Introduction to Free Electron Lasers (Part 1)

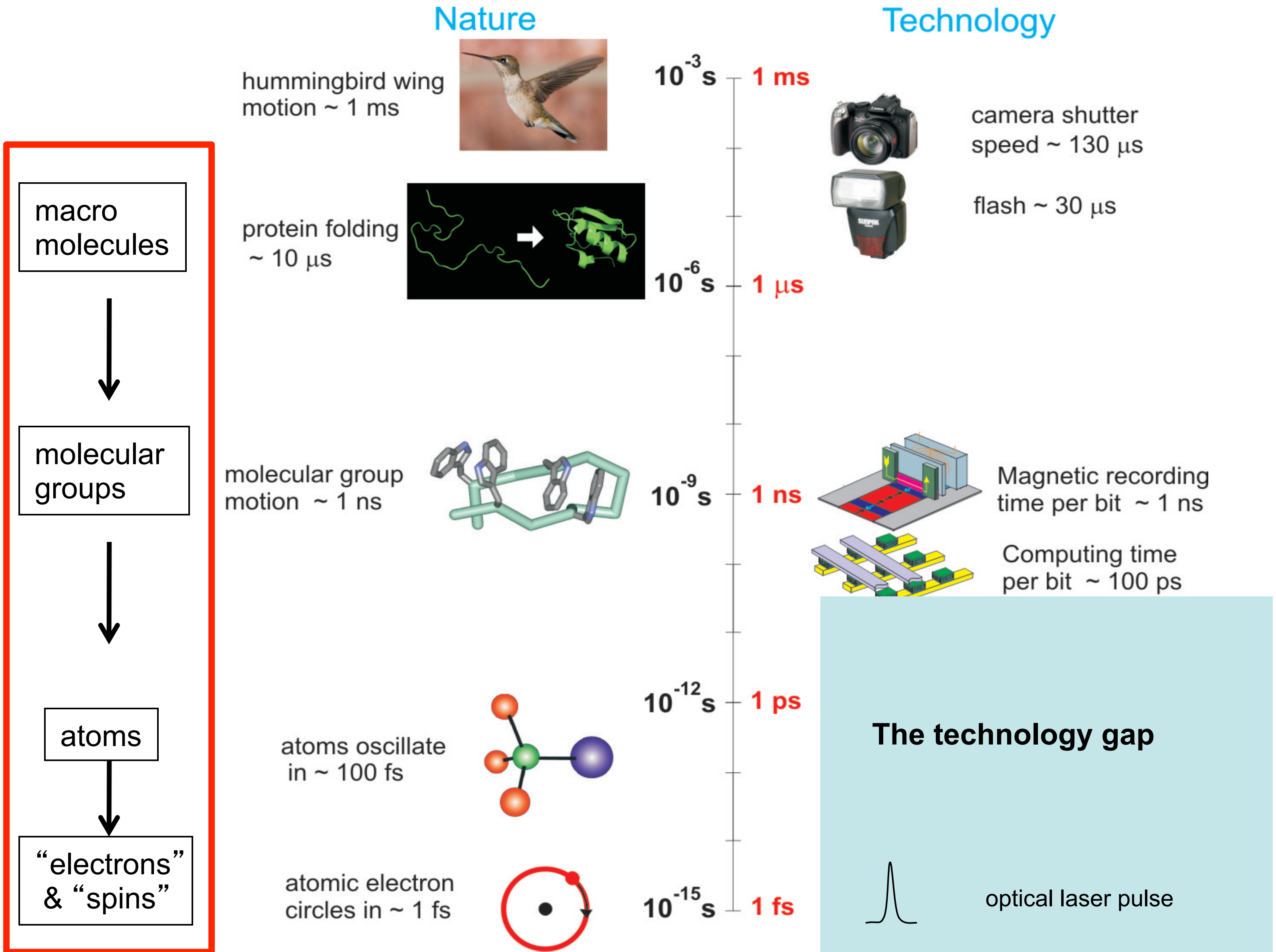
John Byrd
Lawrence Berkeley National Laboratory

Motivation

- **Outline of lecture 1**

1. Frontiers in ultrafast x-ray science
2. What is a Free Electron Laser?
3. 1-D FEL theory

The speed of things – the smaller the faster



macro molecules

molecular groups

atoms

"electrons" & "spins"

Nature

hummingbird wing motion ~ 1 ms

protein folding ~ 10 μs

molecular group motion ~ 1 ns

atoms oscillate in ~ 100 fs

atomic electron circles in ~ 1 fs

Technology

camera shutter speed ~ 130 μs

flash ~ 30 μs

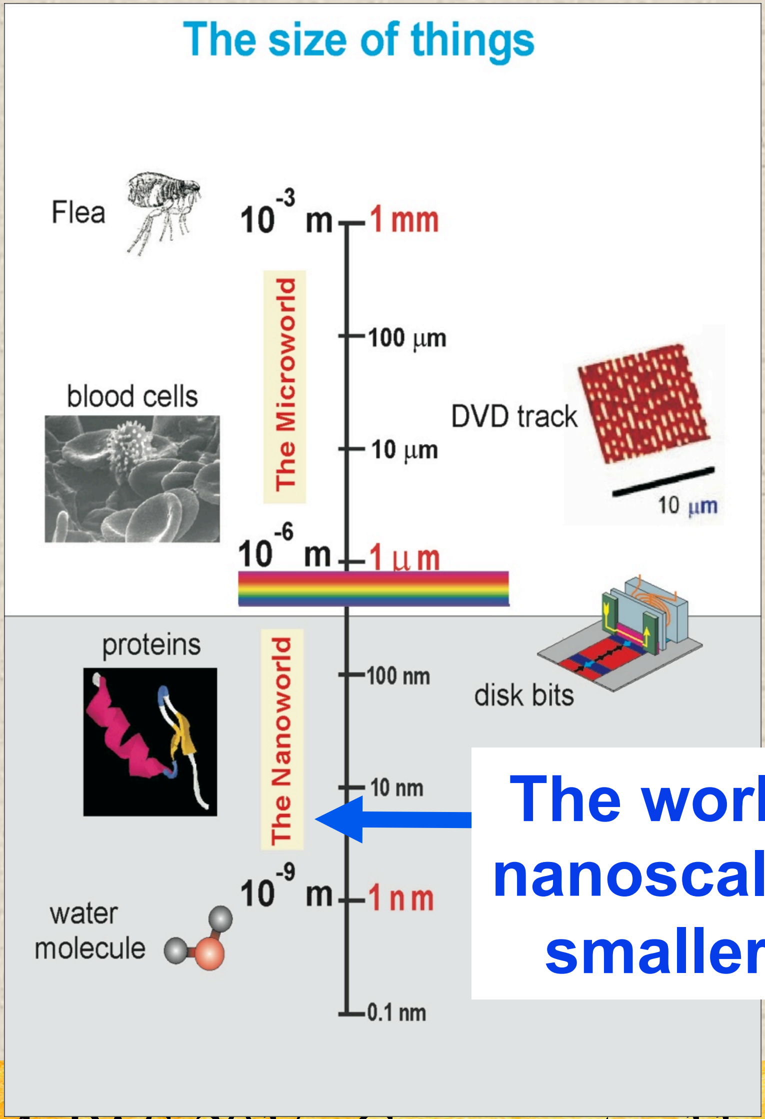
Magnetic recording time per bit ~ 1 ns

Computing time per bit ~ 100 ps

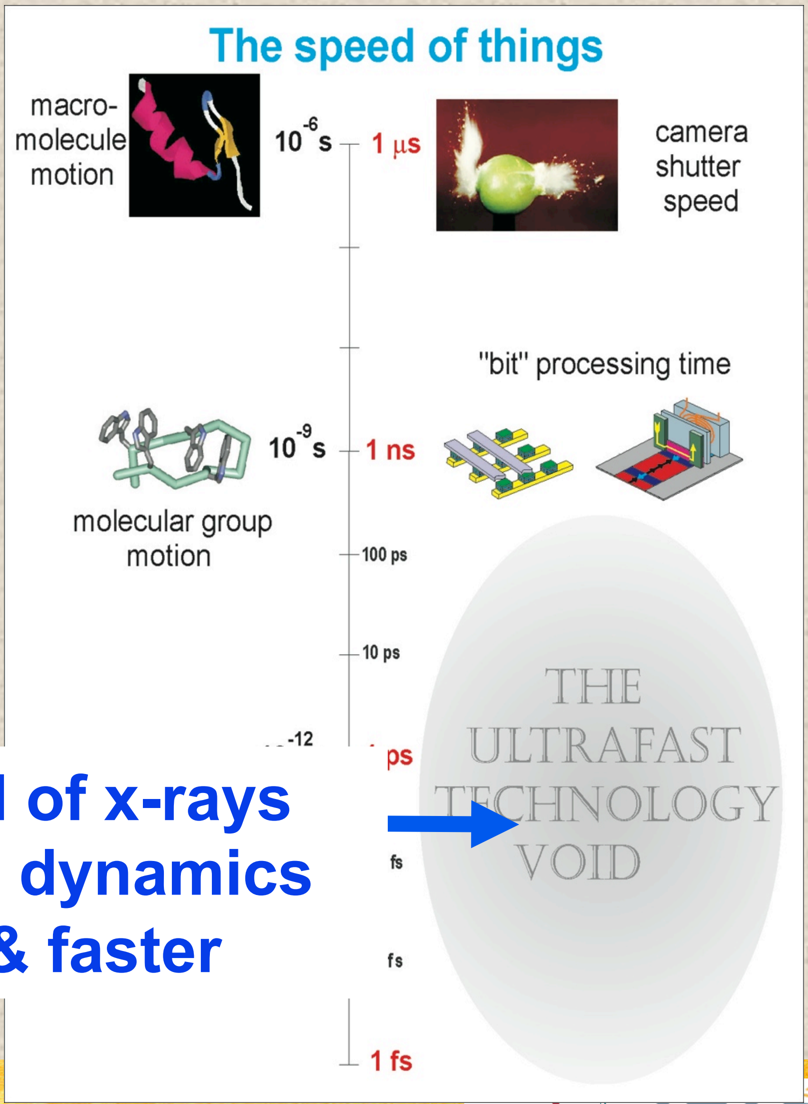
The technology gap

optical laser pulse

The new science paradigm:
Static nanoscale "structure" plus its dynamic "function"



The size of things



The speed of things

The world of x-rays
nanoscale dynamics
smaller & faster

Operational Timescales

Fundamental Timescales

Important areas in ultrafast science

Because of their size, atoms and “bonds” can change fast

but how do systems evolve? key areas of interest:

equilibrium
(“structure”, phase diagram of a system T, P …)

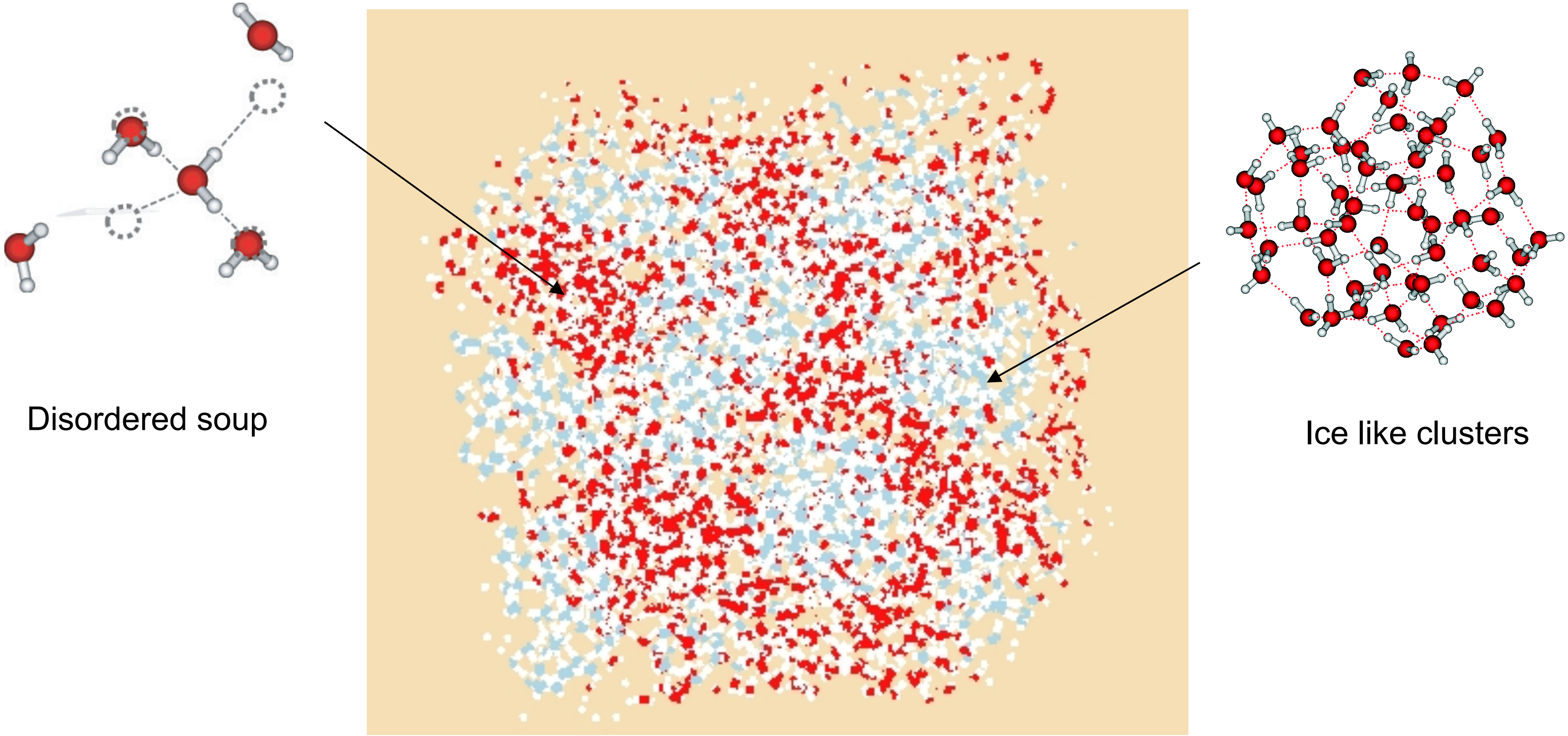
close to equilibrium
(operation or function of a system, e.g. current flow)

far from equilibrium
(transient states after excitation, e.g. chemical reaction)

far-far from equilibrium
(transient states after extreme stimulus, e.g. a plasma)

“Equilibrium”: What is the structure of water?

Small angle x-ray scattering shows inhomogeneity



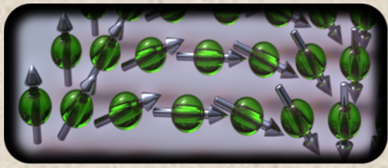
Disordered soup

Ice like clusters

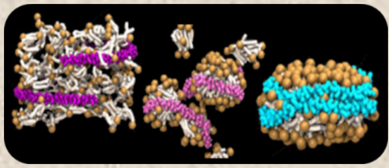
Components probably dynamic – form and dissolve

- can we take an ultrafast snapshot??

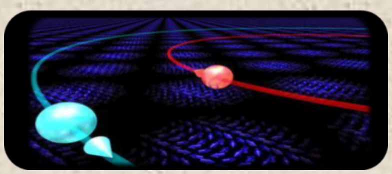
Five Grand Challenges for Science and the Imagination



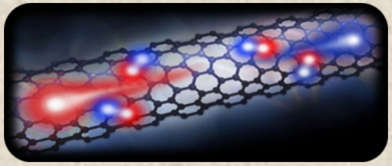
- How do we control materials and processes at the level of electrons?



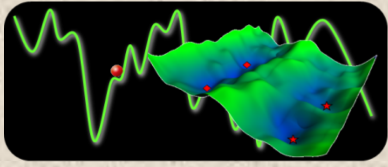
- How do we design and perfect atom-and energy-efficient synthesis of new forms of matter with tailored properties?



- How do remarkable properties of matter emerge from complex correlations of atomic and electronic constituents and how can we control these properties?

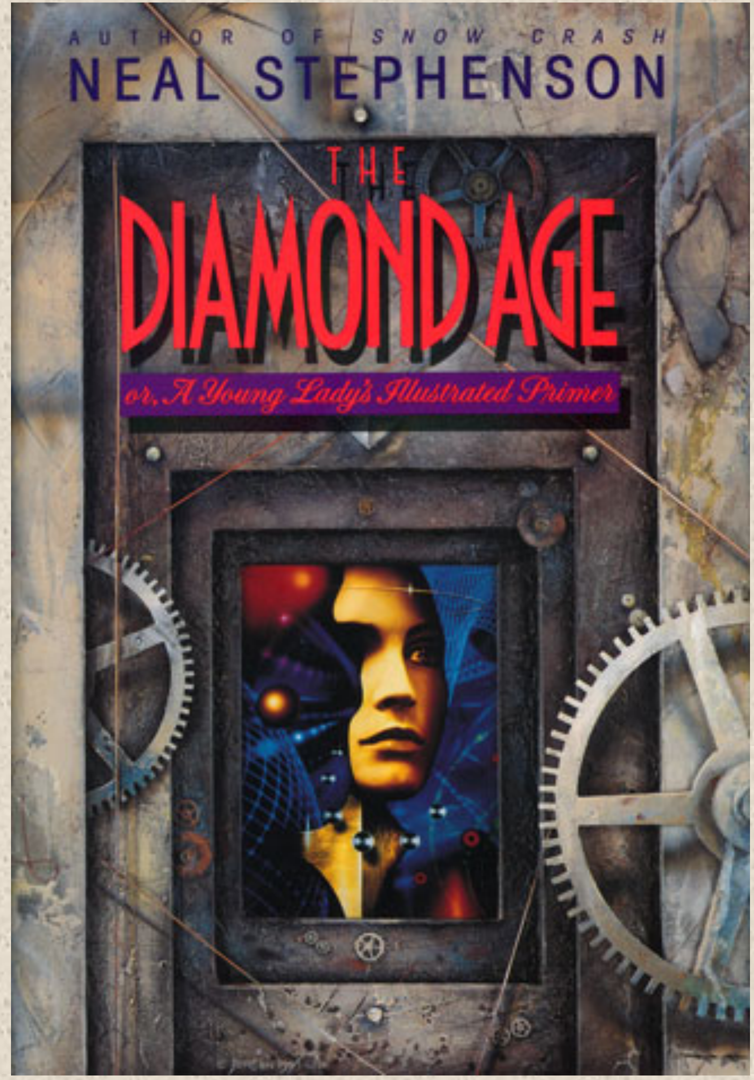


- Can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living systems?

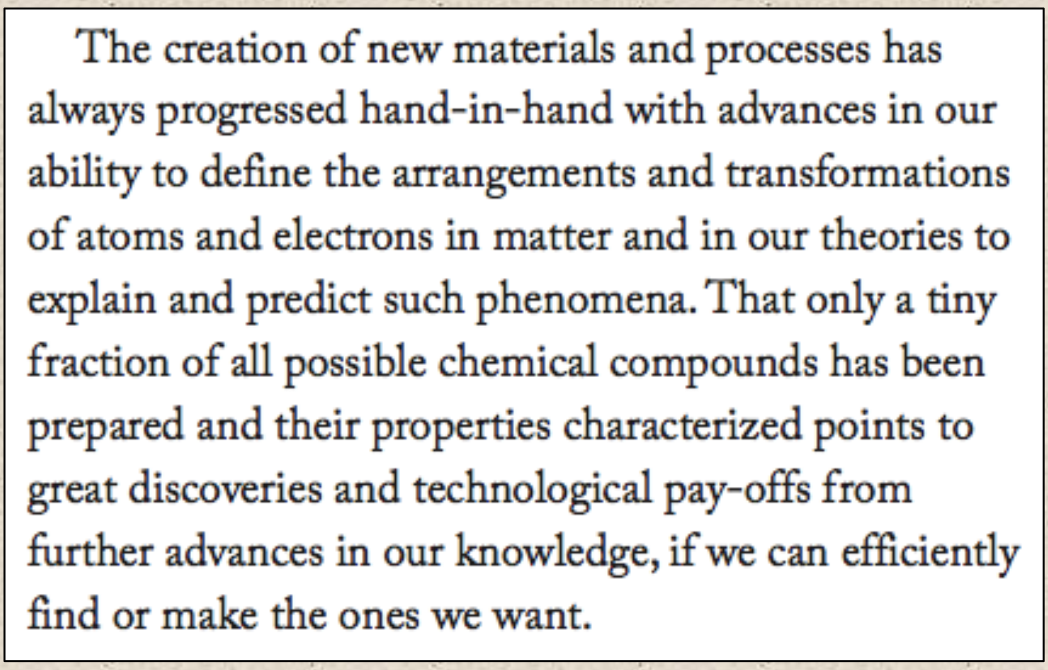


- How do we characterize and control matter away —especially very far away—from equilibrium?

We are entering a “Diamond Age”

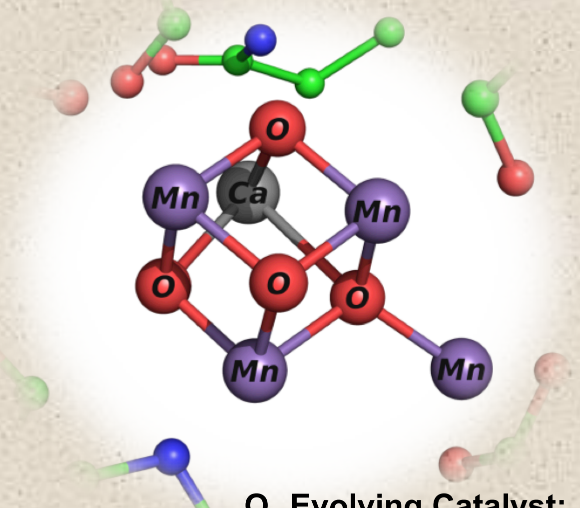


From the DOE/BES report: Directing Matter and Energy: Five Challenges for Science and the Imagination

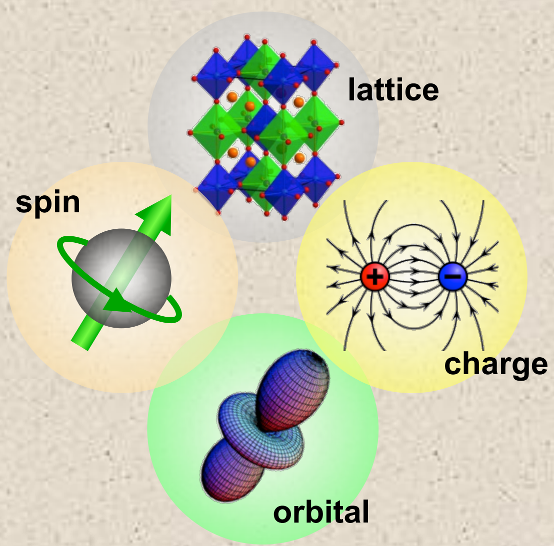


The creation of new materials and processes has always progressed hand-in-hand with advances in our ability to define the arrangements and transformations of atoms and electrons in matter and in our theories to explain and predict such phenomena. That only a tiny fraction of all possible chemical compounds has been prepared and their properties characterized points to great discoveries and technological pay-offs from further advances in our knowledge, if we can efficiently find or make the ones we want.

Underlying questions from the electronic to the mesoscale



O$_2$ Evolving Catalyst: Mn$_4$CaO$_5$

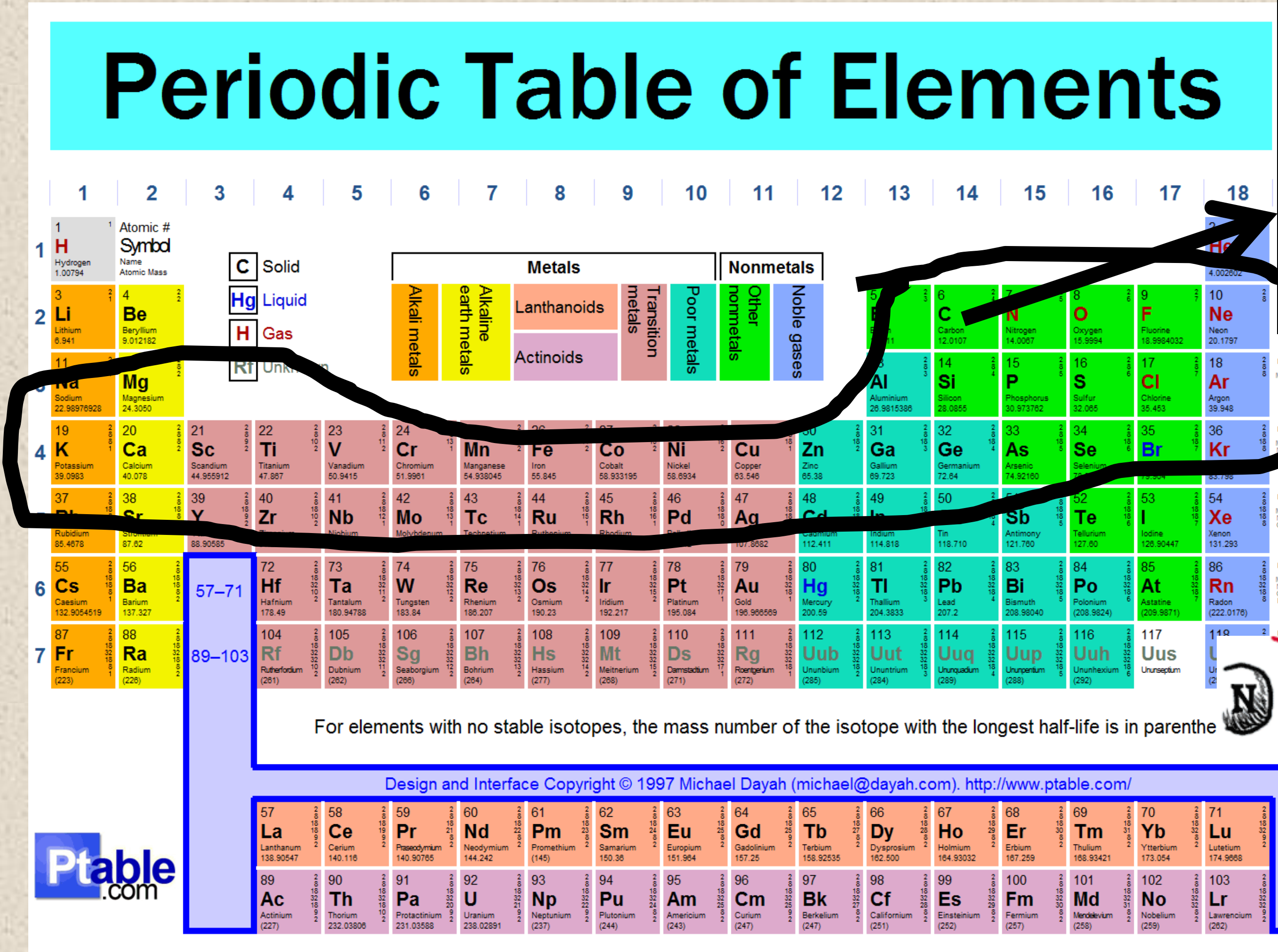


How can we describe correlated electronic degrees of freedom and nuclear displacements in systems like multi-electron catalysts?

How do new material properties emerge from mesoscale ordering & dynamic coupling of
charge, spins,
& phonons?

How do nanoscale components assemble into functional groupings & can we control this?

Fundamentals of X-ray absorption by matter



Periodic Table of Elements

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 **H** Hydrogen 1.00794	Atomic # Symbol Name Atomic Mass																2 **He** 4.002602
2	3 **Li** Lithium 6.941	4 **Be** Beryllium 9.012182											5 **B**	6 **C** Carbon 12.0107	7 **N** Nitrogen 14.0067	8 **O** Oxygen 15.9994	9 **F** Fluorine 18.9984032	10 **Ne** Neon 20.1797
3	11 **Na** Sodium 22.98976928	12 **Mg** Magnesium 24.3050											13 **Al** Aluminium 26.9815386	14 **Si** Silicon 28.0855	15 **P** Phosphorus 30.973762	16 **S** Sulfur 32.065	17 **Cl** Chlorine 35.453	18 **Ar** Argon 39.948
4	19 **K** Potassium 39.0983	20 **Ca** Calcium 40.078	21 **Sc** Scandium 44.955912	22 **Ti** Titanium 47.867	23 **V** Vanadium 50.9415	24 **Cr** Chromium 51.9961	**Mn** Manganese 54.938045	**Fe** Iron 55.845	**Co** Cobalt 58.933195	**Ni** Nickel 58.6934	**Cu** Copper 63.546	**Zn** Zinc 65.38	31 **Ga** Gallium 69.723	32 **Ge** Germanium 72.64	33 **As** Arsenic 74.92160	34 **Se** Selenium	35 **Br**	36 **Kr**
5	37 Rubidium 85.4678	38 Strontium 87.62	39 **Y** 88.90585	40 **Zr**	41 **Nb** Niobium	42 **Mo** Molybdenum	43 **Tc** Technetium	44 **Ru** Ruthenium	45 **Rh** Rhodium	46 **Pd**	47 **Ag** 107.8682	48 Cadmium 112.411	49 Indium 114.818	50 Tin 118.710	**Sb** Antimony 121.760	52 **Te** Tellurium 127.60	53 **I** Iodine 126.90447	54 **Xe** Xenon 131.293
6	55 **Cs** Caesium 132.9054519	56 **Ba** Barium 137.327	57–71	72 **Hf** Hafnium 178.49	73 **Ta** Tantalum 180.94788	74 **W** Tungsten 183.84	75 **Re** Rhenium 186.207	76 **Os** Osmium 190.23	77 **Ir** Iridium 192.217	78 **Pt** Platinum 195.084	79 **Au** Gold 196.966569	80 **Hg** Mercury 200.59	81 **Tl** Thallium 204.3833	82 **Pb** Lead 207.2	83 **Bi** Bismuth 208.98040	84 **Po** Polonium (208.9824)	85 **At** Astatine (209.9871)	86 **Rn** Radon (222.0176)
7	87 **Fr** Francium (223)	88 **Ra** Radium (226)	89–103	104 **Rf** Rutherfordium (261)	105 **Db** Dubnium (262)	106 **Sg** Seaborgium (266)	107 **Bh** Bohrium (264)	108 **Hs** Hassium (277)	109 **Mt** Meitnerium (268)	110 **Ds** Darmstadtium (271)	111 **Rg** Roentgenium (272)	112 **Uub** Ununbium (285)	113 **Uut** Ununtrium (284)	114 **Uuq** Ununquadium (289)	115 **Uup** Ununpentium (288)	116 **Uuh** Ununhexium (292)	117 **Uus** Ununseptium	118

57 **La** Lanthanum 138.90547	58 **Ce** Cerium 140.116	59 **Pr** Praseodymium 140.90765	60 **Nd** Neodymium 144.242	61 **Pm** Promethium (145)	62 **Sm** Samarium 150.36	63 **Eu** Europium 151.964	64 **Gd** Gadolinium 157.25	65 **Tb** Terbium 158.92535	66 **Dy** Dysprosium 162.500	67 **Ho** Holmium 164.93032	68 **Er** Erbium 167.259	69 **Tm** Thulium 168.93421	70 **Yb** Ytterbium 173.054	71 **Lu** Lutetium 174.9668
89 **Ac** Actinium (227)	90 **Th** Thorium 232.03806	91 **Pa** Protactinium 231.03588	92 **U** Uranium 238.02891	93 **Np** Neptunium (237)	94 **Pu** Plutonium (244)	95 **Am** Americium (243)	96 **Cm** Curium (247)	97 **Bk** Berkelium (247)	98 **Cf** Californium (251)	99 **Es** Einsteinium (252)	100 **Fm** Fermium (257)	101 **Md** Mendelevium (258)	102 **No** Nobelium (259)	103 **Lr** Lawrencium (262)

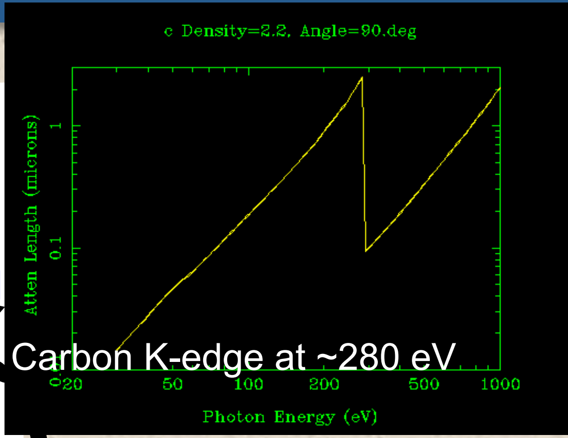
C Solid
Hg Liquid
H Gas
Rf Unkn

Metals: Alkali metals, Alkaline earth metals, Lanthanoids, Actinoids, Transition metals, Poor metals
Nonmetals: Other nonmetals, Noble gases

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parenthe

Design and Interface Copyright © 1997 Michael Dayah (michael@dayah.com). http://www.ptable.com/

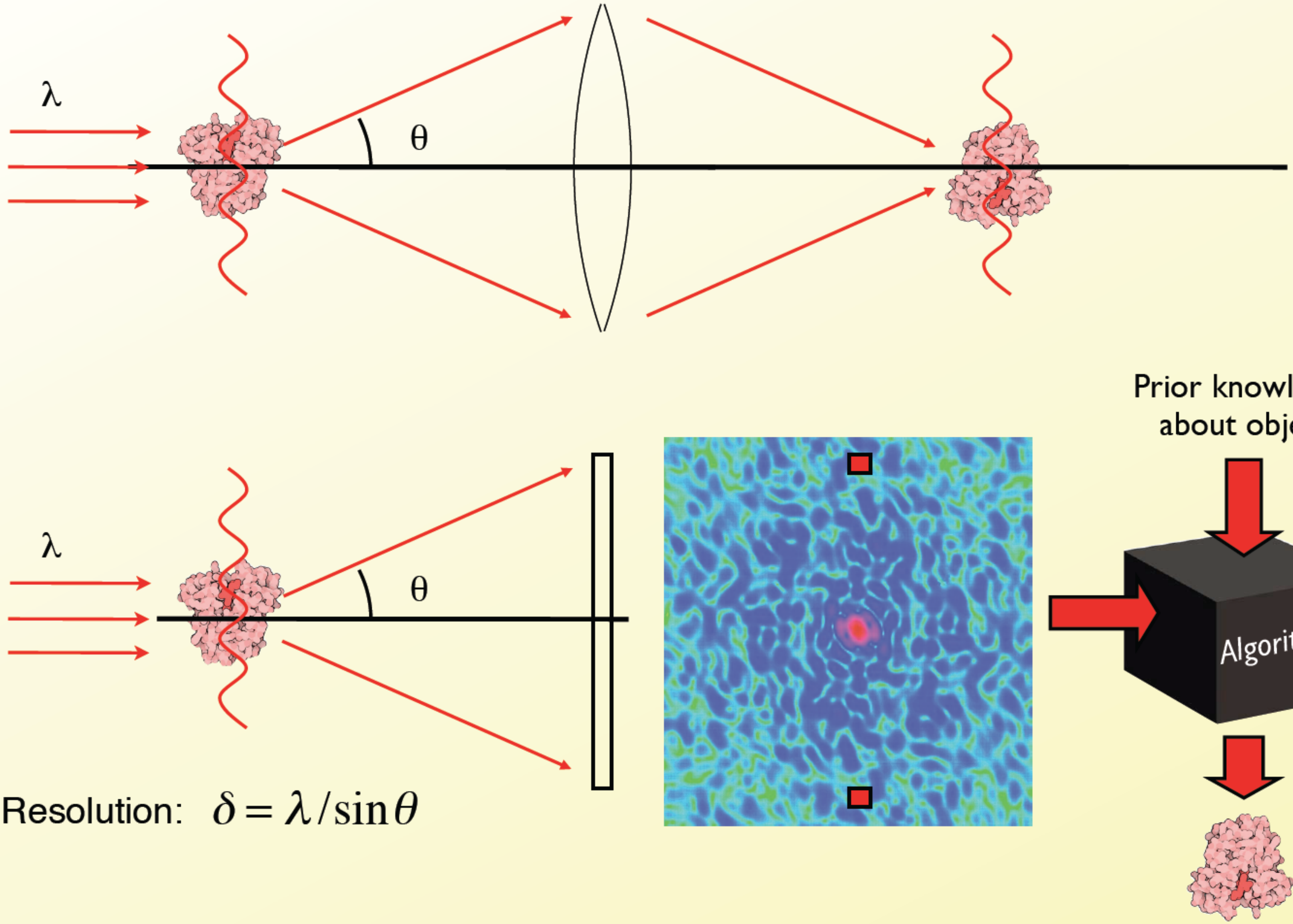
Ptable.com



Carbon K-edge at ~280 eV

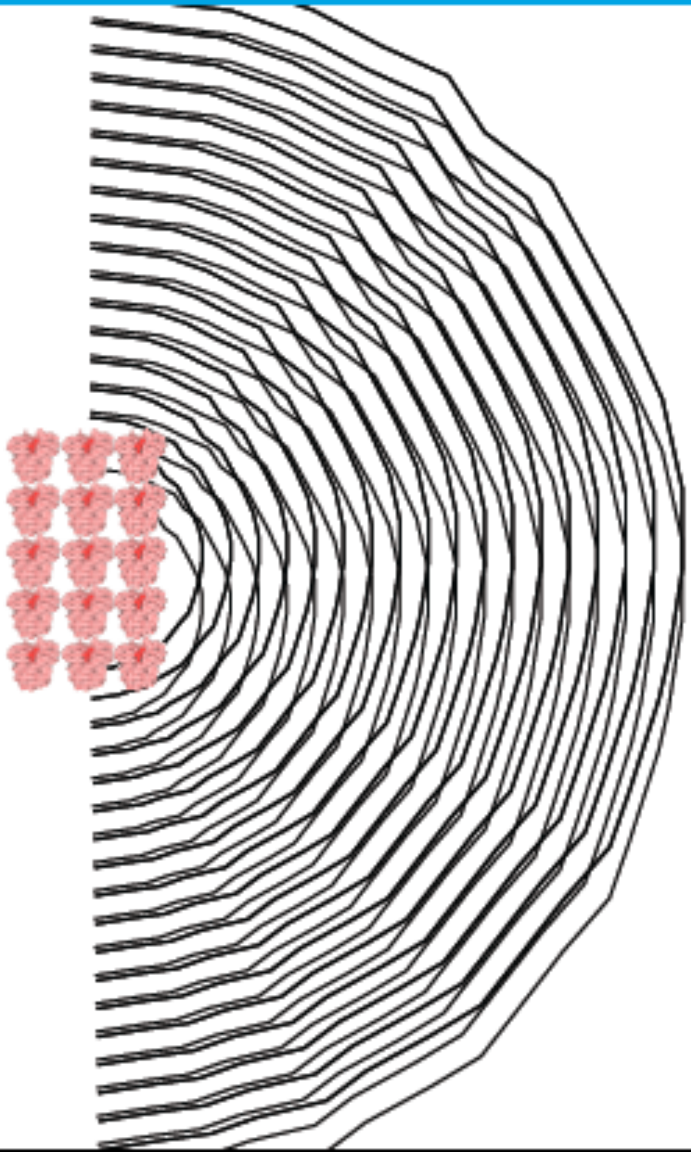
K-shell energies from 100 eV-25 keV

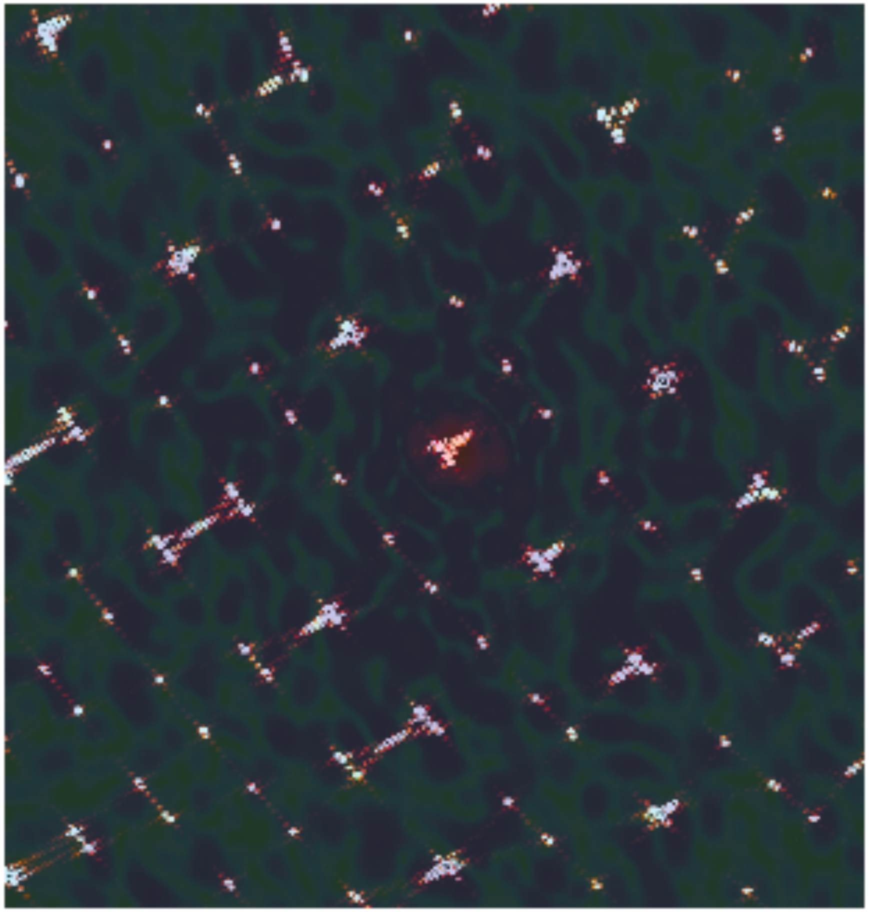
Coherent diffractive imaging (including crystallography) is lensless



Resolution: $\delta = \lambda / \sin\theta$

Diffraction pattern requires enhancement from a crystal

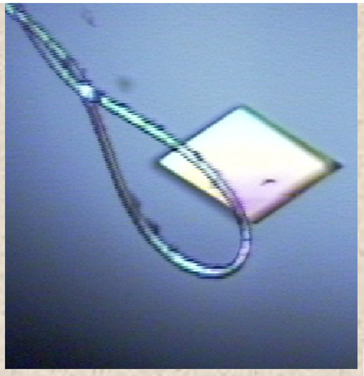


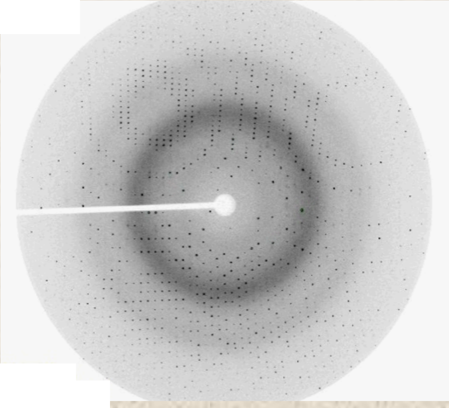


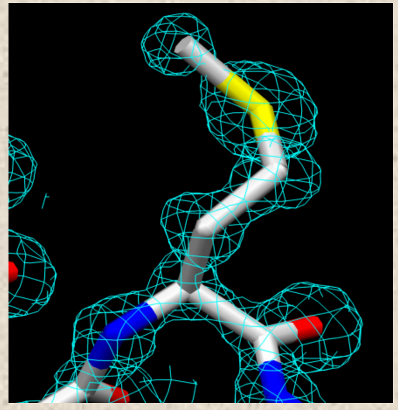
signal is proportional to the number of unit cells

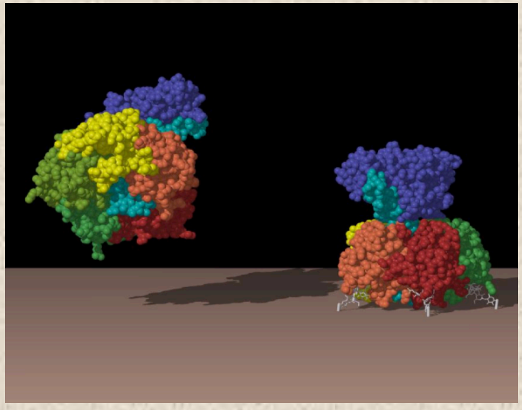
A new Paradigm in Macromolecular Crystallography “beating the speed of sound with the speed of light”

conventional method









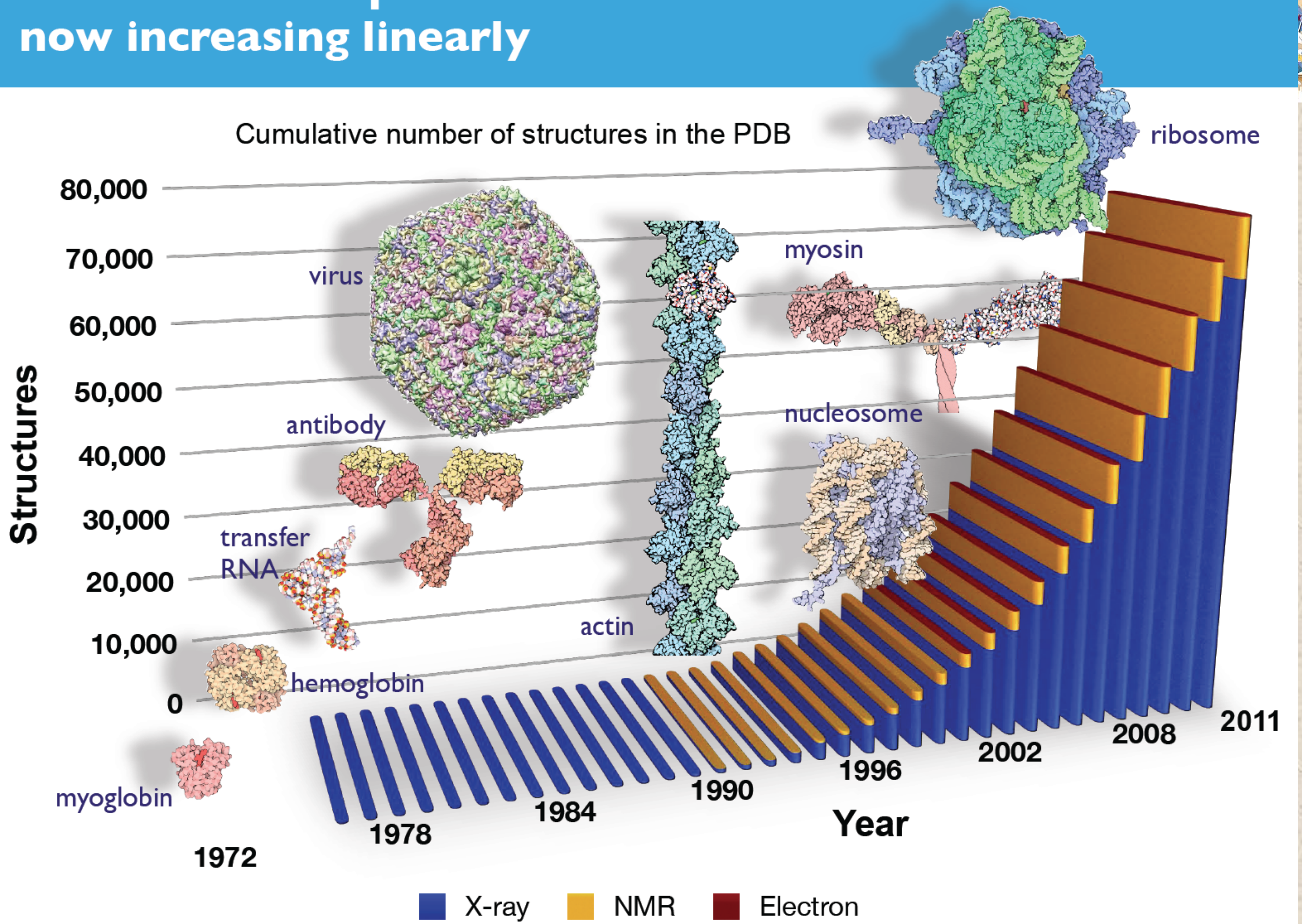
Protein crystal → *Diffraction data* → *Electron density* → *Molecular model of protein suggests its function*

In 1980s synchrotron x-rays revolutionized macromolecular crystallography

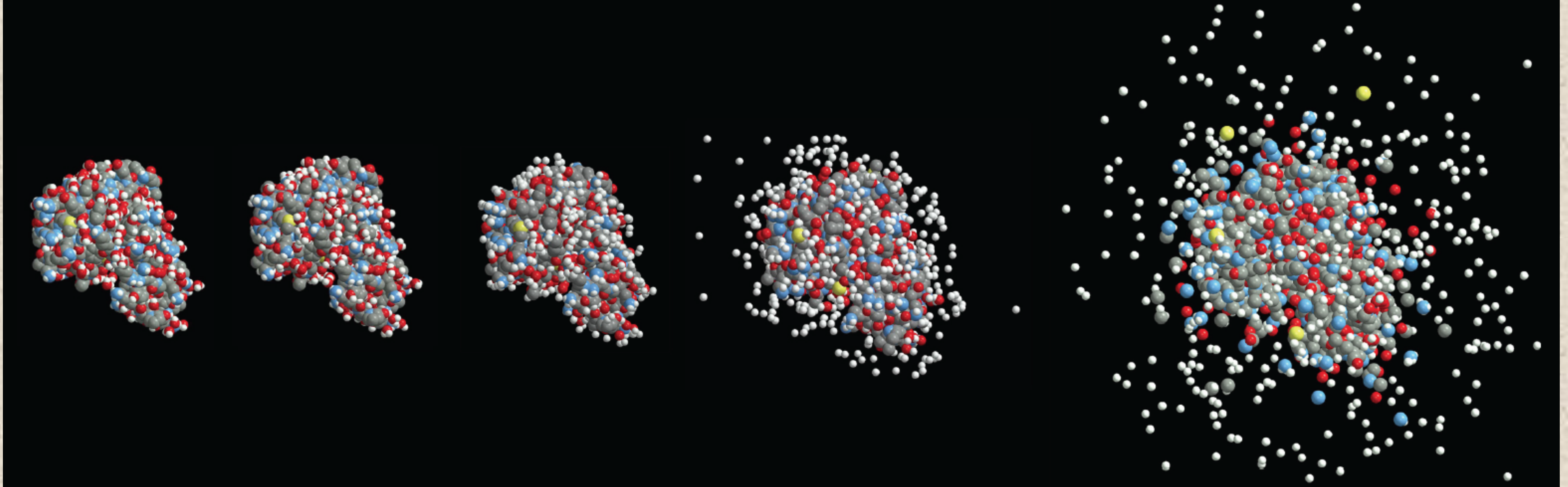
- Protein structure has allowed the developments of drugs
- However, synchrotron studies limited to large (> 5 microns) crystals
- Data for smaller crystals limited by x-ray beam damage

Studies of nanocrystals at X-FELs leads to a new paradigm

The number of protein structures solved is now increasing linearly

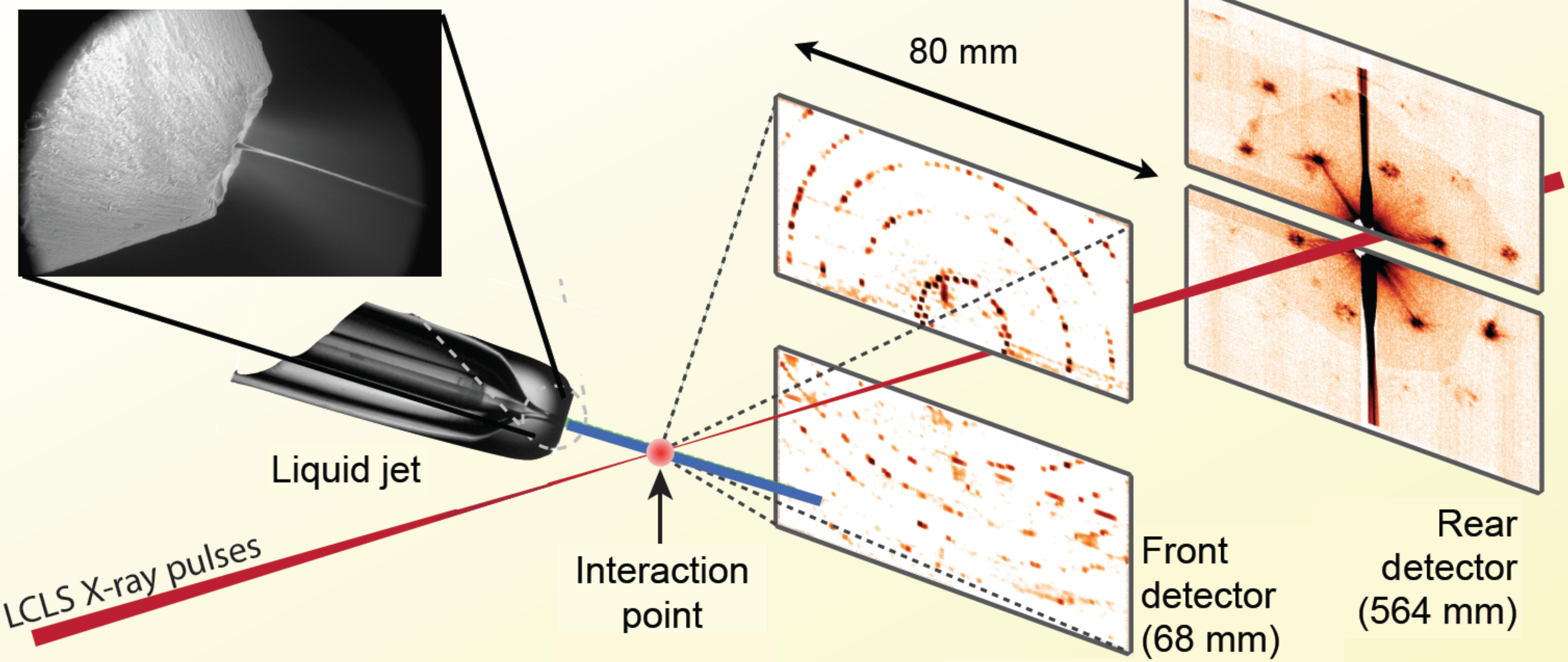


X-ray free-electron lasers may enable atomic-resolution imaging of biological macromolecules

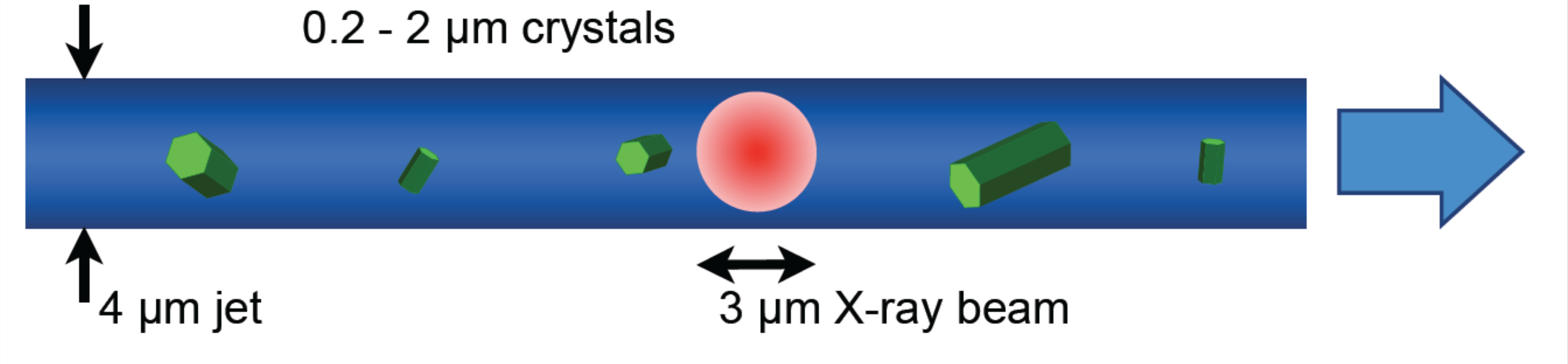


R. Neutze, R. Wouts, D. van der Spoel, E. Weckert, J. Hajdu, Nature **406** (2000)

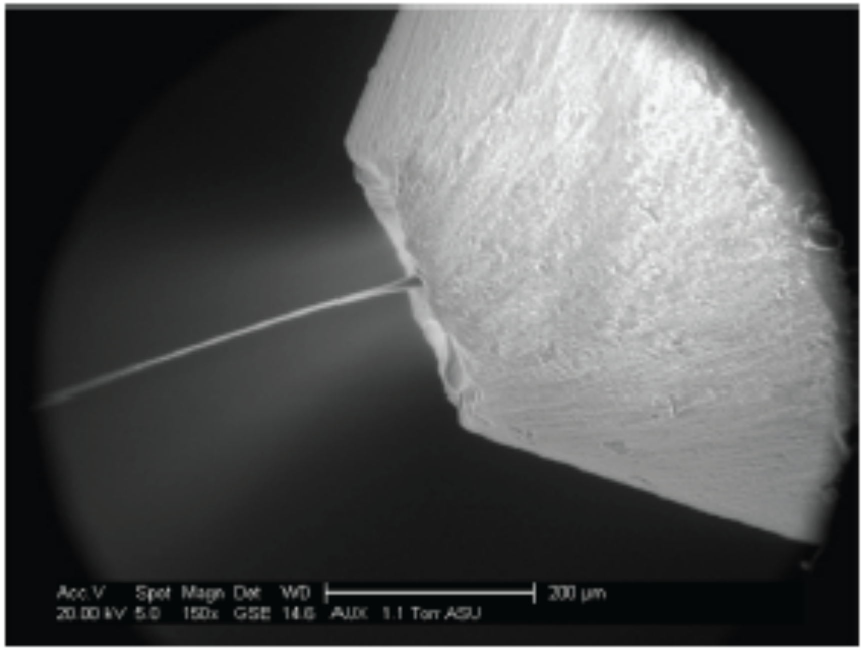
Nanocrystallography is carried out in a flowing water microjet

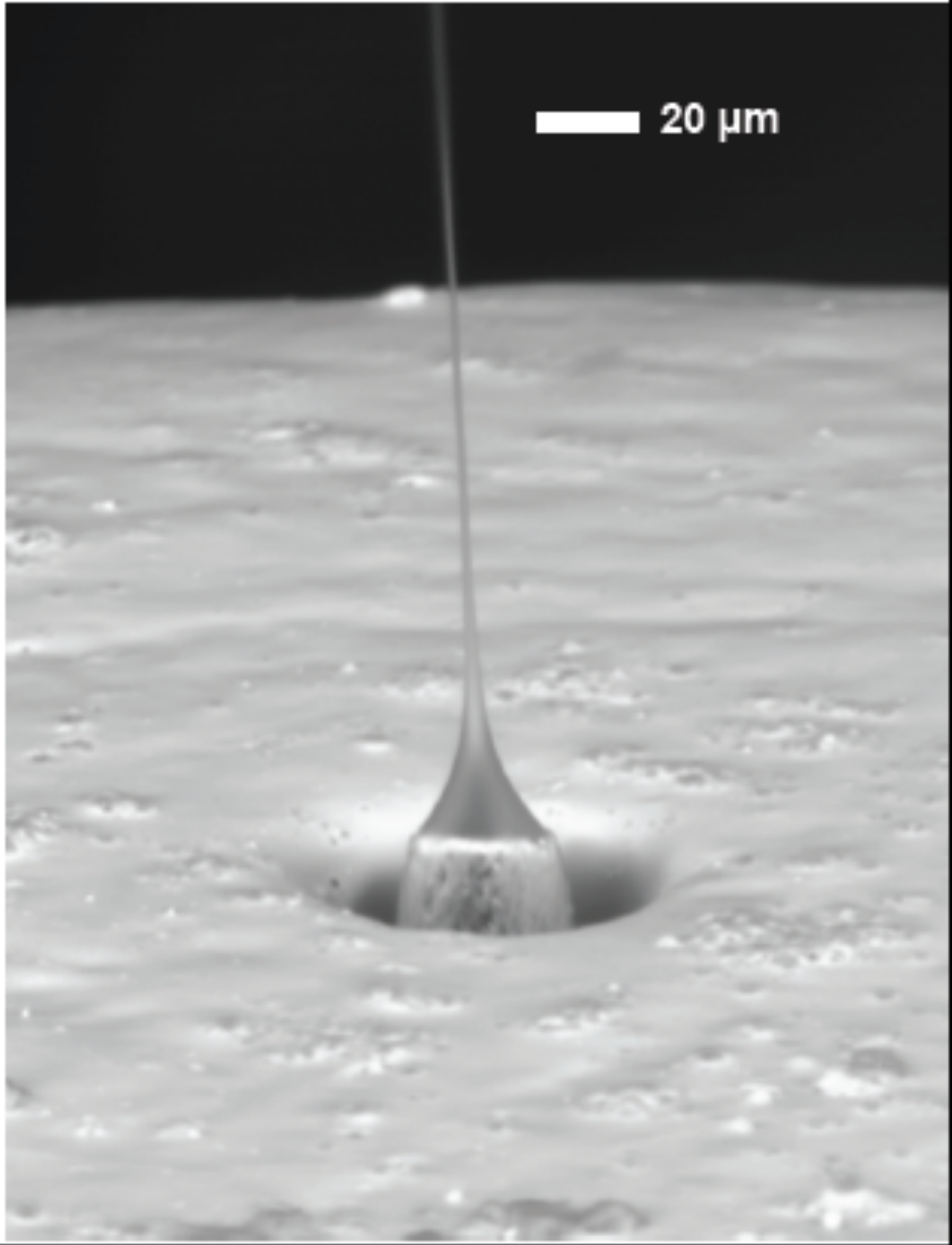


CAMP Chamber: L. Struder *et al.*



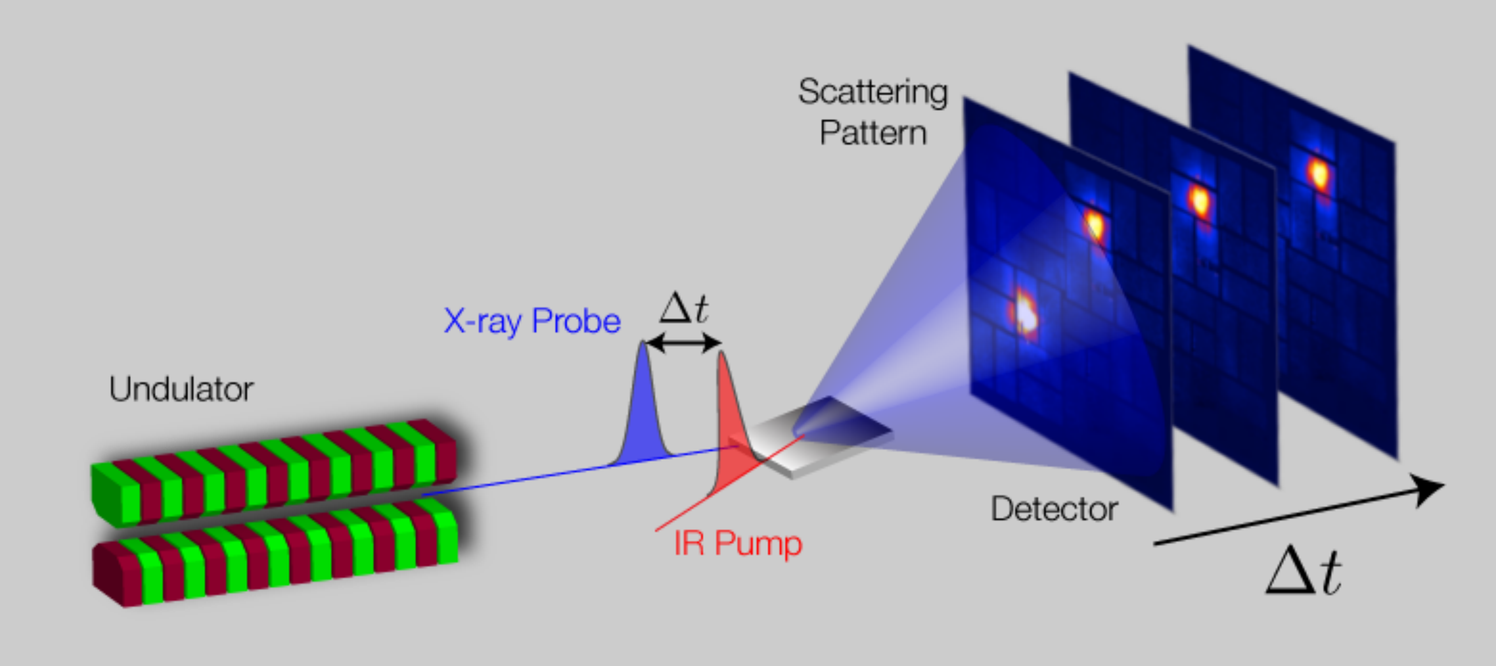
Samples are delivered to the beam in a liquid jet





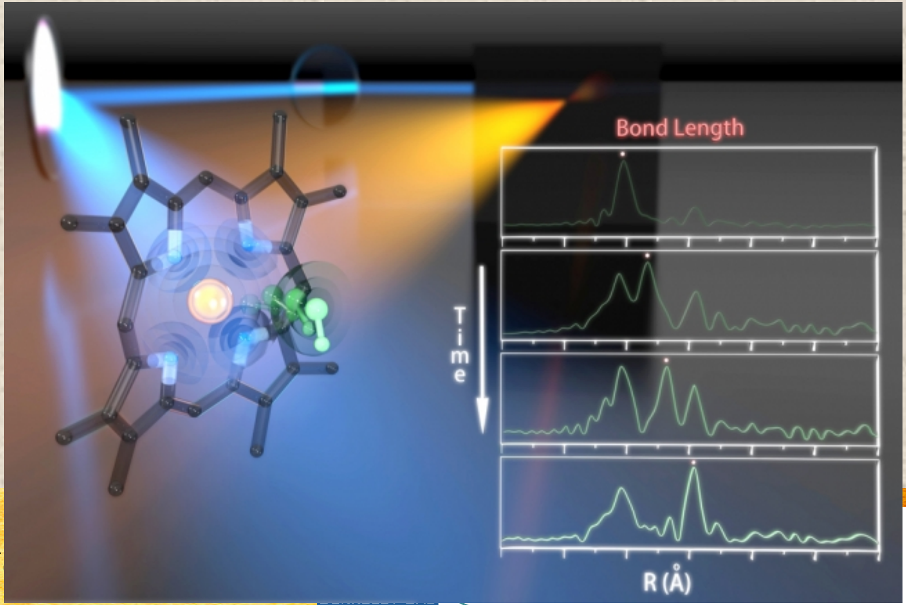
Dan Deponte, CFEL

Molecular Movies: X-ray Pump-Probe Techniques

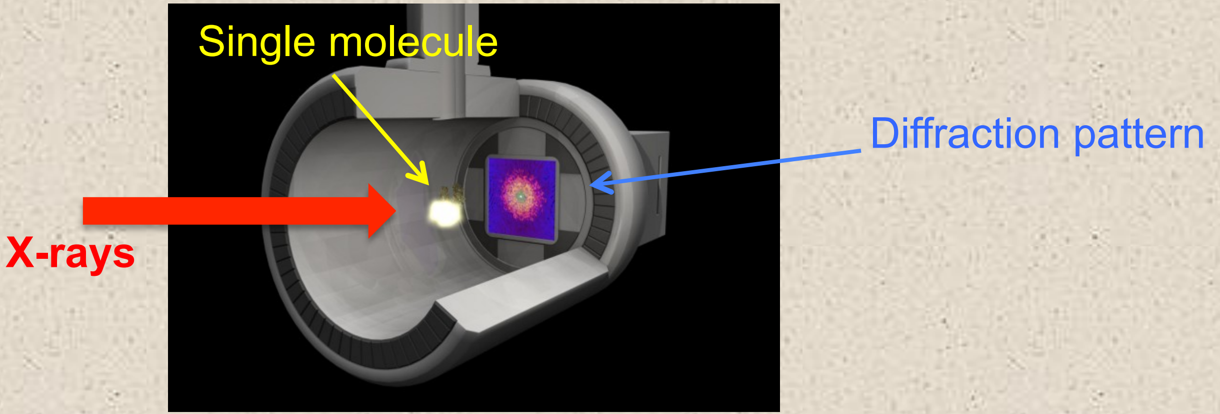


An input x-ray, optical, or THz pump can initiate an electronic or molecular motion. The x-ray probe measures the structure some time later.

Requires precision synchronization of pump and x-ray pulse.



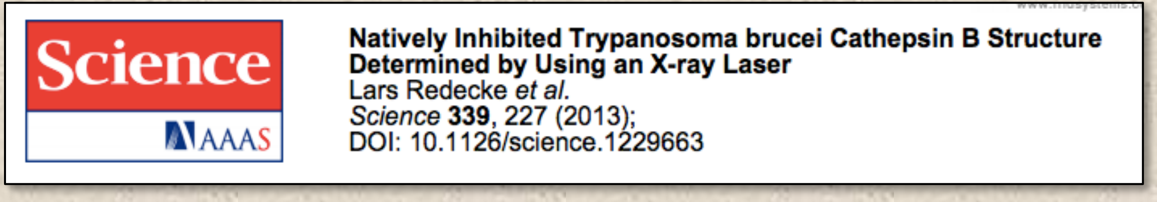
The dream of imaging single molecules!



… or at least really really small crystals: **nanocrystallography**

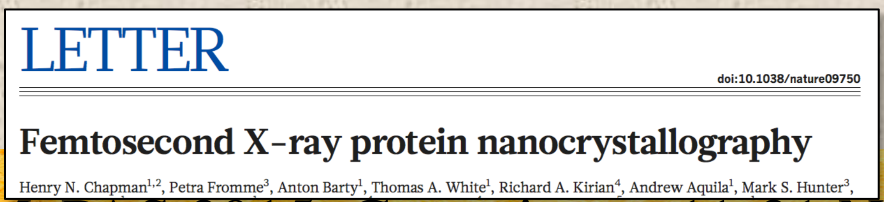
Simultaneous Femtosecond X-ray Spectroscopy and Diffraction of Photosystem II at Room Temperature

Jan Kern,[1,2] Roberto Alonso-Mori,[2] Rosalie Tran,[1] Johan Hattne,[1] Richard J. Gildea,[1]



Science AAAS

Natively Inhibited Trypanosoma brucei Cathepsin B Structure Determined by Using an X-ray Laser
Lars Redecke *et al.*
Science **339**, 227 (2013);
DOI: 10.1126/science.1229663

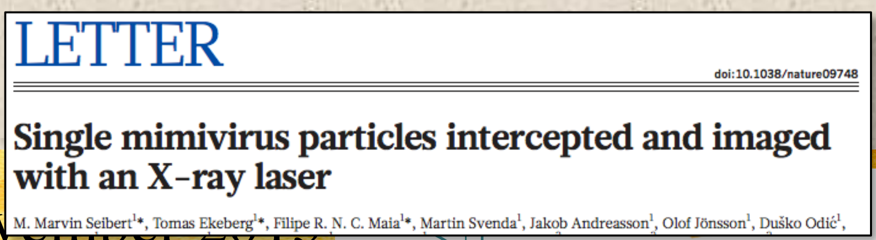


LETTER

doi:10.1038/nature09750

Femtosecond X-ray protein nanocrystallography

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],



LETTER

doi:10.1038/nature09748

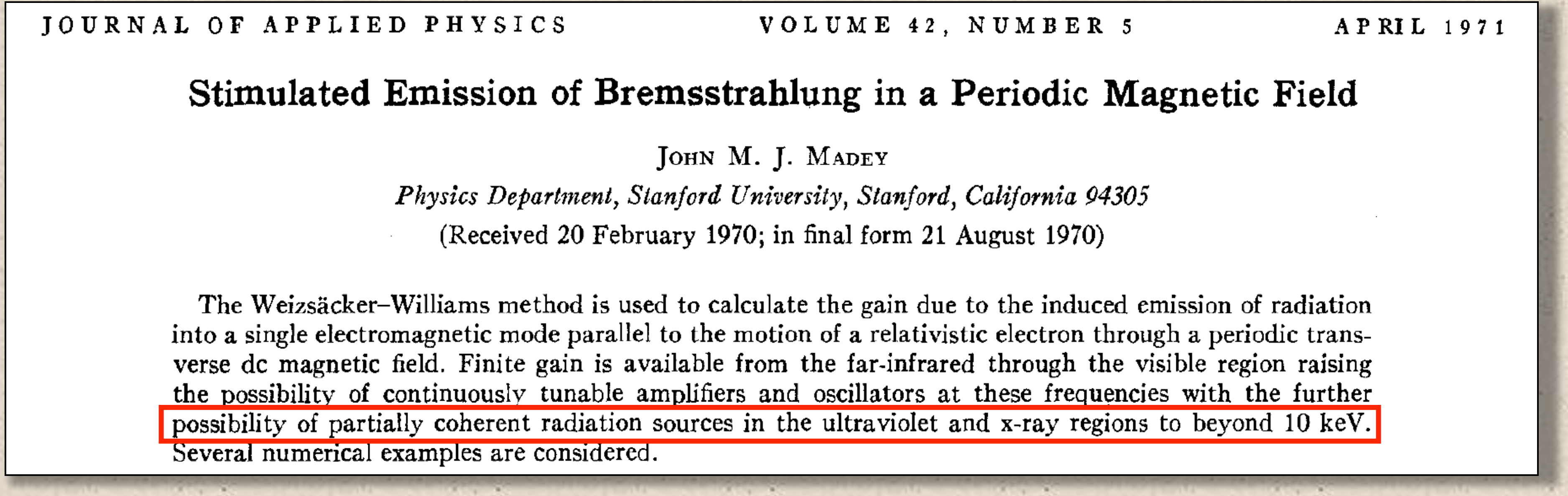
Single mimivirus particles intercepted and imaged with an X-ray laser

M. Marvin Seibert[1]*, Tomas Ekeberg[1]*, Filipe R. N. C. Maia[1]*, Martin Svenda[1], Jakob Andreasson[1], Olof Jönsson[1], Duško Odić[1],

Enter the FEL

The Free Electron Laser

John Madey, 1971



JOURNAL OF APPLIED PHYSICS VOLUME 42, NUMBER 5 APRIL 1971

Stimulated Emission of Bremsstrahlung in a Periodic Magnetic Field

John M. J. Madey
Physics Department, Stanford University, Stanford, California 94305

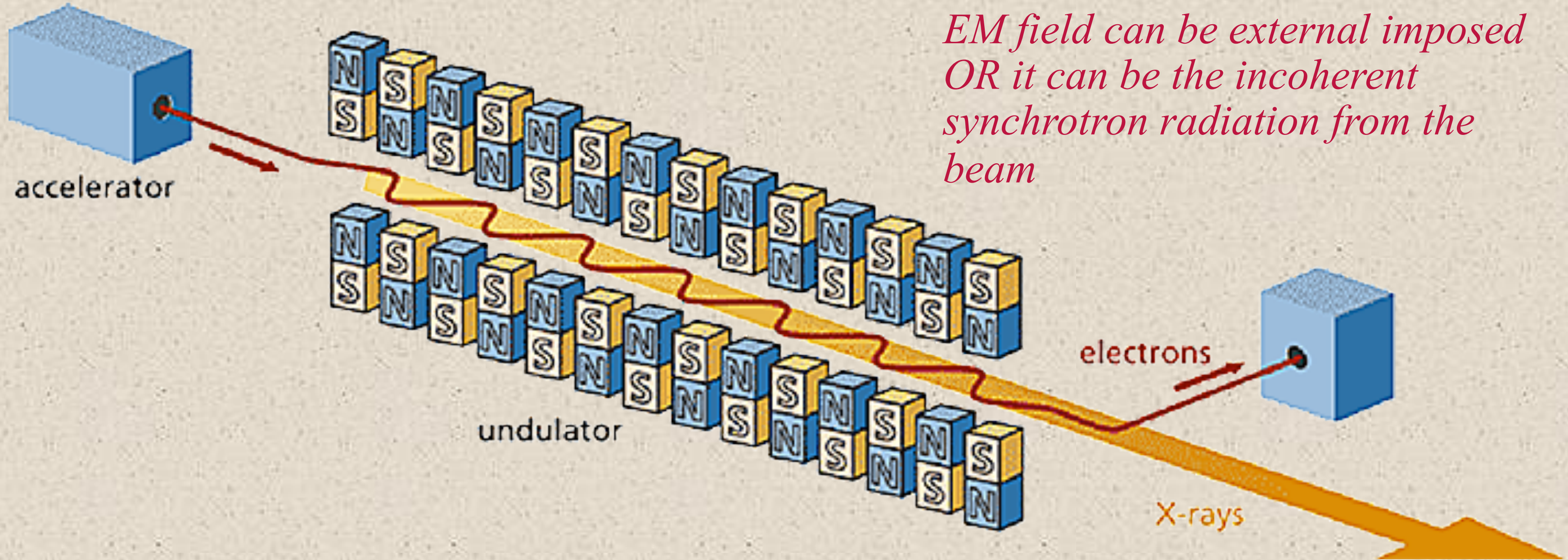
(Received 20 February 1970; in final form 21 August 1970)

The Weizsäcker–Williams method is used to calculate the gain due to the induced emission of radiation into a single electromagnetic mode parallel to the motion of a relativistic electron through a periodic transverse dc magnetic field. Finite gain is available from the far-infrared through the visible region raising the possibility of continuously tunable amplifiers and oscillators at these frequencies with the further possibility of partially coherent radiation sources in the ultraviolet and x-ray regions to beyond 10 keV. Several numerical examples are considered.

What is an FEL?

A beam of relativistic electrons co-propagating with **an optical field**
Through **a spatially periodic magnetic field**

- Undulator causes transverse electron oscillations
- Transverse electron velocity couples to E-component (transverse) of optical field giving *energy transfer*
- **Interaction between electron beam and optical field** causes *microbunching* of electron beam on scale of radiation wavelength, leading to *coherent emission of radiation*



EM field can be external imposed OR it can be the incoherent synchrotron radiation from the beam

Two types of FELs

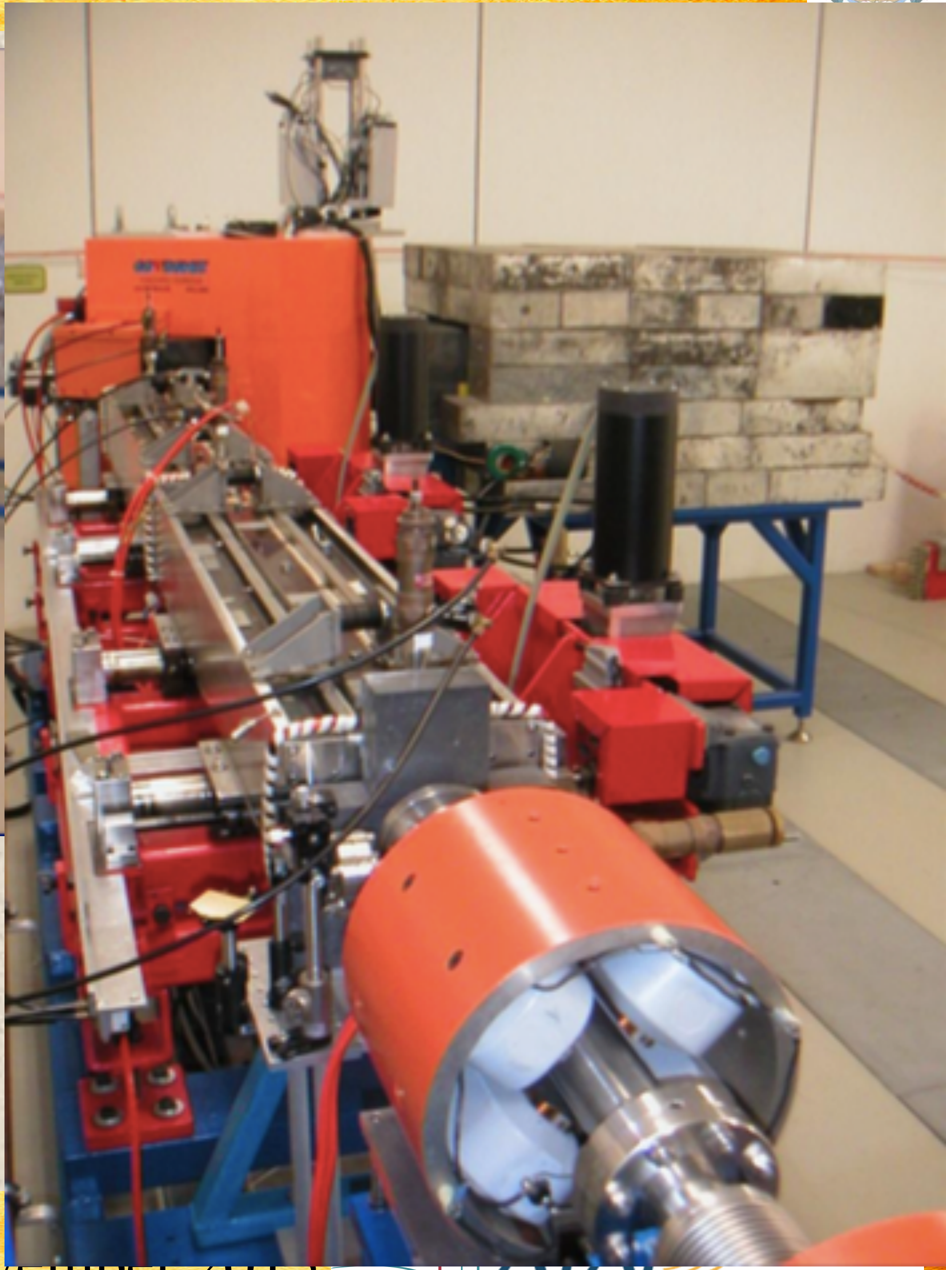
AMPLIFIER (HIGH GAIN) FEL

- Long undulator (no optical cavity *)
- Spontaneous emission from start of undulator interacts with electron beam.
- Interaction between light and electrons grows, producing microbunching
- Increasing intensity gives stronger bunching, yielding stronger emission
- High optical intensity achieved in **single pass (SASE)**

OSCILLATOR (LOW GAIN) FEL

- Short undulator
- Spontaneous emission trapped in an optical cavity
- Trapped light interacts with successive electron bunches leading to
- microbunching and coherent emission
- High optical intensity achieved over **many passes**

FELs can be small….



FELIX Facility, Rijnhuizen, The Netherlands

Or big!

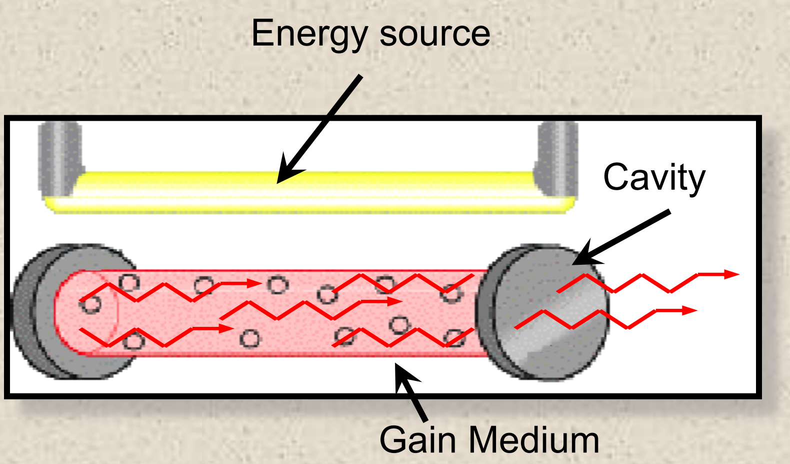
Laser Components

What makes a conventional laser special?

1. Spatial coherence
2. Temporal coherence (narrow bandwidth)
3. High brightness (flux/phase space area)

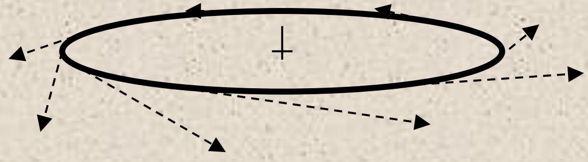
Components of a laser

1. Energy Source (e.g. flashlamp)
2. Radiation Source (electronic transition)
3. Wavelength Selection (gain medium):
4. Gain (oscillator cavity)



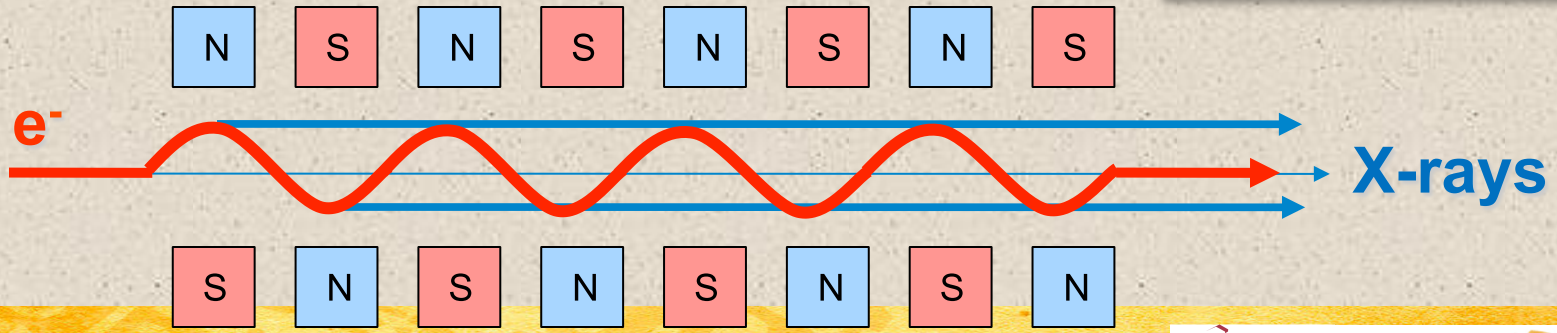
Free Electron Laser Basics: Radiation Source

- Bending high energy electrons ➔ X-rays



Synchrotron Radiation

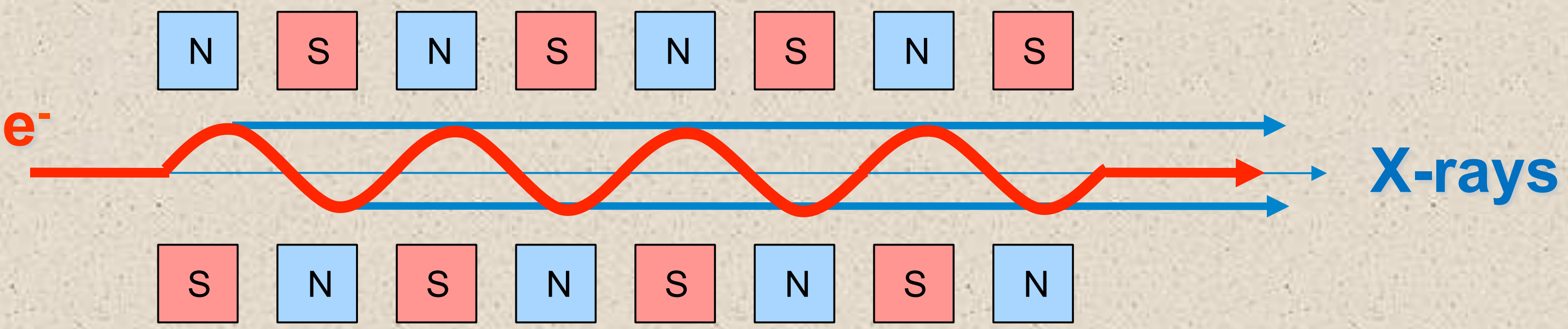
- Modern light sources use Undulators:

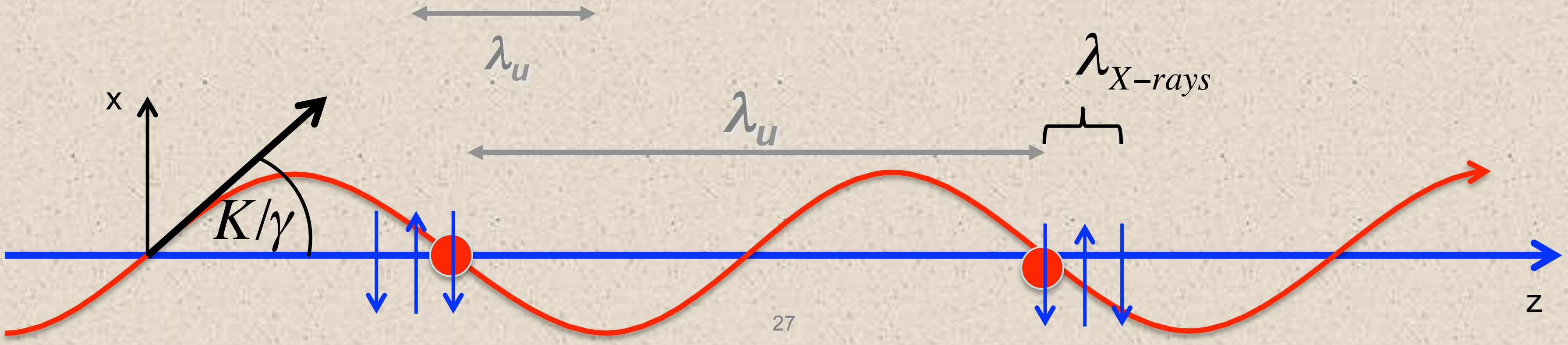


Free Electron Laser Basics: Resonant Condition

Resonant condition

- Electron slippage selects one radiation wavelength





Free Electron Laser Basics: Resonant Condition

Slippage from difference in speed:

$$\Delta z_{speed} = \lambda_u (1-\beta)$$

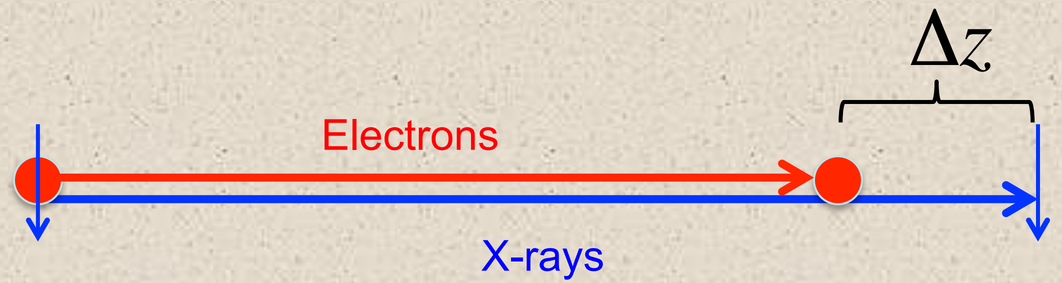
$$\Rightarrow \Delta z_{speed} \approx \frac{\lambda_u}{2\gamma^2}$$

Relativity review:

$$\beta \equiv v/c \qquad \gamma^2 = 1/\left(1-\beta^2\right)$$

$$\Rightarrow \beta \approx 1 - 1/2\gamma^2$$

e- energy = $\gamma m_e c^2$



Free Electron Laser Basics: Resonant Condition

Slippage from length of path:

$$\Delta z_{path} = L_{e-} - L_{X-ray}$$

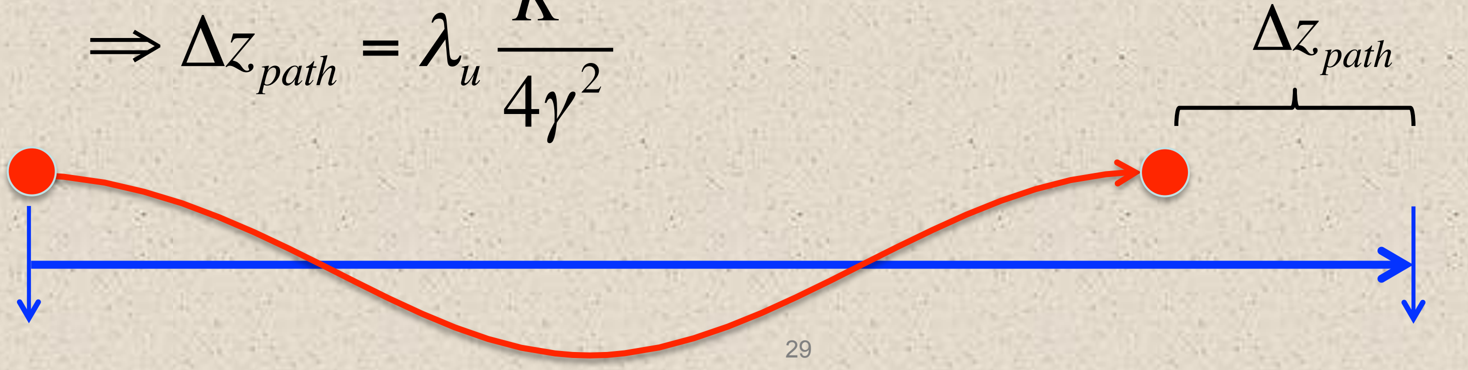
$$L_{X-ray} = \lambda_u$$ (One period)

Geometry review:

$$L_{e-} = \int_0^{\lambda_u} \sqrt{1 + K/\gamma \cos(k_u z)} \approx \lambda_u \left(1 + \frac{K^2}{4\gamma^2}\right)$$

$$K = eB_0/(mck_u) = 0.94 B_0[\text{Tesla}]\lambda_u[\text{cm}]$$

$$\Rightarrow \Delta z_{path} = \lambda_u \frac{K^2}{4\gamma^2}$$



Free Electron Laser Basics: Resonant Condition

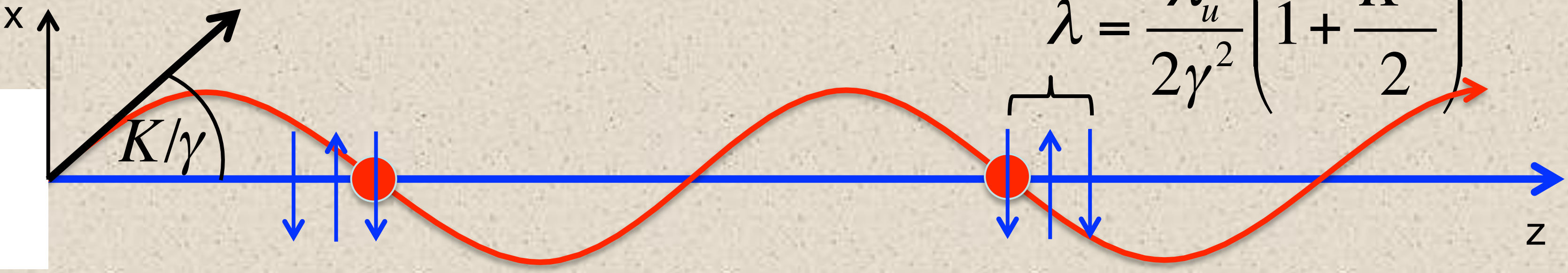
Total slippage:

(approximately) sum of path and speed effects

$$\Delta z_{path} = \lambda_u \frac{K^2}{4\gamma^2}$$

$$\Delta z_{speed} = \frac{\lambda_u}{2\gamma^2}$$

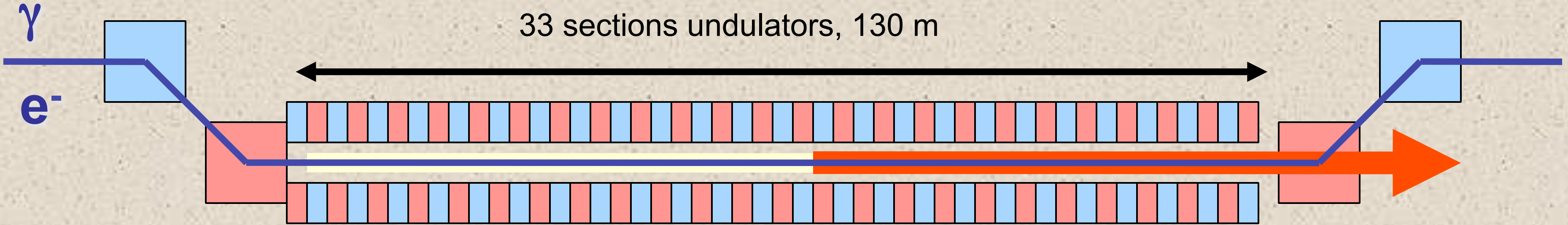
$$\longrightarrow \boxed{\Delta z = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2}\right)}$$



Free Electron Laser Basics: Gain

High Gain FEL: single pass for electrons

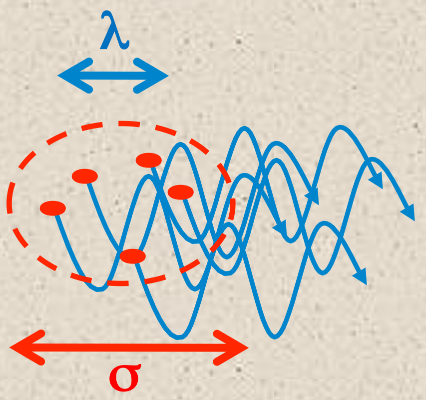
- No mirrors, no cavity
- LCLS uses ~3000 periods



Free Electron Laser Basics: Gain

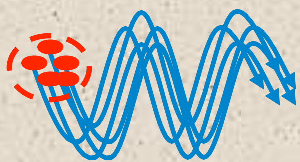
Radiation and bunching

Incoherent Bunch



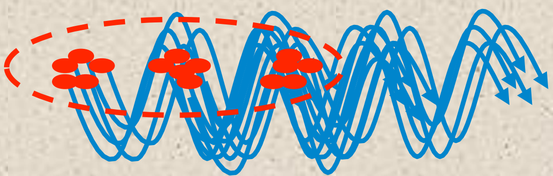
$$P_{rad} \propto N_e$$

Coherent Bunch



$$P_{rad} \propto N_e^2$$

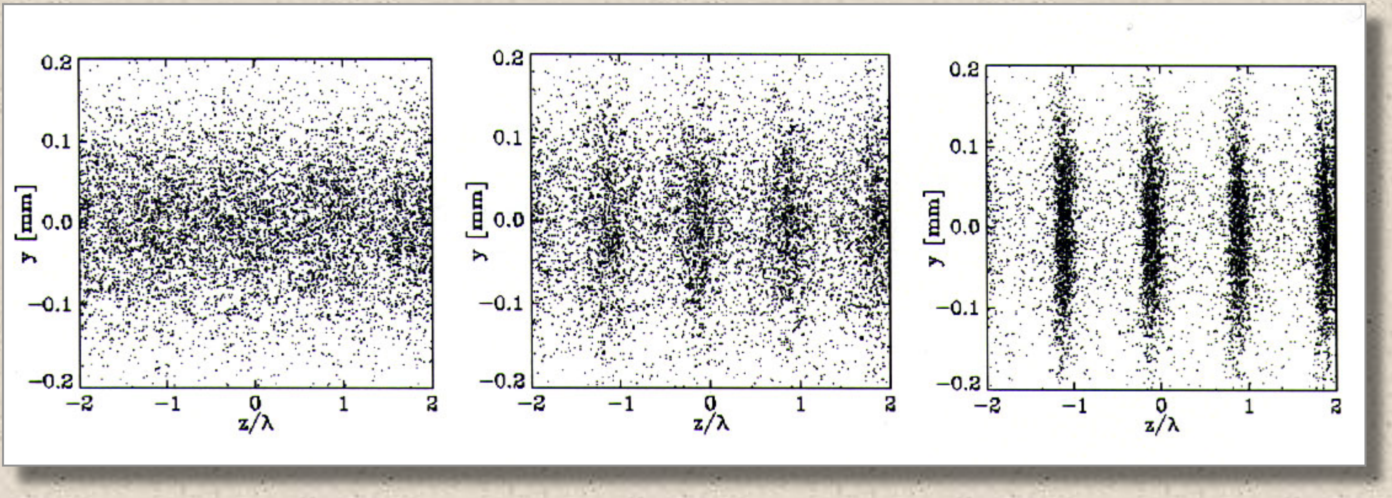
Microbunching



$$P_{rad} \propto N_e^2$$

Intro to FEL Theory

- Simulation of an X-ray FEL



Intro to 1D FEL Theory

Time for recap…

1. GeV electron beam is energy source and lasing medium
2. Undulators produce radiation
3. Resonant condition selects single wavelength
4. Microbunching occurs in a single pass
5. Brightness increases by factor of 10 billion!

Intro to 1D FEL Theory

Goal: solve for exponential X-ray growth

➔ describe evolution of 3 variables

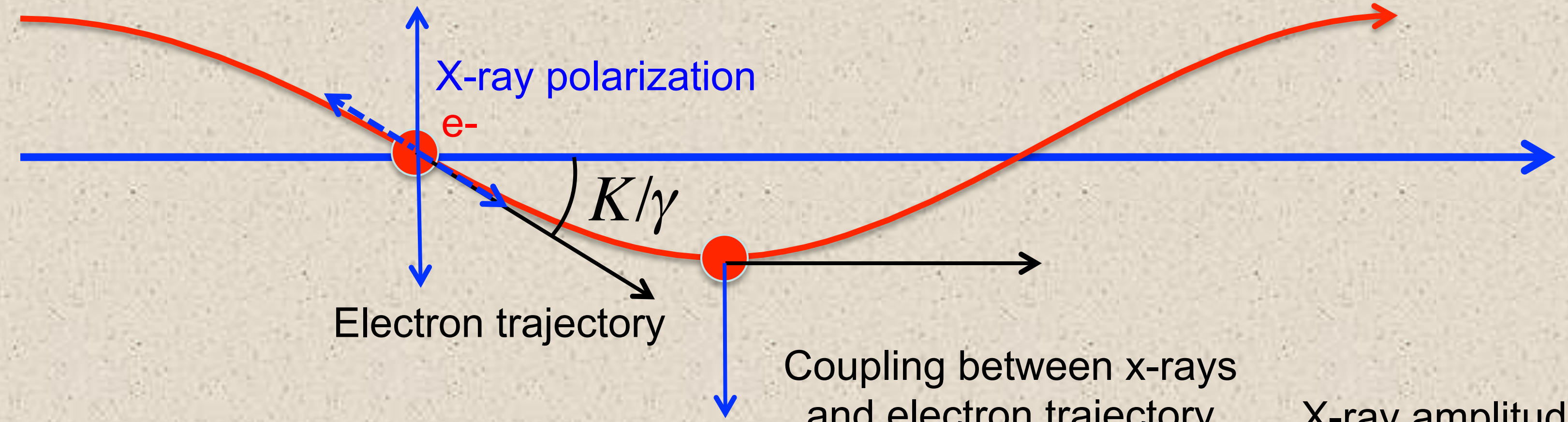
Electron energy $\eta=(\gamma-\gamma_0)/\gamma_0$

Electron phase $\theta=(k_r+k_u)z-\omega_r t$

X-ray amplitude $E=|\mathbf{E}_{\text{X-ray}}|$

Intro to 1D FEL Theory

Electron energy $\eta=(\gamma-\gamma_0)/\gamma_0$



Electron trajectory

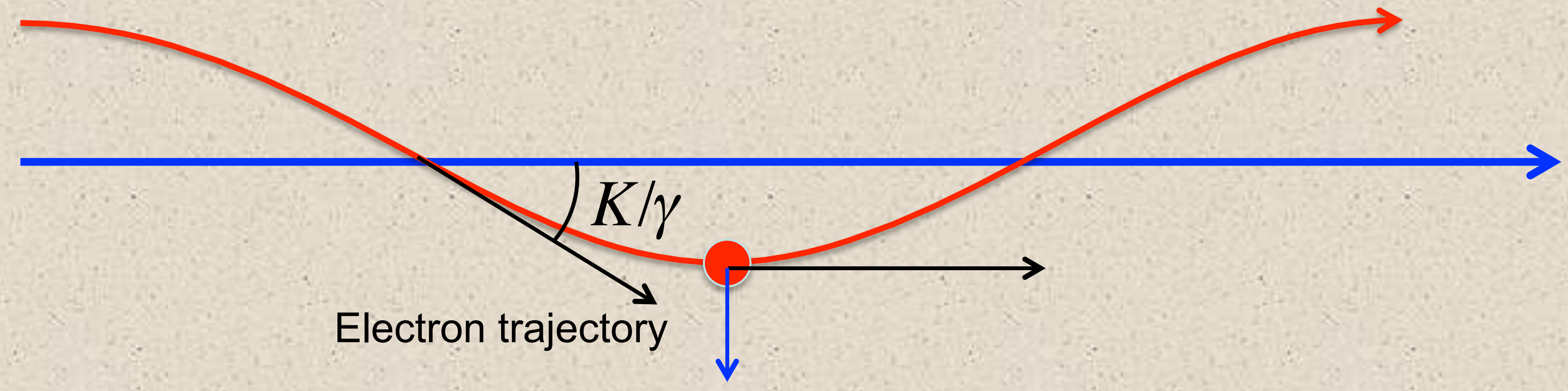
Instantaneous change in energy:

$$\frac{d\eta}{dz}=\frac{eEK}{\gamma^2mc^2}\overbrace{\cos\left[k_uz\right]}^{\text{Coupling between x-rays and electron trajectory}}\overbrace{\cos\left[kz-\omega t+\phi\right]}^{\text{X-ray amplitude}}$$

$$=\frac{eEK}{2\gamma^2mc^2}\cos\underbrace{\left[(k+k_u)z-\omega t+\phi\right]}_{=\delta+\pi/2}\quad+\quad\ldots$$

Intro to 1D FEL Theory

Electron energy $\eta=(\gamma-\gamma_0)/\gamma_0$



Instantaneous change in energy:

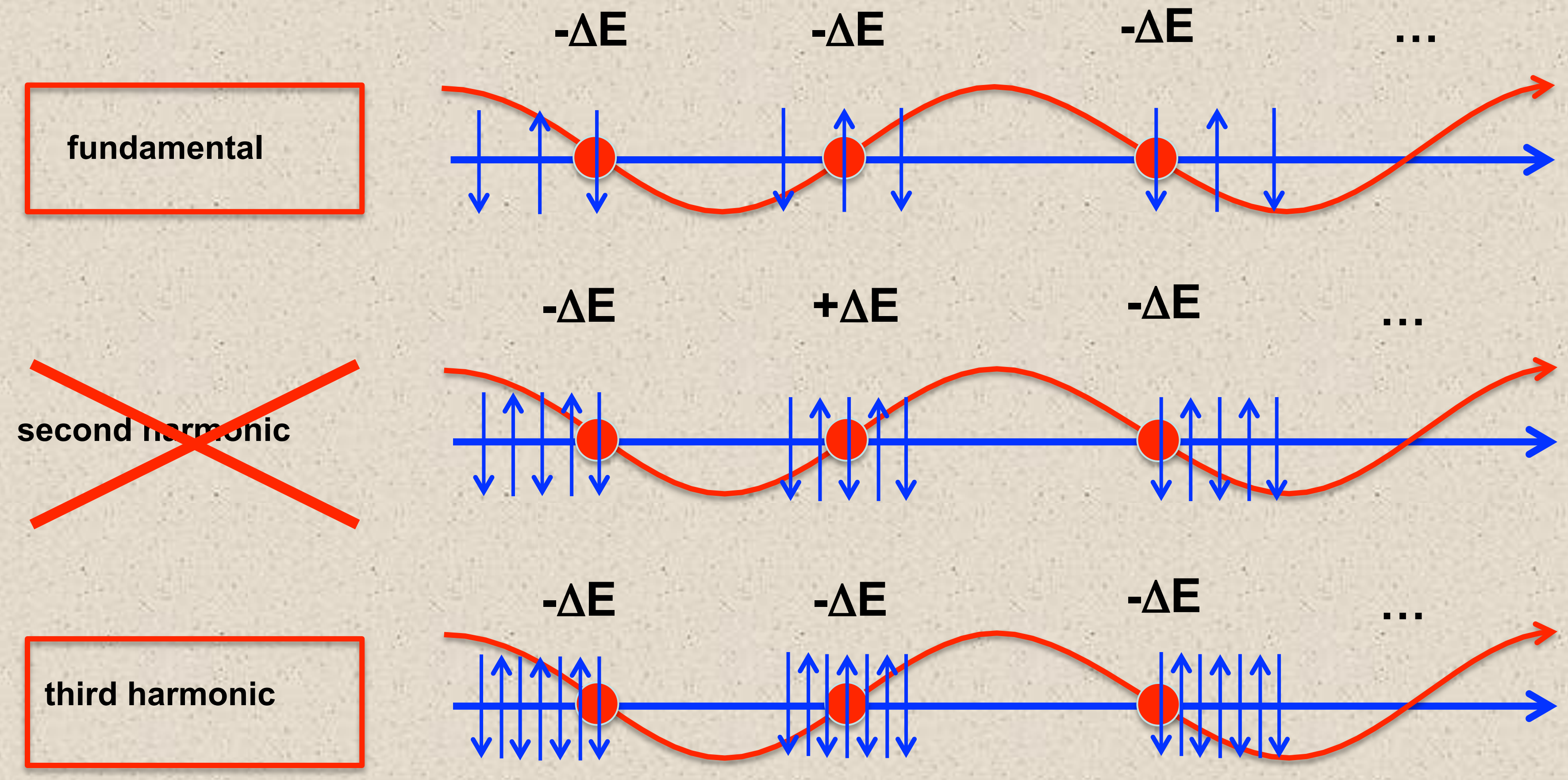
$$\frac{d\eta}{dz}=\frac{eEK}{2\gamma^2}\cos\left[\theta+\pi/2\right]$$

Position in the bunch

Position in accelerator ~ time

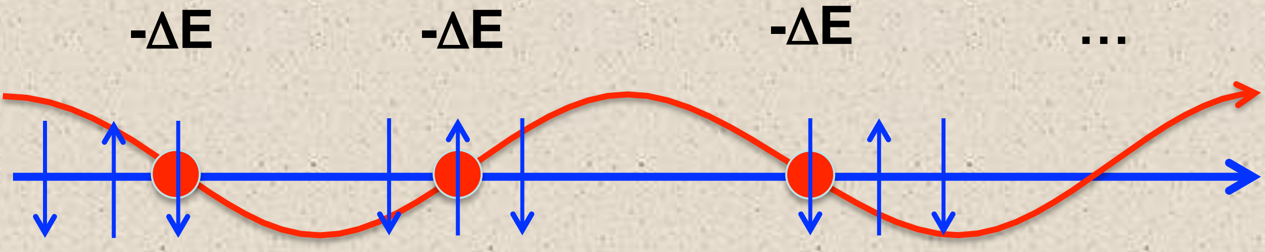
Free Electron Laser Basics: Resonant Condition

Undulator harmonics



Intro to 1D FEL Theory

Electron energy $\eta=(\gamma-\gamma_0)/\gamma_0$



Instantaneous change:

$$\frac{d\eta}{dz}=\frac{eEK}{2\gamma^2}\cos\left[\theta+\pi/2\right]$$

Wiggle averaged change:

$$\boxed{\frac{d\eta}{dz}=\chi_1 E\sin\theta}$$

$$\chi_1=\frac{eK[\mathrm{JJ}]}{(2\gamma_0^2 mc^2)}$$

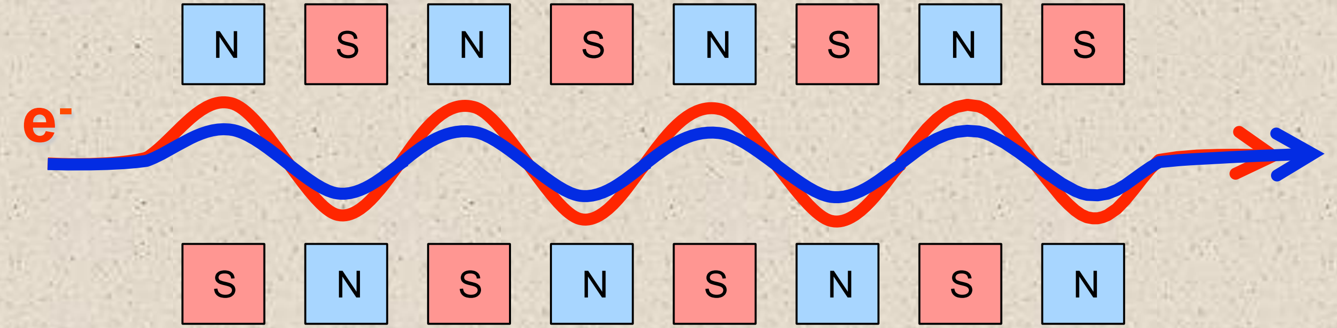
$$[\mathrm{JJ}]=J_0\left(\frac{K^2}{4+2K^2}\right)-J_1\left(\frac{K^2}{4+2K^2}\right)$$

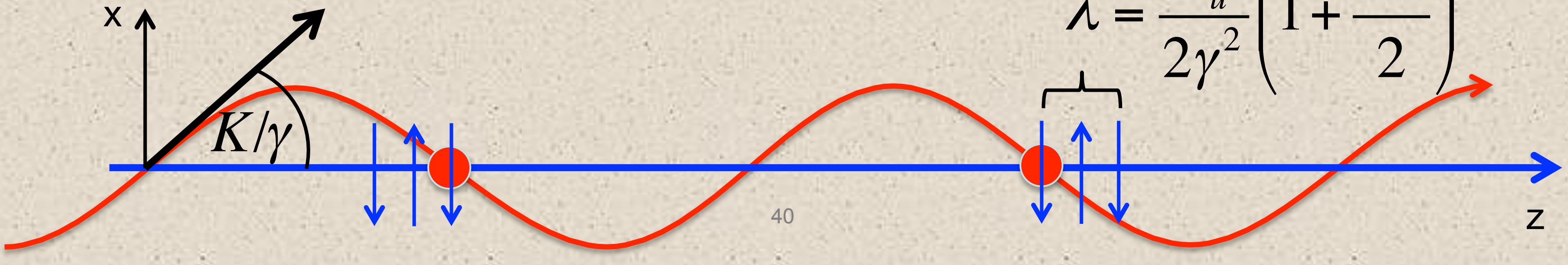
(planar undulator)

Intro to 1D FEL Theory

Electron phase $\theta=(k_r+k_u)z-\omega_r t+\pi/2$

Dispersion in accelerators





$$\lambda=\frac{\lambda_u}{2\gamma^2}\left(1+\frac{K^2}{2}\right)$$

An FEL is a feedback of the beam interacting with its own radiation

- The current creates an EM field (or adds to an external field)

$$\frac{dA}{dt} = -J\left\langle e^{-ix} \right\rangle$$

- Therefore the beam can couple to itself non-linearly to begin bunching the beam
  - Bunching comes from the non-linear terms in the pendulum equation
- Fields ==> Acceleration ==> Radiation ==> Fields ==> Acceleration ==> Radiation ==> Fields ==> Acceleration ==> Radiation ==> Fields ==> **ETC**
- This description is the pendulum model of the free electron laser

The pendulum equation of the FEL

- The equation of motion for individual electrons in an EM-field:

$$\frac{d^2x}{dt^2} = |A|\sin(x+\varphi)$$

- Is coupled to the wave equation for the electromagnetic field.

$$\frac{dA}{dt} = -J\left\langle e^{-ix}\right\rangle$$

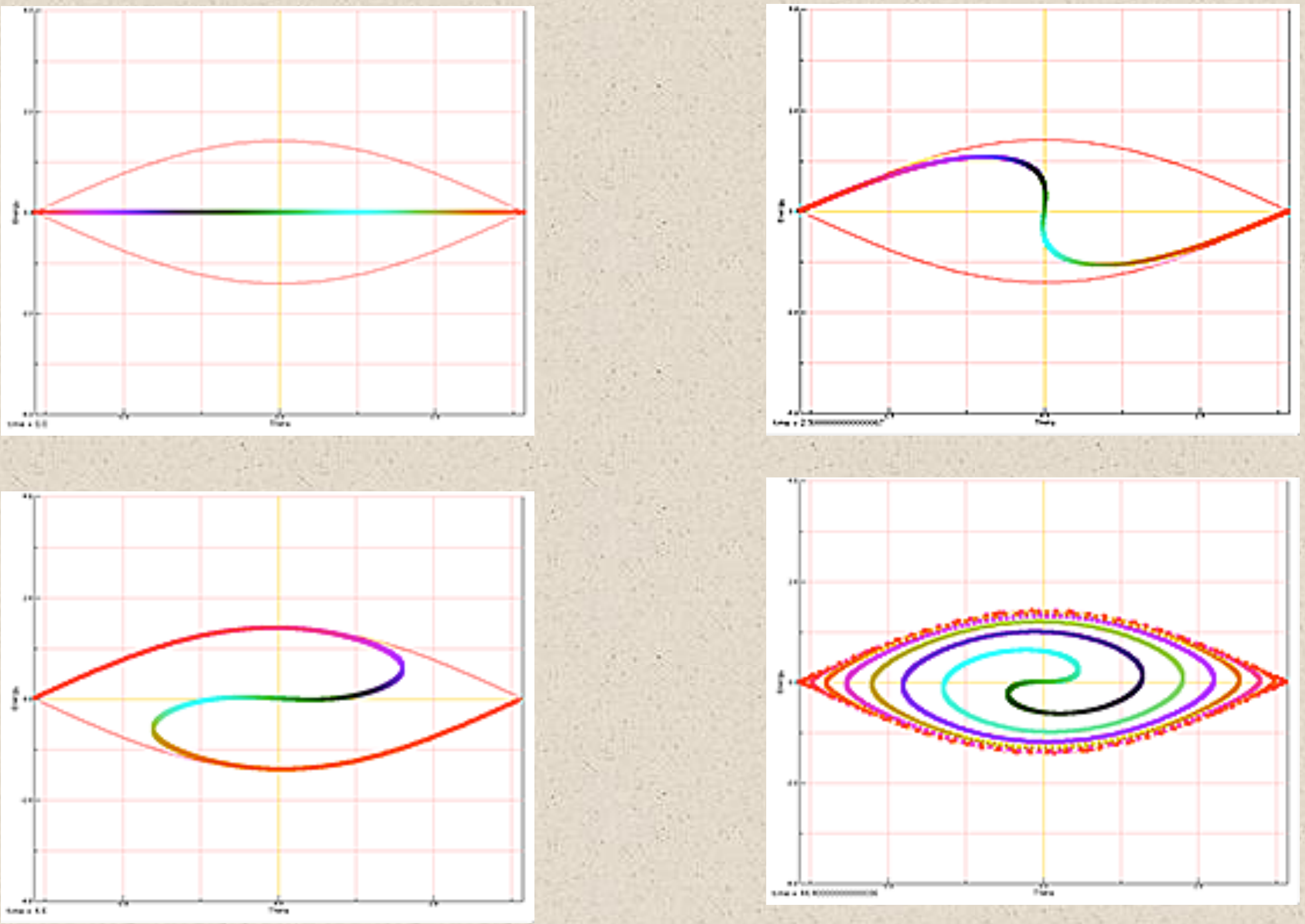
- Non-dimensional parameters, A and J, are proportional to the optical field strength and the current density, respectively.
  - The current density, J, determines the rate of change of the laser field, A.
  - The EM field phase, ϕ, is the phase of the complex scalar, A.
  - The electron phase, x, with respect to the EM and wiggler field is

$$x = (k_w - k)\, z - \omega t.$$

A simulation will show us the bunching & signal growth

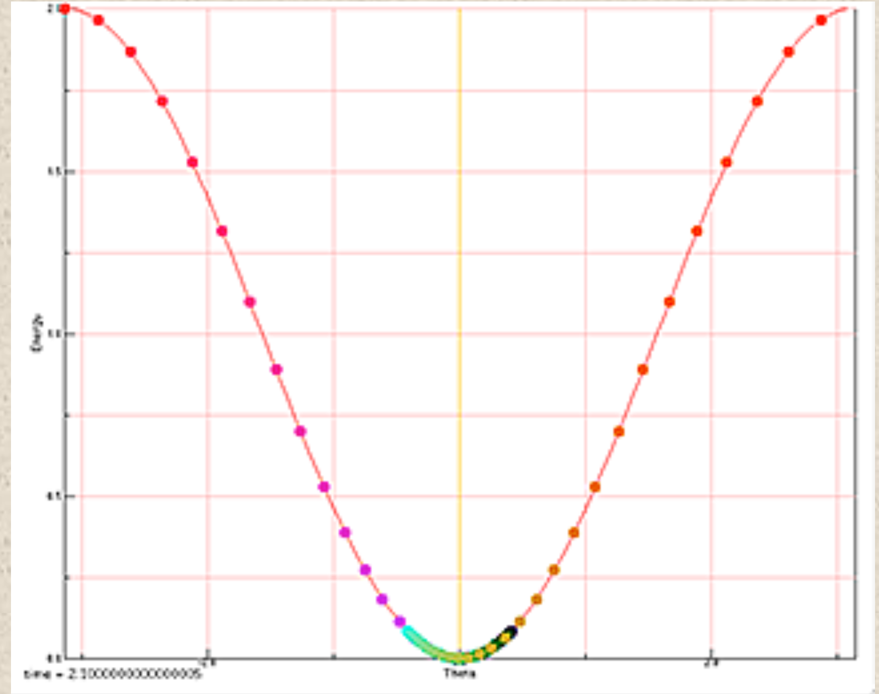
Ex. 1) Turn off the coupling: J = 0

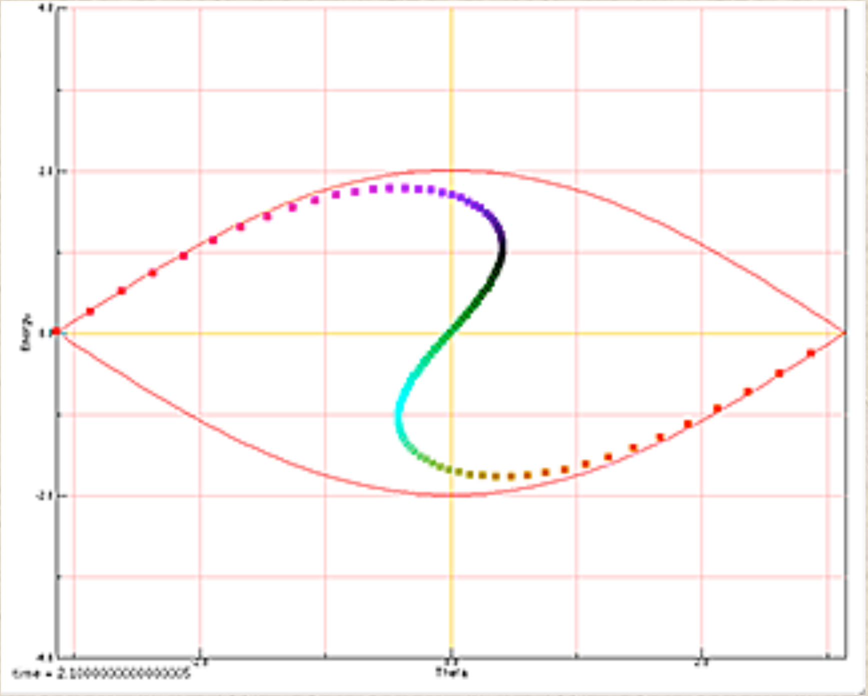
Synchrotron oscillations in the rf-bucket



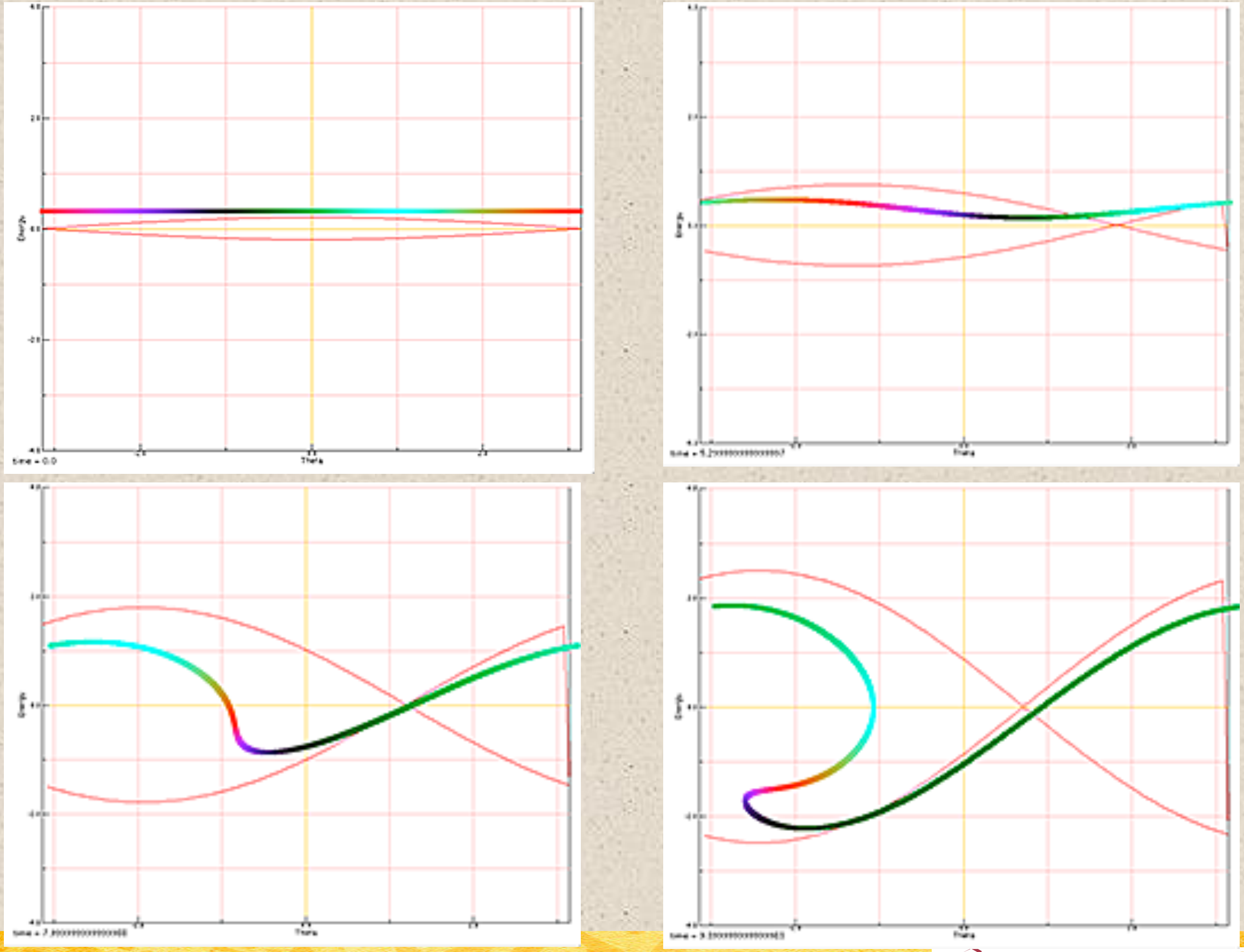
http://webphysics.davidson.edu/applets/felpart/felode.html

Bunching comes from the non-linearity of the pendulum equation



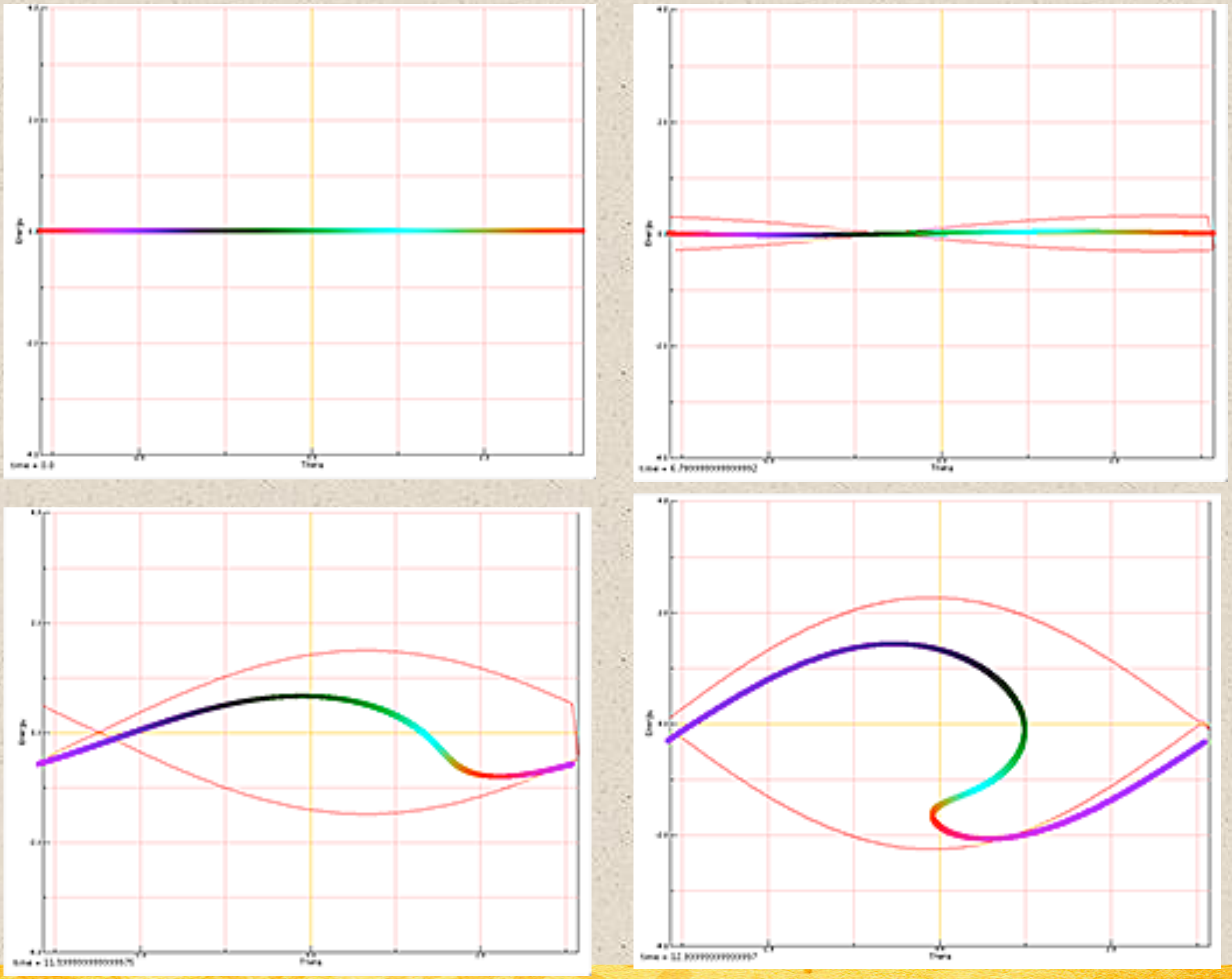


As particles radiate the separatrix grows and bunches the beam



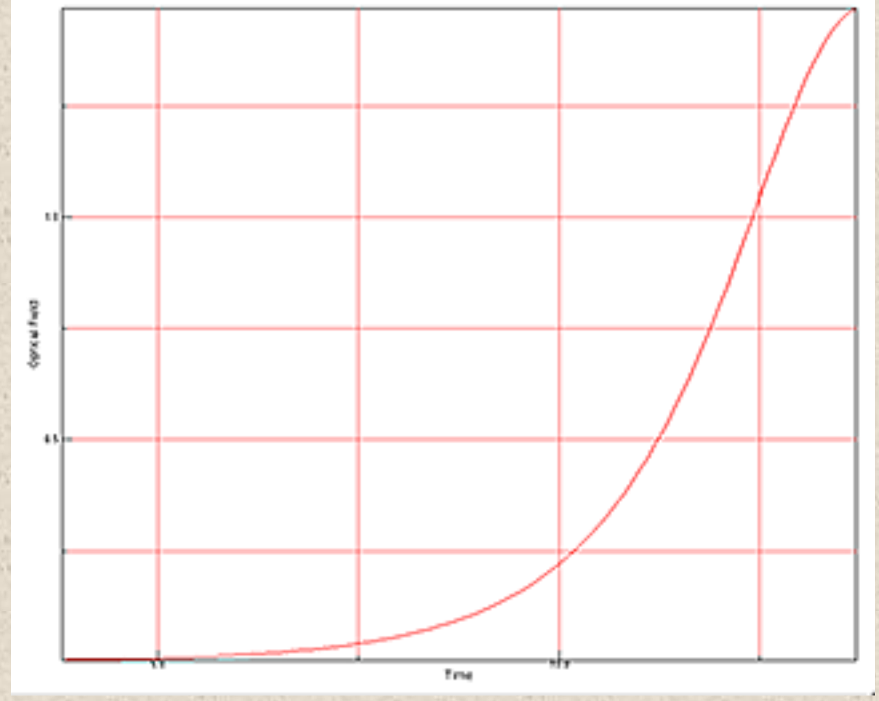
The FEL can start spontaneously

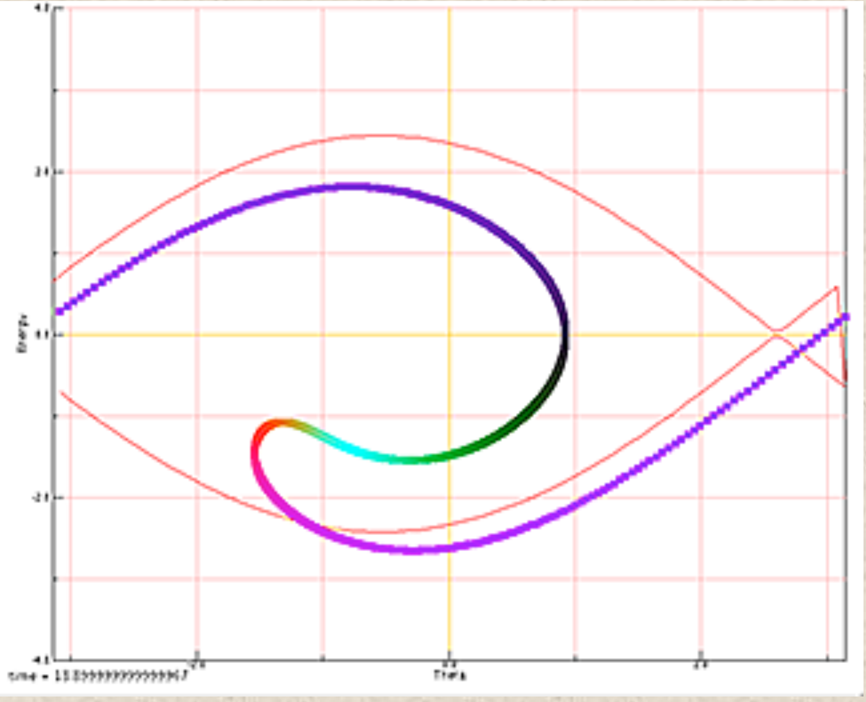
from incoherent synchrotron radiation



The optical field

grows exponentially to saturation



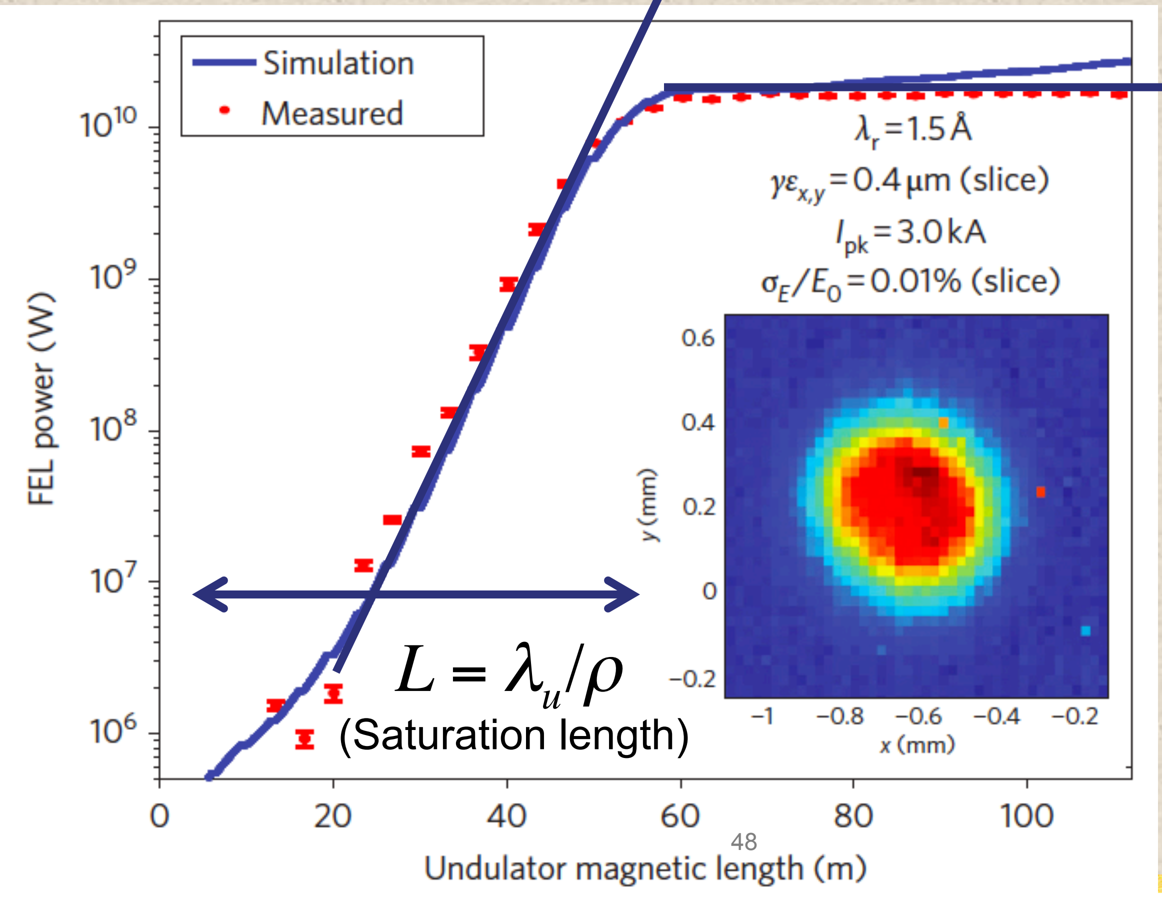


The beam has lost energy to the field

FEL Optical field grows exponentially

Exponential growth until saturation

$$L_{G0} = \frac{\lambda_u}{4\pi\sqrt{3}\rho}$$ (Gain length)



$$L = \lambda_u/\rho$$

(Saturation length)

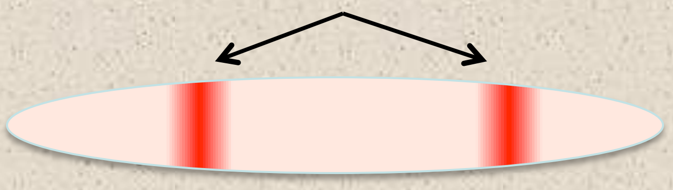
$$P_{X-rays} = \rho P_{e-}$$

(Power)

SASE FELs start growth from shot noise

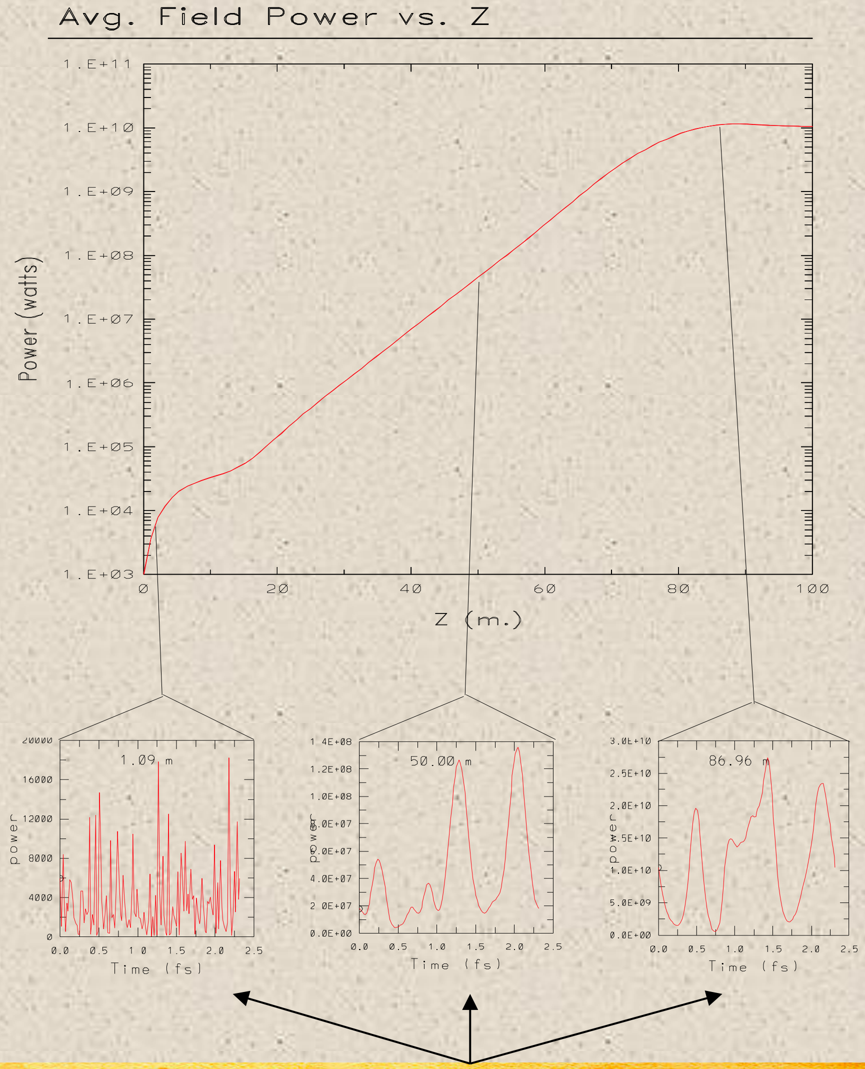
Implications of shot noise

Different slices don't communicate



Each slice lases independently!

Upshot: SASE FELs have complicated temporal structure



1 % of X-Ray Pulse Length

Intro to SASE FELs

Summary

1. Studied evolution of the three FEL parameters (electron position and energy, X-ray amplitude)

2. Found exponentially growing X-ray power

3. …But some complications for starting the SASE process