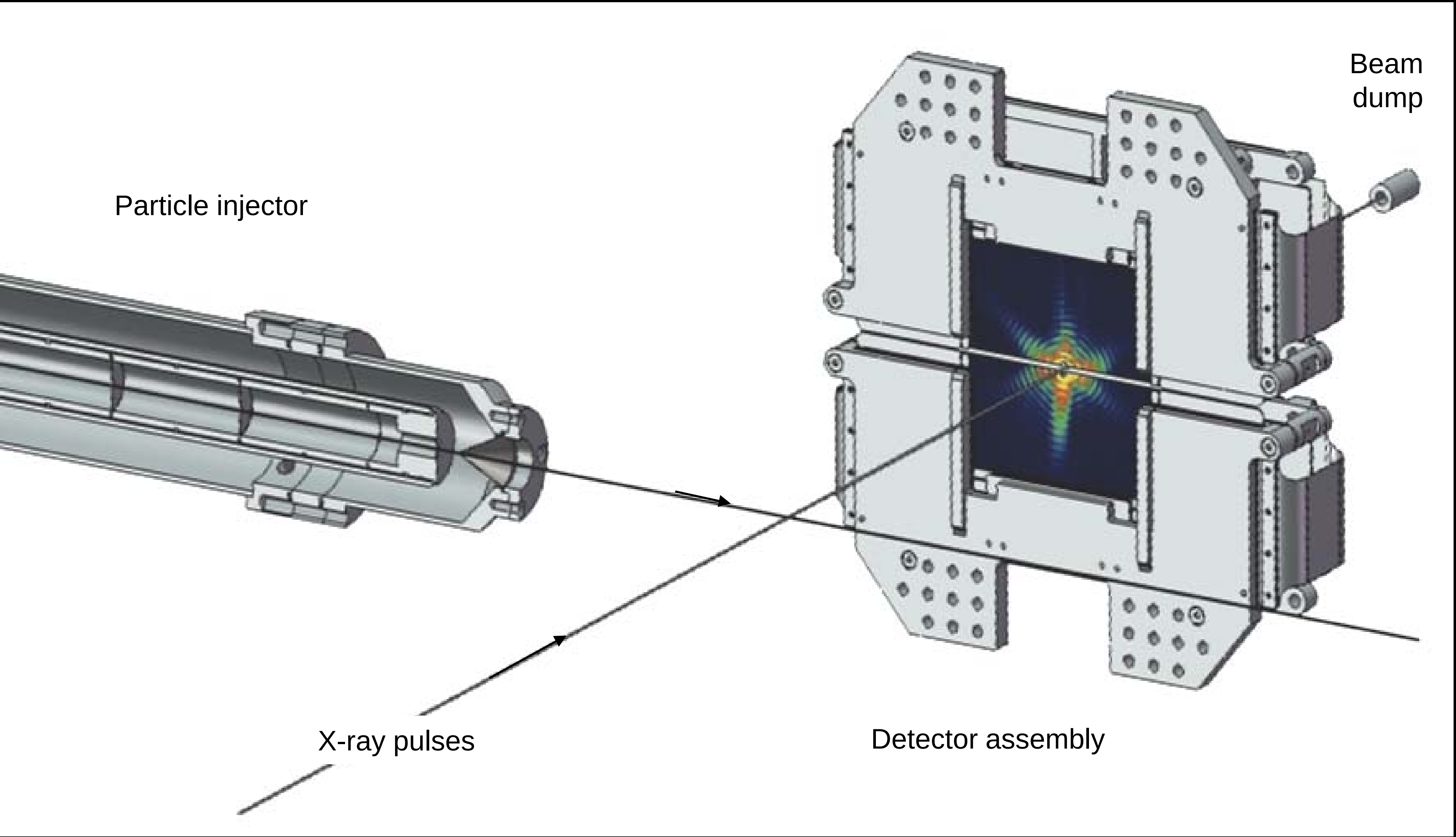


Artist’s impression of

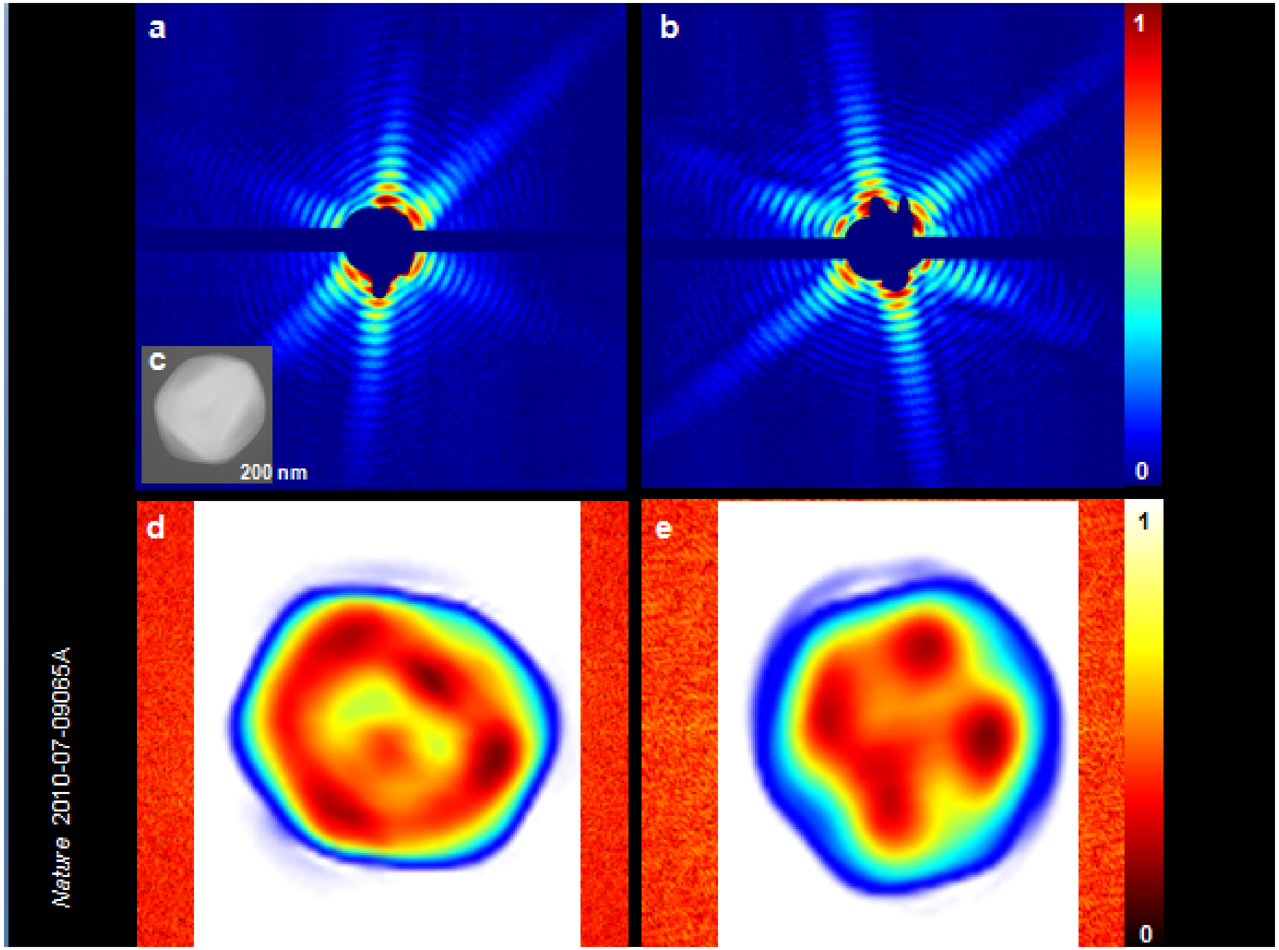
acanthamoeba polyphaga mimivirus

Wikipedia

The Experimental Setup



Single Shot Images of Mimivirus from LCLS



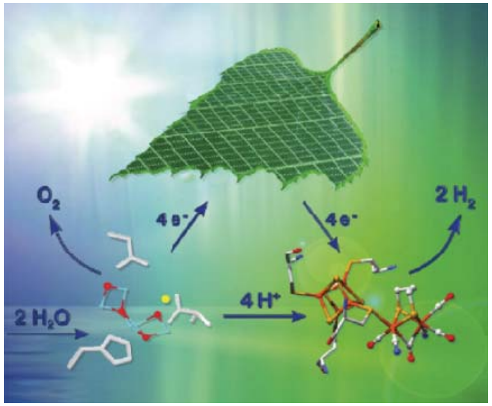
- **2-D reconstructions of Single shot LCLS images (32 nm resolution)**
- **Reveal inhomogeneous interior structure of virion which does not follow the pseudo-icosahedral shell**

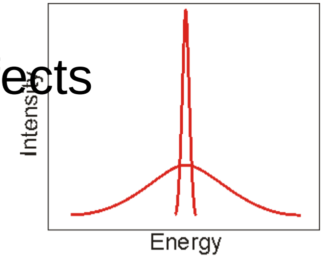
Looking Forward: LCLS-II and Beyond

Desired Extensions to LCLS-I

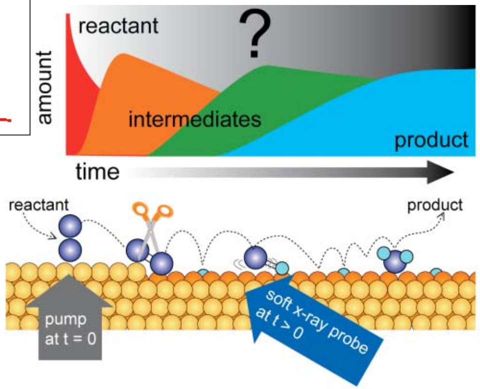
- Extended spectral range down to the carbon absorption edge at 280eV
  - study of chemical transformations of key carbon based molecular complexes
- Extension to harder x-rays >10 keV
  - study of thick 3D materials with increased x-ray penetration & spatial resolution
- Ultrashort x-ray pulses < 1 fs
  - explore attosecond temporal region for molecular dynamics
- Variable polarization
  - allows separation of charge and spin effects
- Enhanced intensity in narrow energy window through seeding
  - improved signal to noise
- Combination of THz excitation with x-ray probe
  - understanding and control of thermally induced chemical reactions

Light excitation:
photosynthesis

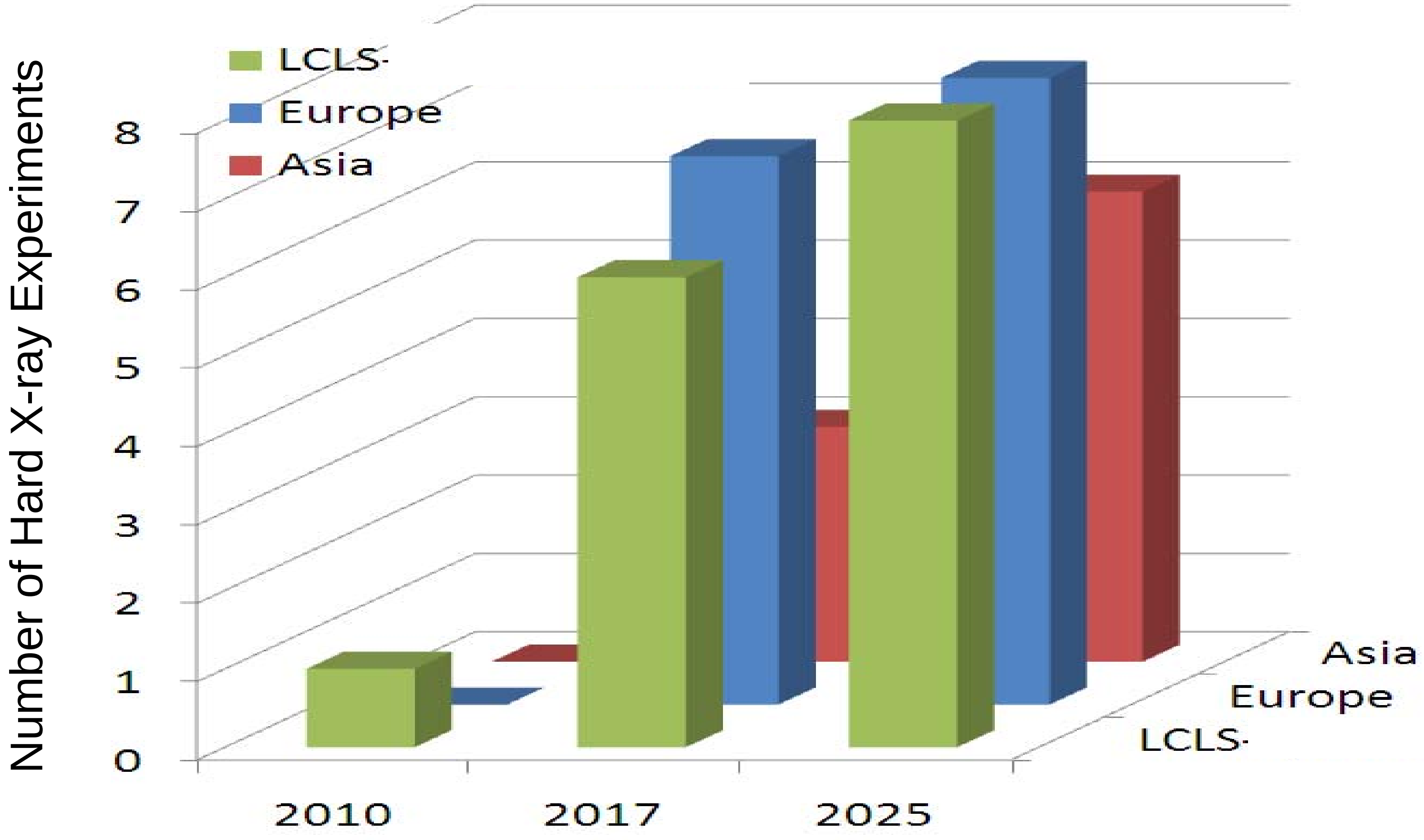




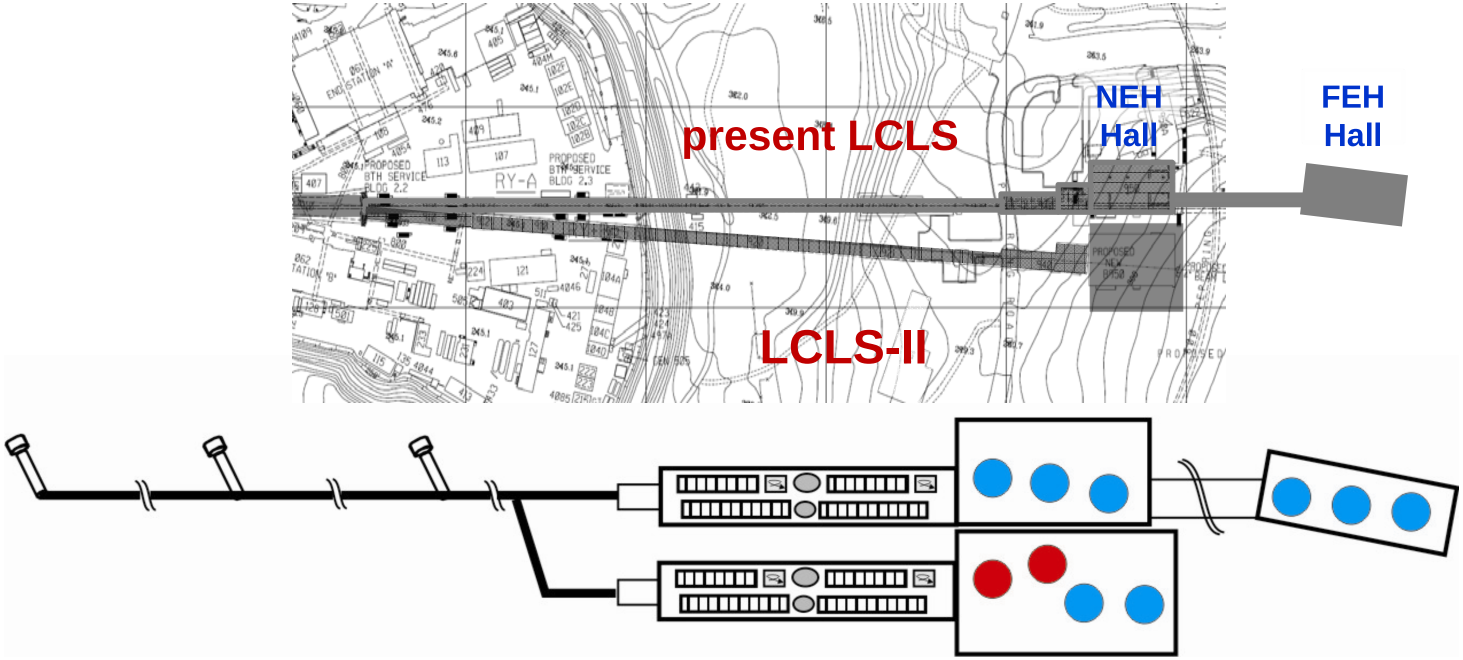
THz (heat) excitation:
Industrial catalysis



The Competition



LCLS Upgrades: What we Envision



- **3 injectors up to 360 Hz & 3 linac sections up to 14 GeV each**
- **4 seeded undulator x-ray sources**
- **10 experimental stations operating simultaneously**

Summary

- Near term is very exciting
  - – LCLS-I is in operation
    - Operation with capability undreamt of before first lasing (4/10/09)
  - – LCLS-II is moving forward
    - Adding capability and capacity undreamt of before 4/10/09
- A new scientific frontier is being opened
  - – Time of extraordinary opportunity
    - Structure → Dynamics @ fs scale
    - Observation → Understanding → Control
- Biggest surprises are yet to come!