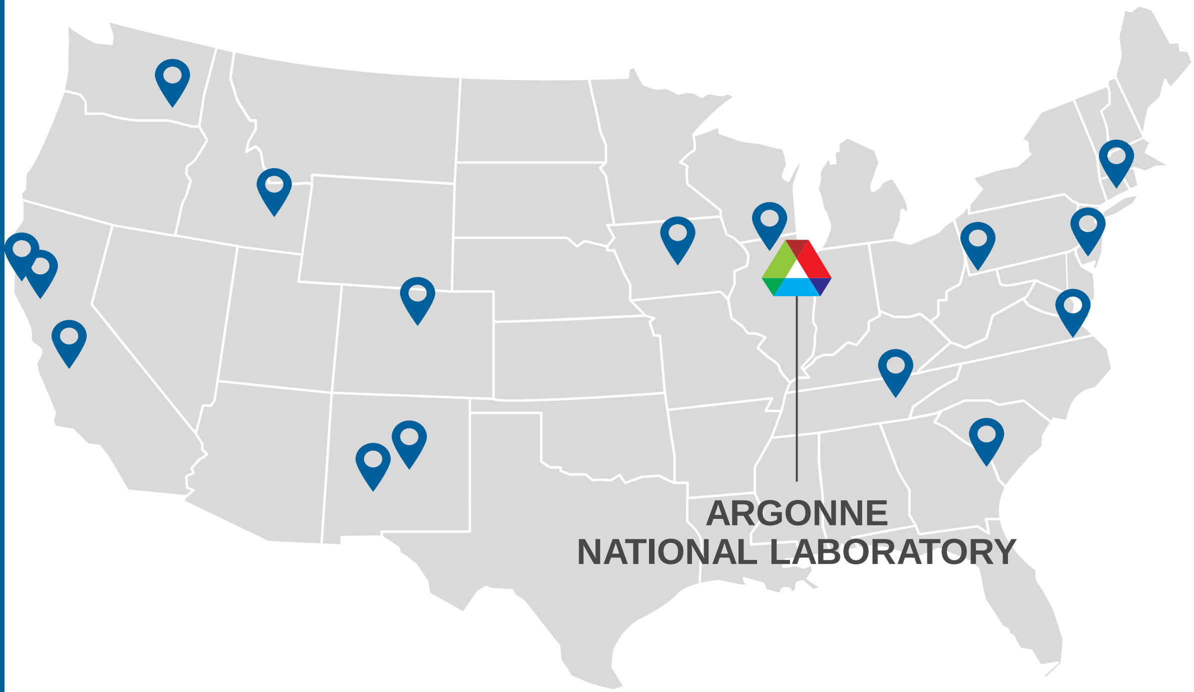
WELCOME & OVERVIEW OF

ADVANCED PHOTON SOURCE (APS)

LAURENT C. CHAPON
Associate Laboratory Director for Photon Sciences
Advanced Photon Source Director

ARGONNE NATIONAL LABORATORY



Contractor
- UChicago Argonne LLC

Physical assets
- 1,517 acres
- 156 buildings

Human capital
- 3,500 FTE employees
- 500+ students
- 8,035 facility users

Location
- Lemont, Illinois, near Chicago

Type
- Multiprogram laboratory

We integrate our domain strengths to achieve impactful team science and engineering

Advanced Energy Technologies

- Applied materials
- Energy systems and infrastructure analysis
- Transportation and power systems

Computing, Environment & Life Sciences

- Applied mathematics & computer science
- Computational science
- Data science & learning
- Biosciences
- Environmental science

Physical Sciences & Engineering

- Chemical sciences & engineering
- Materials science
- Nanoscience & nanotechnology
- Nuclear & particle physics

Photon Sciences

- X-ray science
- Accelerator systems & engineering

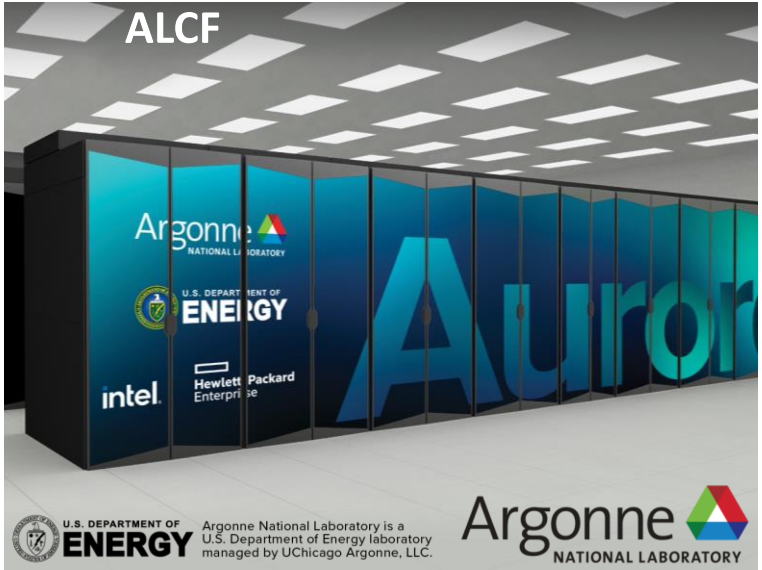
Nuclear Technologies and National Security

- Chemical & fuel cycle technologies
- Decision & infrastructure sciences
- Nuclear science & engineering
- Strategic security sciences

Science and Technology Partnerships and Outreach


ARM


APS


ALCF
Argonne
U.S. DEPARTMENT OF ENERGY
Hewlett Packard Enterprise
intel
U.S. DEPARTMENT OF ENERGY
Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.
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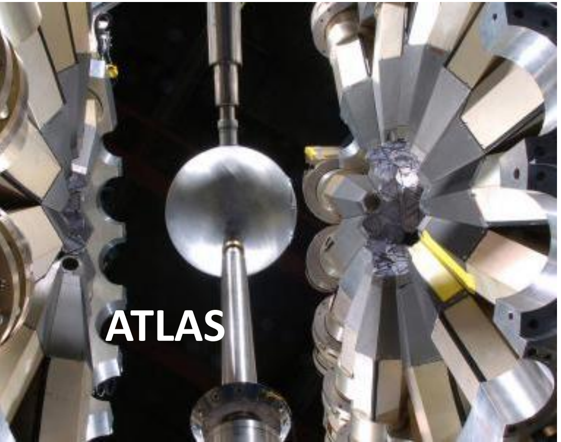
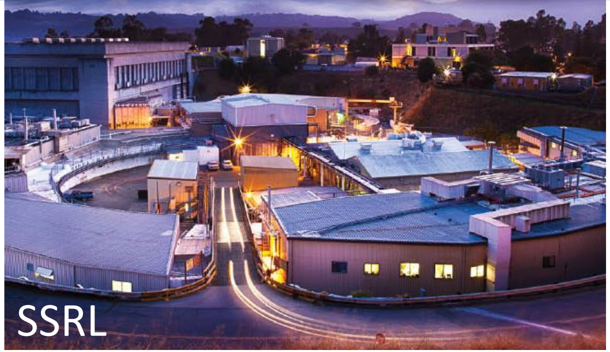
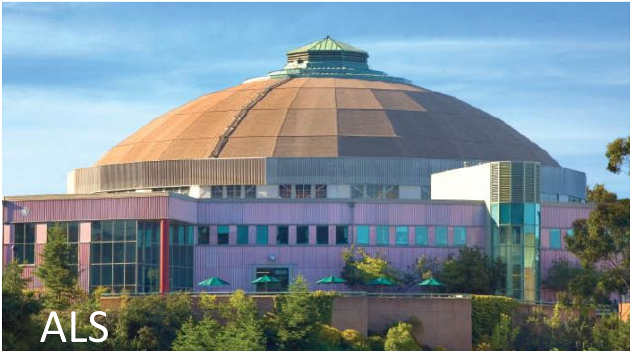

ATLAS


CNM





Basic Energy Science – DOE light sources

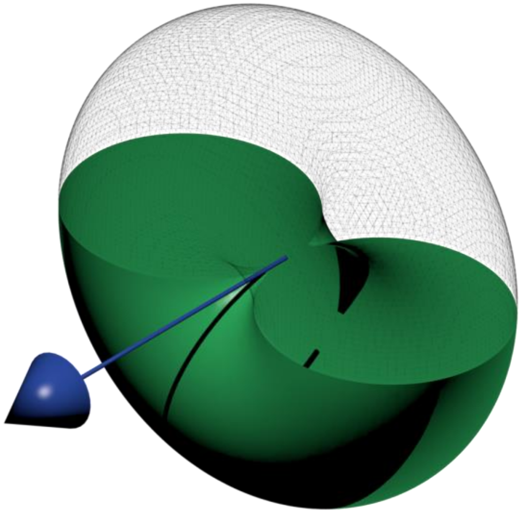
U.S. DEPARTMENT OF ENERGY
Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

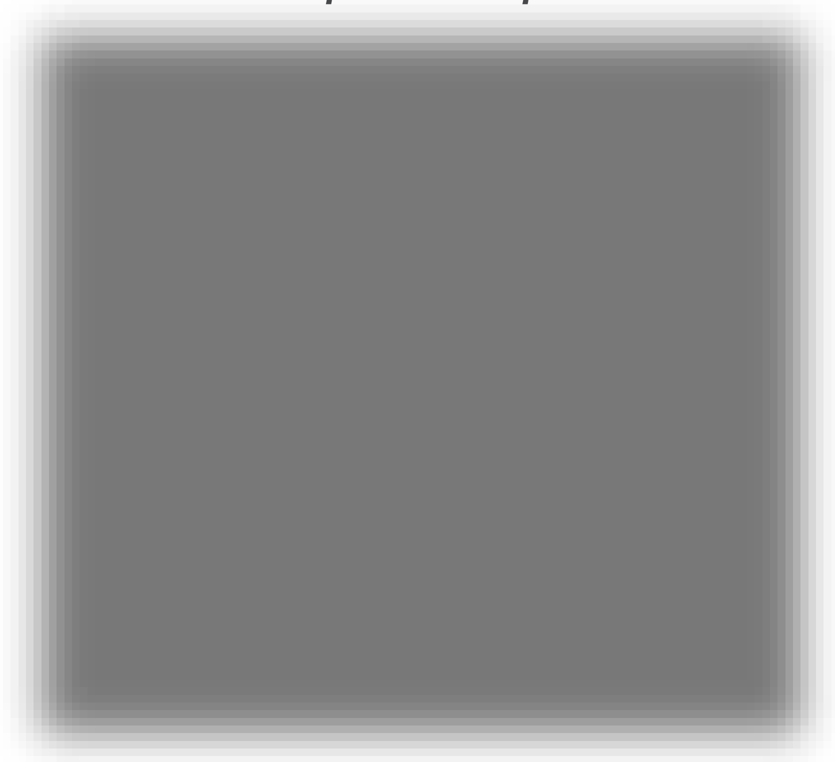
Argonne NATIONAL LABORATORY

RADIATION FROM ACCELERATED CHARGES

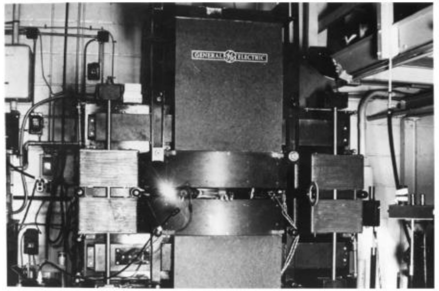
From β=0 to β~1

$$\beta = \frac{v}{c}$$





Jackson "Classical Electromagnetism"



General Electric Research Lab

1947

APS

3rd Generation (1994-2007)

1995

APS-U

2024

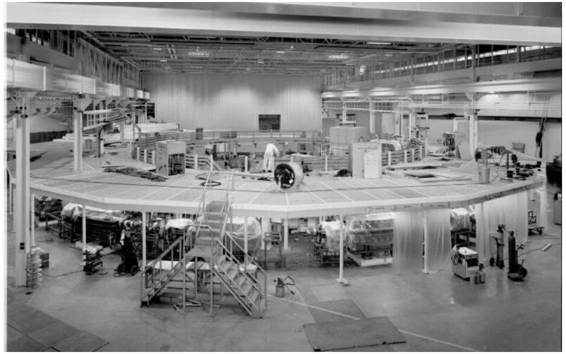
1945 | 1952 | 1959 | 1966 | 1973 | 1980 | 1987 | 1994 | 2001 | 2008 | 2015 | 2022

Today

1981

2nd Generation (1981-1986)

SRS



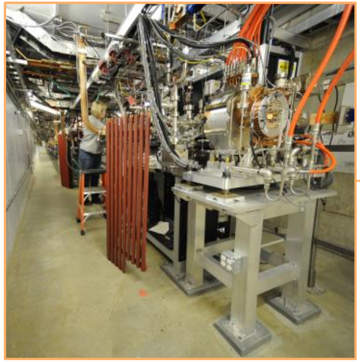
2016

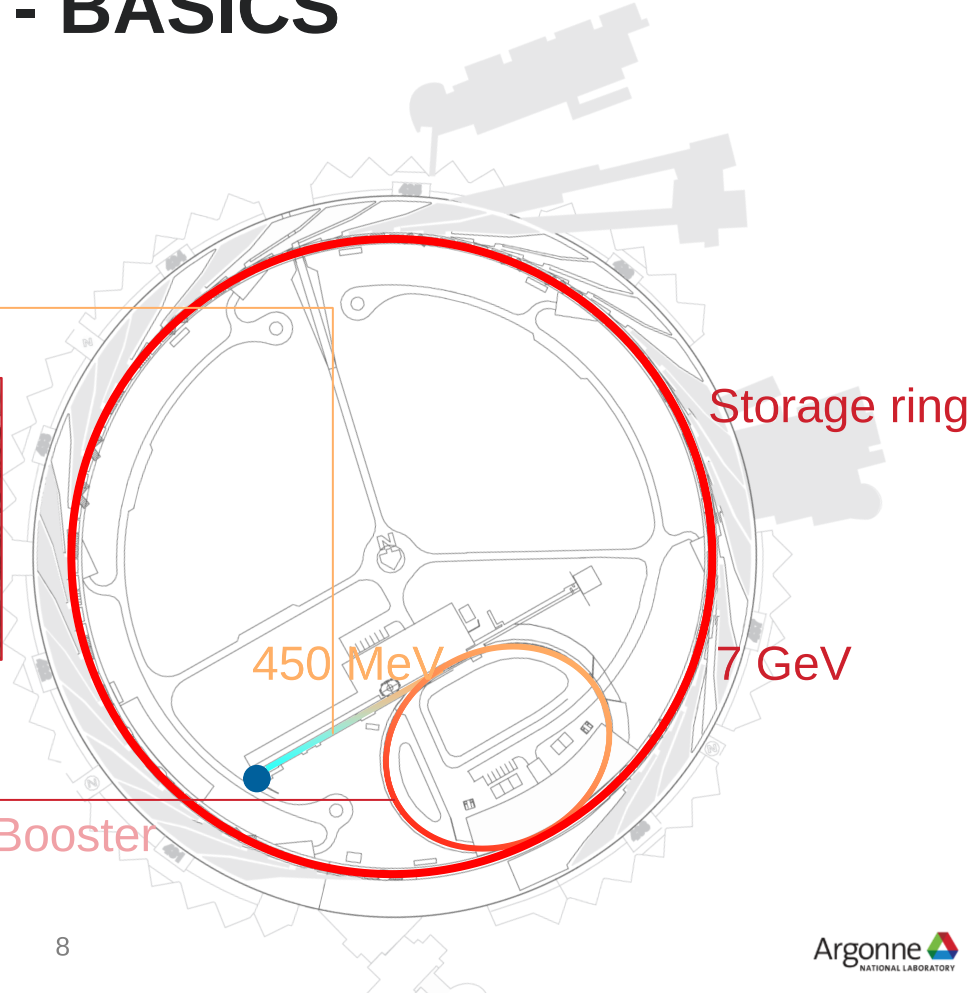
4th Generation (2016- ...)

Max-IV

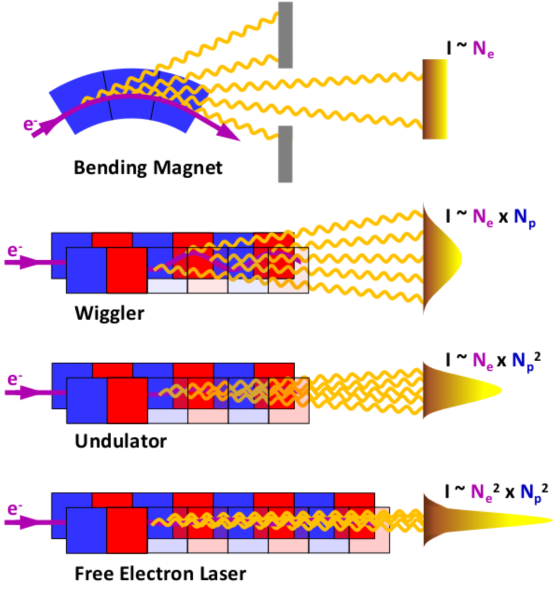
For early history : Blewett, J. P. (1998). 50 YEARS OF SR Synchrotron Radiation ± Early History. *Journal of Synchrotron Radiation*, *5*, 135–139.

X-RAY SYNCHROTRON - BASICS





SOURCES



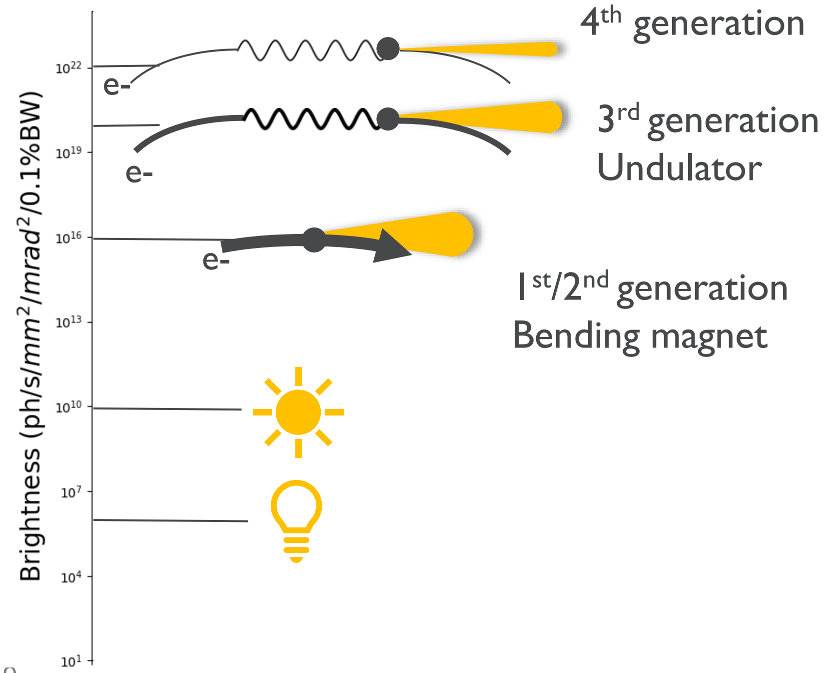
Anatoly Shabalin, PhD thesis

Flux

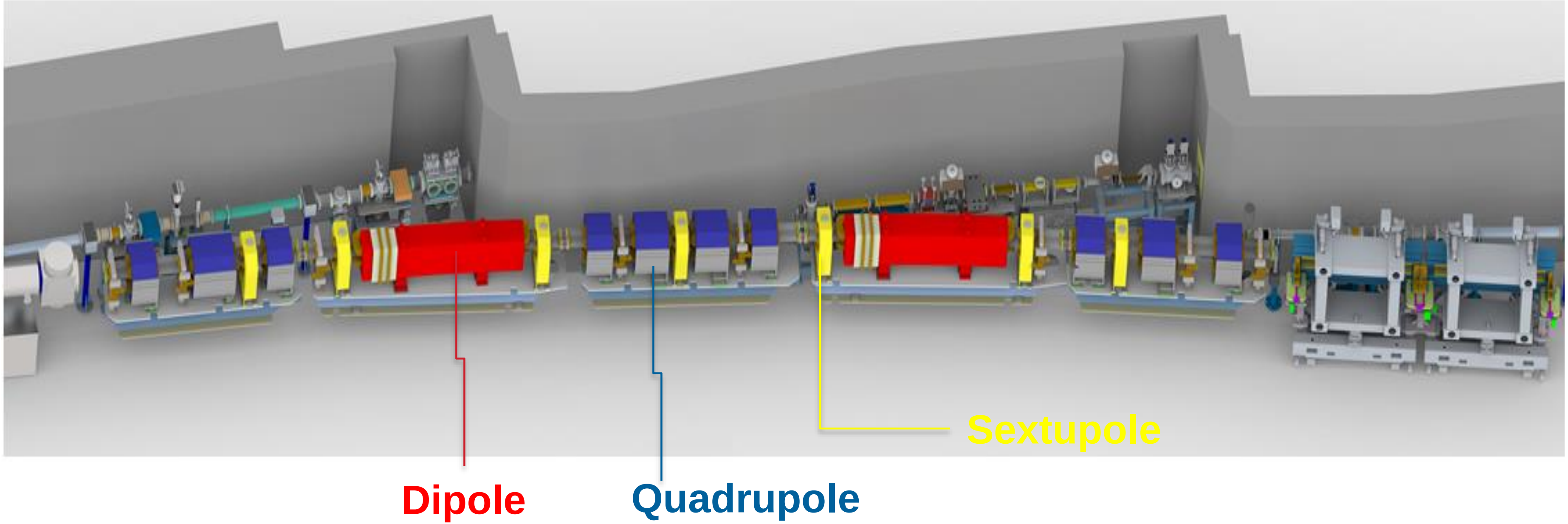
$$\boxed{\Phi = \frac{n_{ph}}{\Delta t \cdot \frac{\Delta\omega}{\omega}}}$$

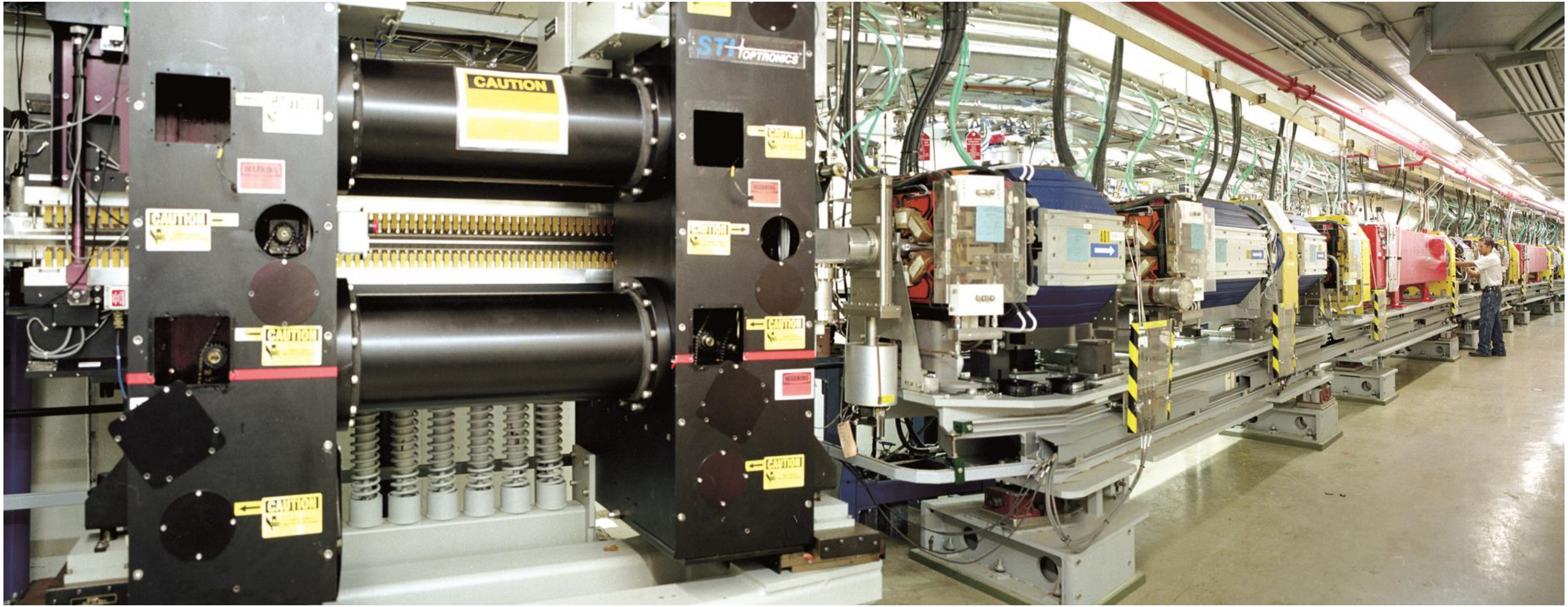
Spectral brightness

$$\boxed{\mathcal{B} = \frac{\Phi}{4\pi^2 \Sigma_x \Sigma_{x'} \Sigma_y \Sigma_{y'}}}$$



MAGNETIC LATTICE

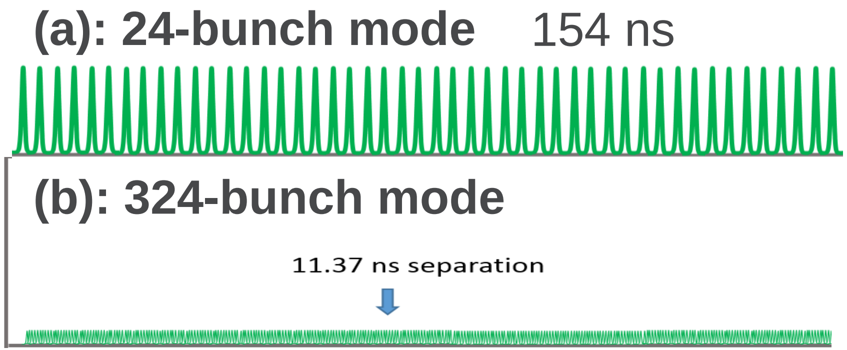




APS storage ring

PROPERTIES OF SYNCHROTRON RADIATION

- High brightness.
- Wide energy spectrum: from 10s of eV to >100 keV.
- Tunable energy
  - Elemental sensitivity by tuning to specific absorption edges
- Highly polarized radiation
  - Which can be manipulated
- Coherence
  - High degree of spatial and longitudinal coherence
- Short pulses, typically ~100 ps
  - Different filling patterns

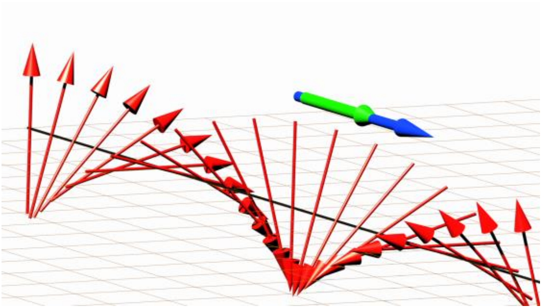


POLARIZATION

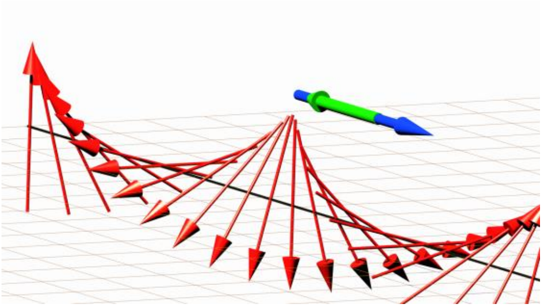
Naturally polarized in the
horizontal plane with a planar undulator

E-field from accelerated charge

$$\vec{E} = \frac{q}{4\pi\epsilon_0 c(1-\vec{\beta}.\vec{n})^3}\frac{\vec{n}\times(\vec{n}-\vec{\beta})\times\dot{\vec{\beta}}}{R}$$

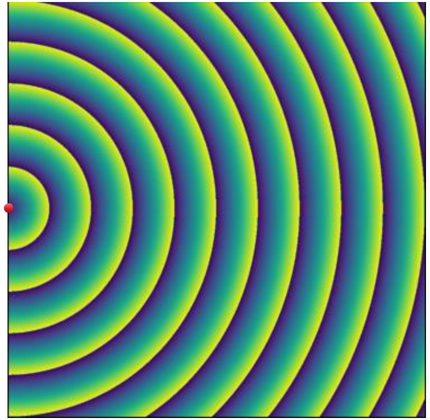


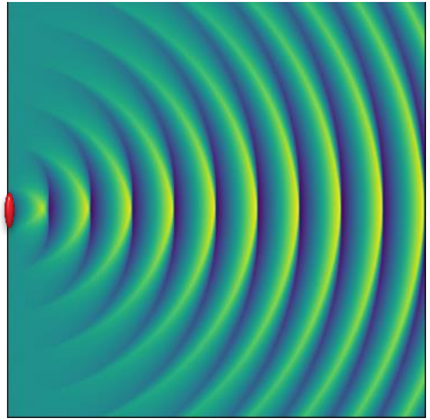
$$|\psi\rangle_L = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\\ 0\end{pmatrix}$$



$$|\psi\rangle_R = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\\ 0\end{pmatrix}$$

SPATIAL COHERENCE





Spatial coherence from ducks
https://physicstoday.scitation.org/doi/pdf/10.1063/1.3366225
https://www.youtube.com/watch?v=4o48J4streE

ADVANCED PHOTON SOURCE

- Highest Energy: 7 GeV
- High Brilliance
  - ✓ Small beams (≲µm) & Coherence
- Unique timing structure
- Polarized in the horizontal plane

Beamlines:

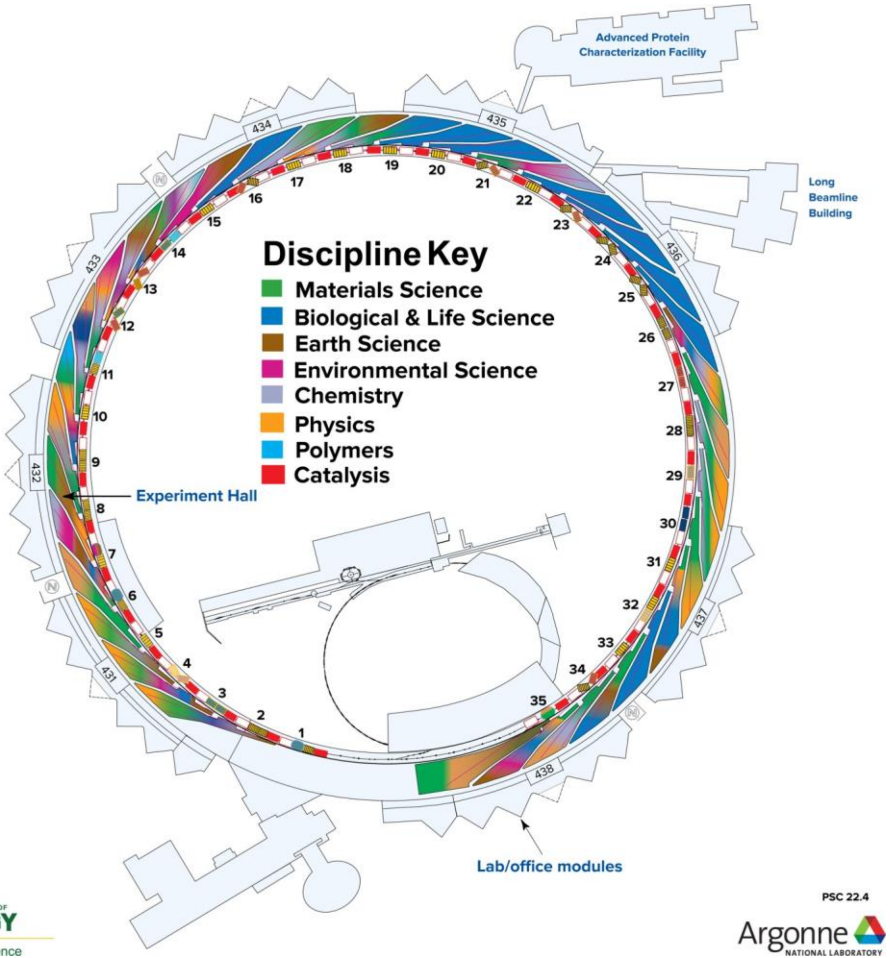
67 beamlines, 47 ID, 20 BM

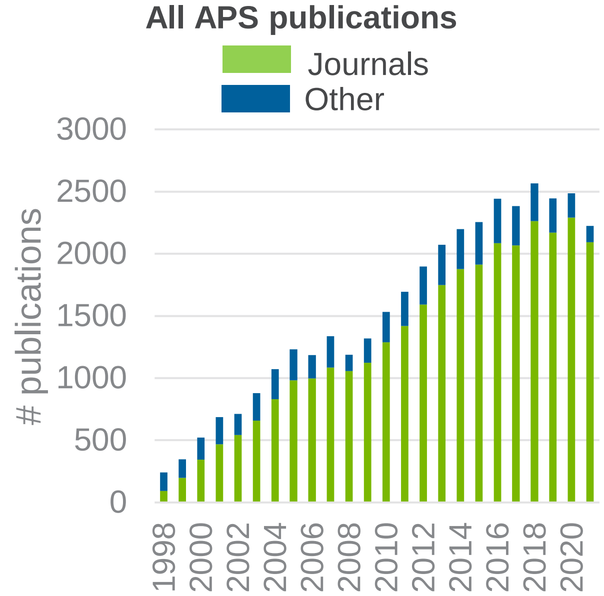
35 DOE-BES funded (base APS budget)

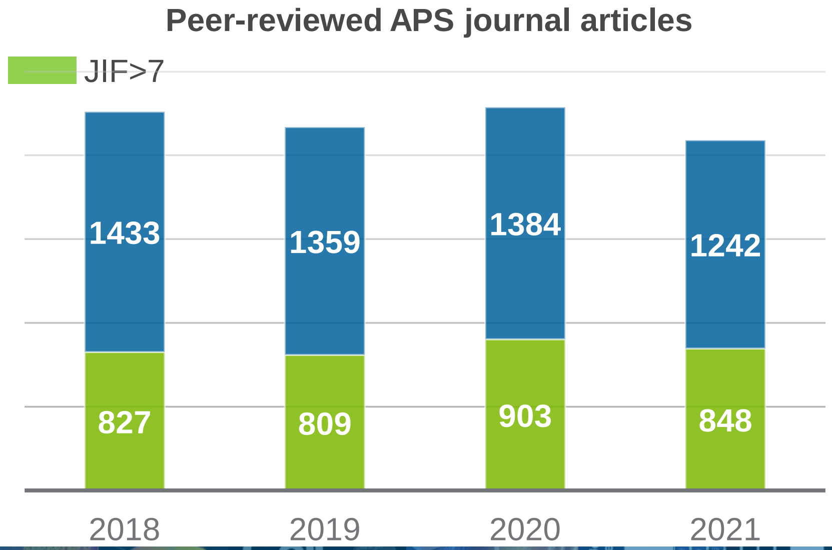
32 CATs (DOE-BER, NNSA, NIH, Industry)

8 APS operated

General user access via peer reviewed proposals

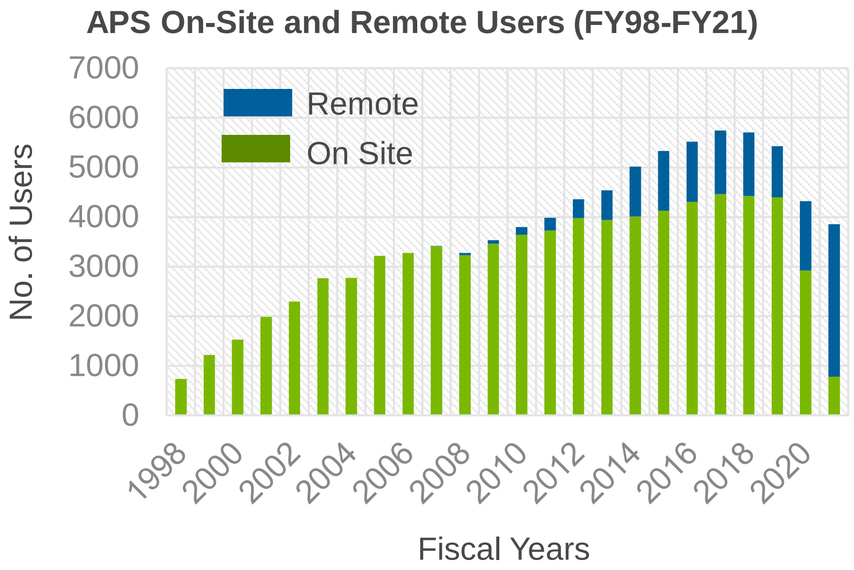


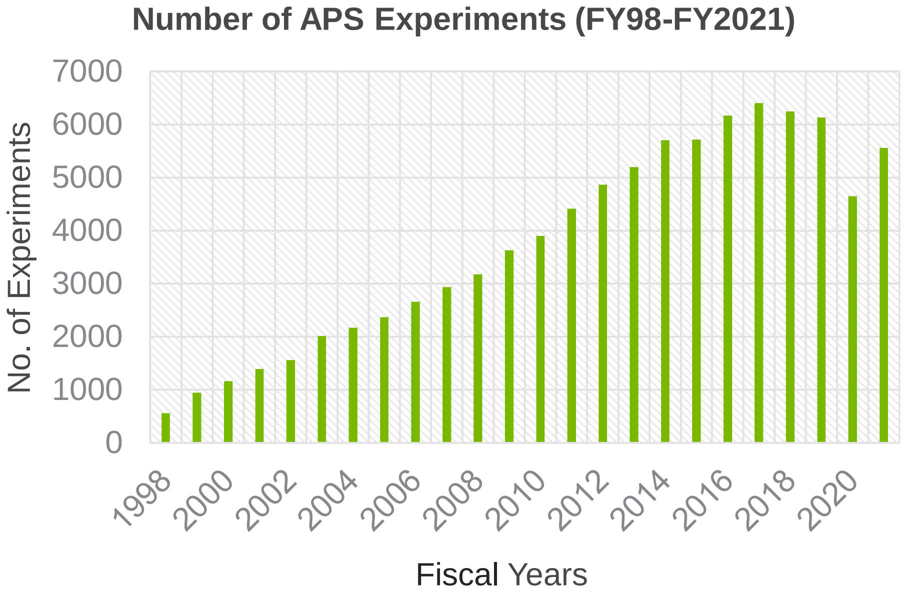

All APS publications
Journals
Other
publications
3000
2500
2000
1500
1000
500
0
1998
2000
2002
2004
2006
2008
2010
2012
2014
2016
2018
2020


Peer-reviewed APS journal articles
JIF>7
1433
827
1359
809
1384
903
1242
848
2018
2019
2020
2021

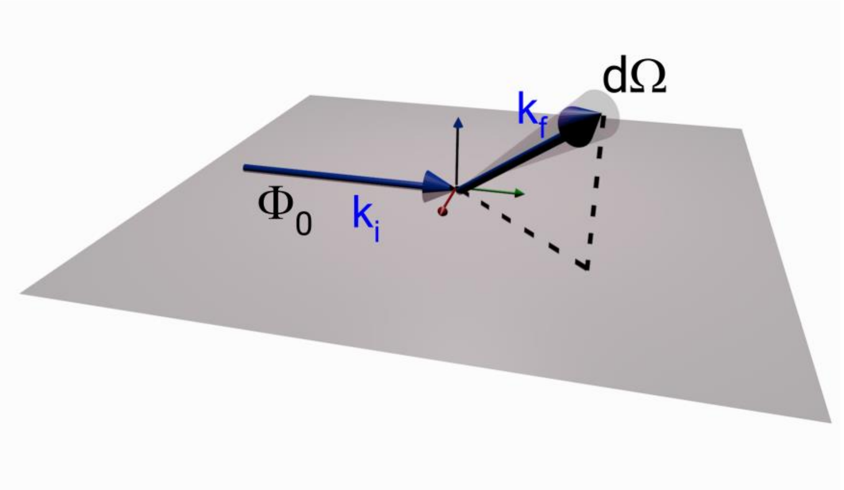
200 PhDs

APS USER DATA





TRANSITION RATE AND CROSS SECTIONS



Transition rate

$$w_{i\to f} = \frac{2\pi}{\hbar}\left|\langle f|\,H'\,|i\rangle + \sum_g \frac{\langle f|\,H'\,|g\rangle\,\langle g|\,H'\,|i\rangle}{E_i - E_g}\right|^2 \delta(E_i - E_f)$$

$$|i\rangle = |a; k_i \epsilon_i\rangle \qquad E_i = E_a + \hbar\omega_i$$

$$|f\rangle = |b; k_f \epsilon_f\rangle \qquad E_f = E_b + \hbar\omega_f$$

HAMILTONIAN ELECTRON IN EMF

X-rays couple to charge, and to spin

$$\mathcal{H} = \underbrace{\sum_j \frac{(\boldsymbol{p_j} + e\boldsymbol{A}(\boldsymbol{r_j}))^2}{2m}}_{\text{Kinetic}}$$

$$+ \underbrace{\frac{e\hbar}{2m}\boldsymbol{\sigma_j} \cdot \vec{\boldsymbol{\nabla}} \times \boldsymbol{A}(\boldsymbol{r_j})}_{\text{Zeeman}}$$

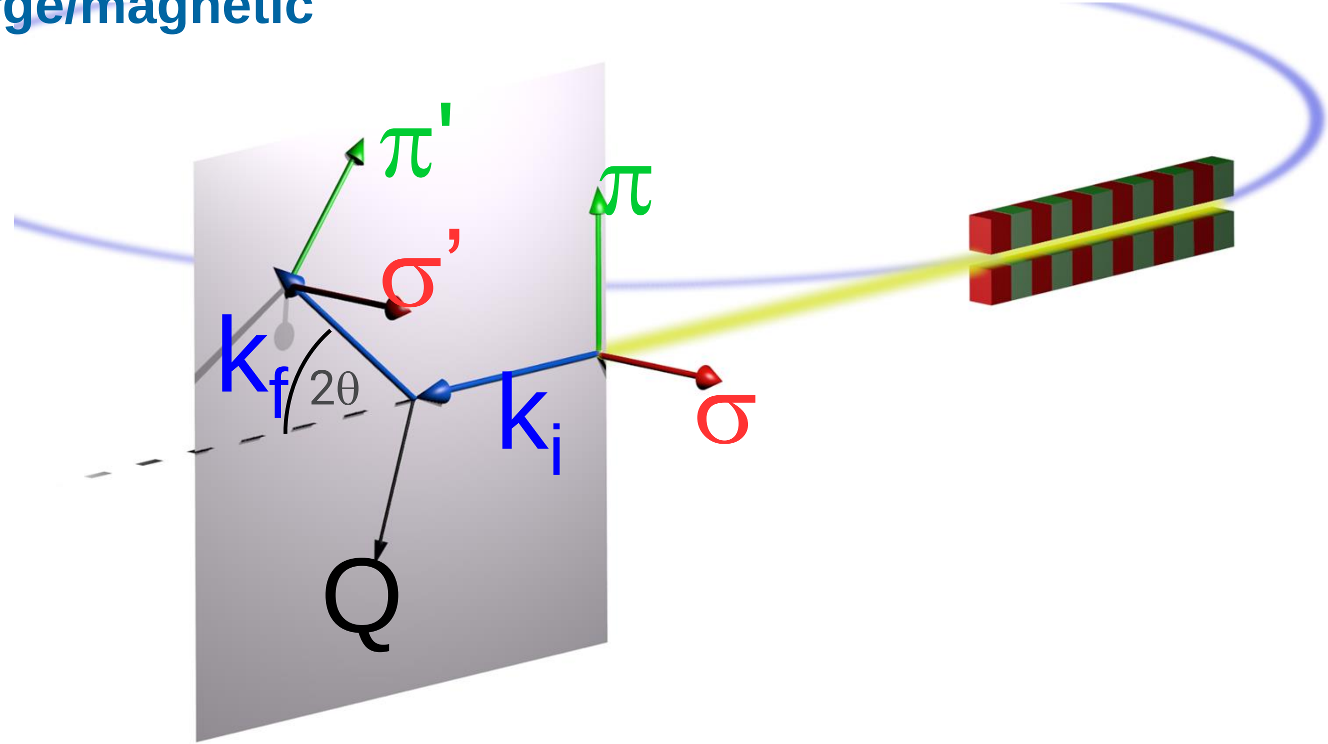
$$+ \underbrace{\frac{e\hbar}{2(2mc)^2}\boldsymbol{\sigma_j} \cdot [(\boldsymbol{p_j} + \boldsymbol{eA}(\boldsymbol{r_j})) \times \partial_t \mathbf{A_j} - \partial_t \mathbf{A_j} \times (\boldsymbol{p_j} + \boldsymbol{eA}(\boldsymbol{r_j}))]}_{\text{SO coupling}}$$

$$+ \underbrace{\sum_n V_{jn}}_{\text{Coulomb}}$$

$$+ \underbrace{\sum_{\boldsymbol{k},\epsilon} \hbar\omega_k \left(a^\dagger_{\boldsymbol{k},\epsilon} a_{\boldsymbol{k},\epsilon} + \frac{1}{2}\right)}_{\text{EMF self-energy}}$$

EXPLOITING POLARIZATION DEPENDENCE TO SEPARATE CONTRIBUTIONS

L/S or charge/magnetic

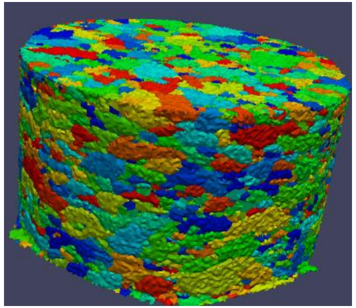


APS BEAMLINES - SCATTERING

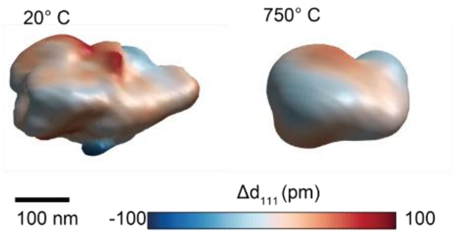
Structure of matter on length scales from atomic to μm.

- XRD, PDF
- SAXS/USAXS/WAXS
- High Energy Diffraction Microscopy
- Single Crystal Diffraction
- **Surface scattering (in-situ growth)**

maging

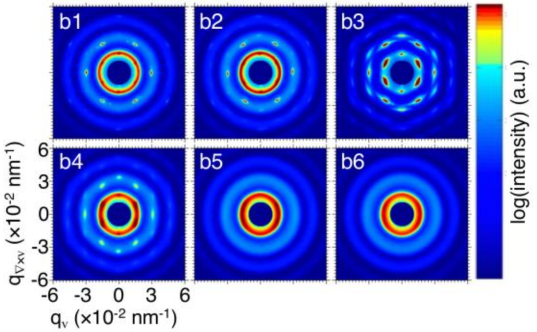


HEDM of material under thermomechanical load



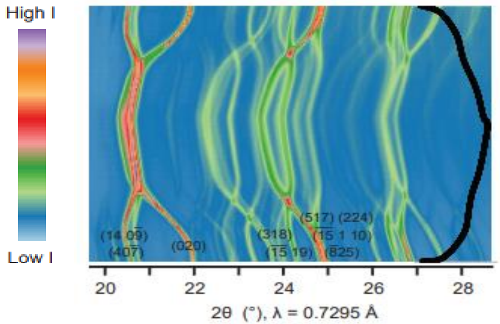
Hruszkewycz, *et al., APL Materials*, **5**, 026105 (2017).

Bragg-CDI of diamond nanocrystals during annealing



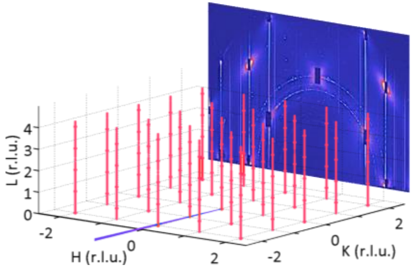
Jonghun Lee *et al., Phys. Rev. Lett*. **120**, 028002 (2018)

SAXS of colloids under shear



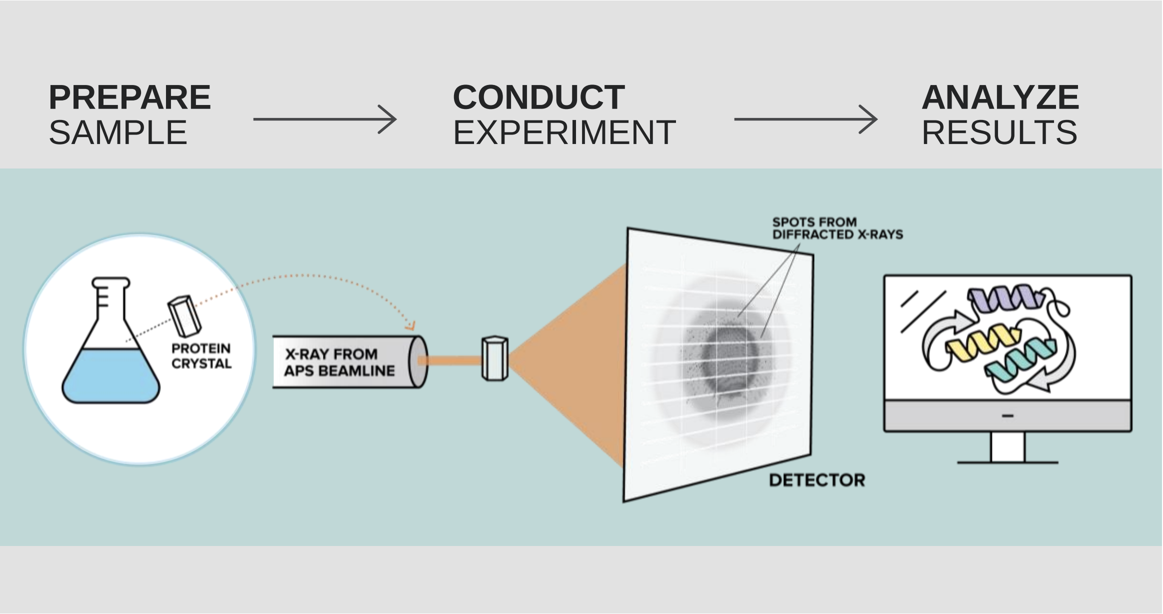
K. Griffin, et al., *Nature*, **559**, 556 (2020).

XRD of $Nb_{16}W_5O_{55}$ electrode

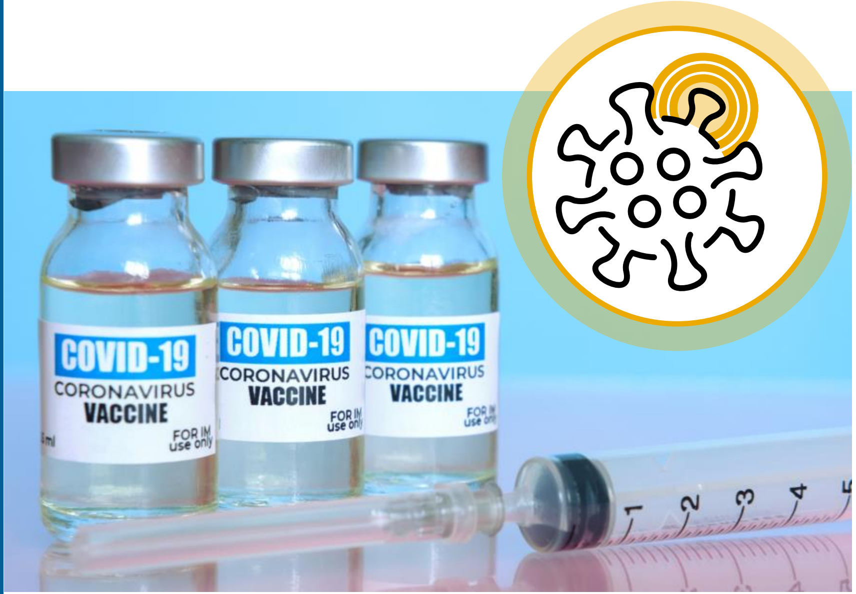


Coherent crystal truncation Bragg rods

PROTEIN CRYSTALLOGRAPHY



RESEARCH ON COVID

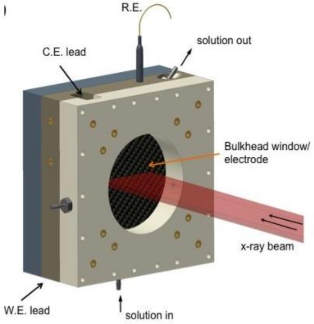


Development of Paxlovid enabled by data collected at the IMCA-CAT beamline at the APS.

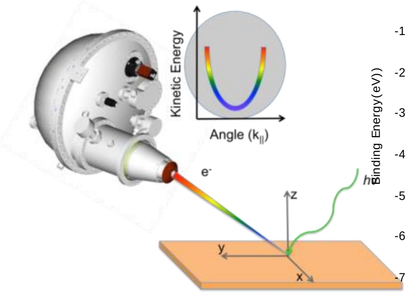
APS BEAMLINES - SPECTROSCOPY

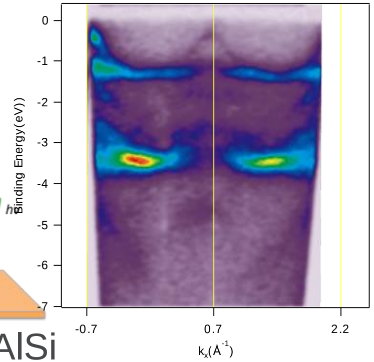
Chemical, electronic, and magnetic states and dynamics (IXS) during reactions and applied external stimuli

- XAS/ UltraFast-XAS, XMCD
- Nuclear Resonance Scattering
- **Inelastic Scattering, RIXS**
- **ARPES**

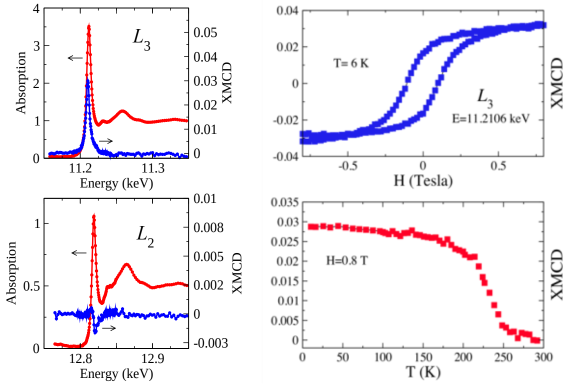


XAS during battery cycling

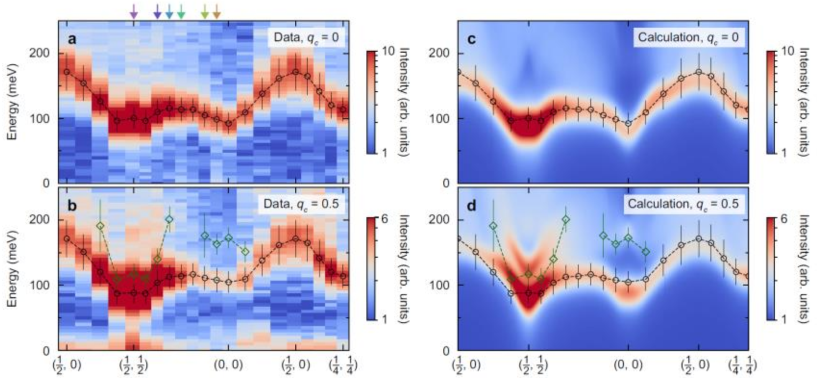




ARPES of LaAlSi

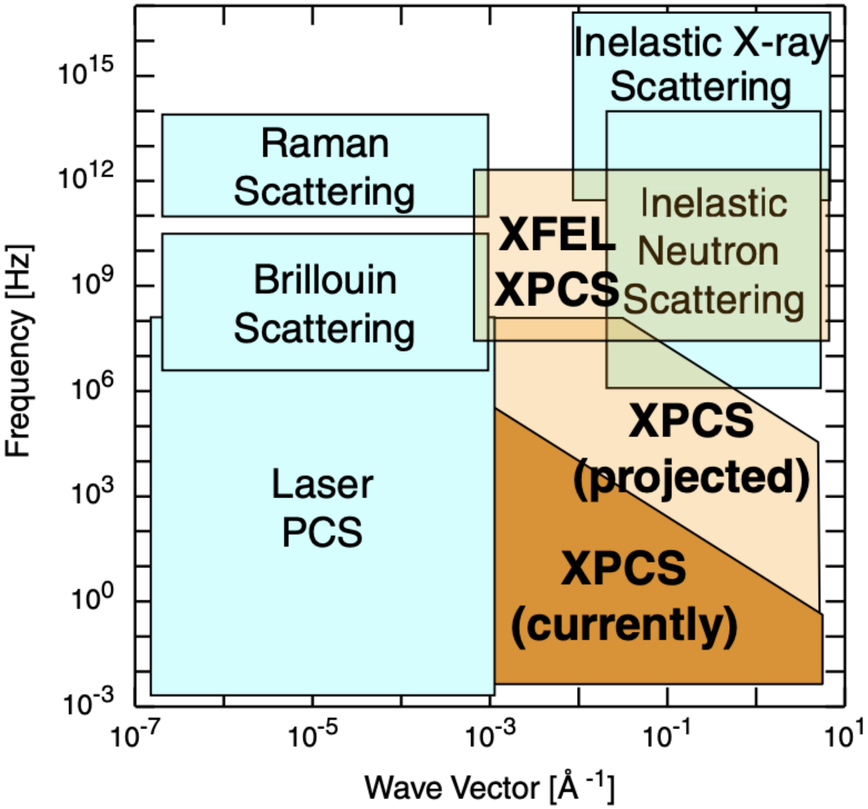


XMCD of Sr_2IrO_4



Mazzone, Det *al.* *Nat Commun* **13,** 913 (2022)

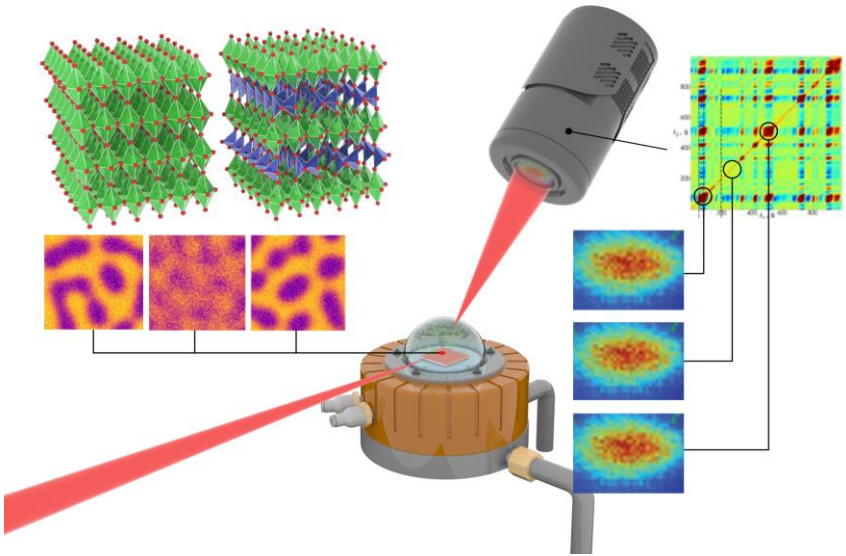
X-RAY PHOTON CORRELATION SPECTROSCOPY



- Dynamic structure factor probed in the time domain.
- Measuring speckle patterns at different time.
- Computing the intensity-intensity correlation function.

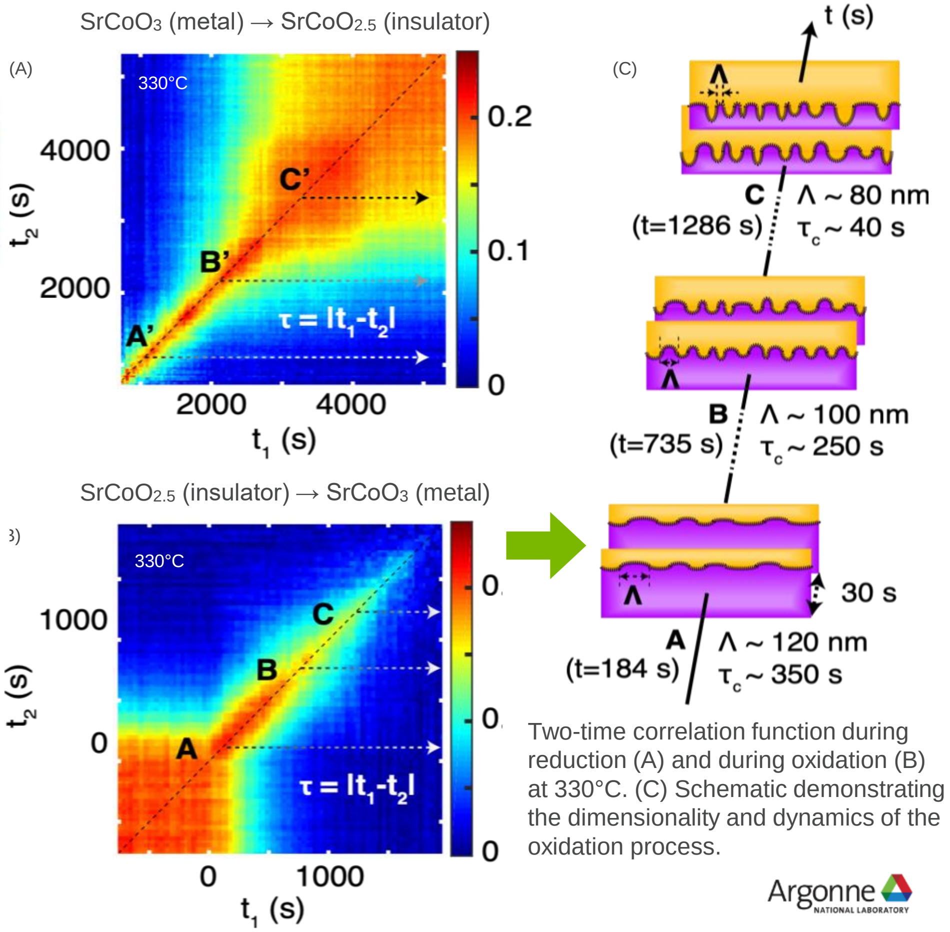
$$g_2(q,\tau) = \frac{\langle I(q,t)I(q,t+\tau)\rangle_t}{\langle I(q,t)\rangle_t}$$

DYNAMICS DURING PHASE TRANSITION IN A RESISTIVE SWITCHING OXIDE



Research Detail

In situ redox, wide-angle XPCS measurements conducted at 8-ID-E in a complex oxide heterostructure

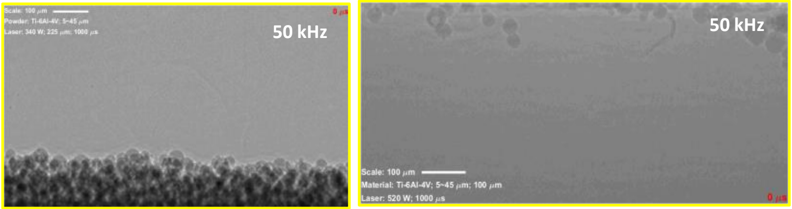


Two-time correlation function during reduction (A) and during oxidation (B) at 330°C. (C) Schematic demonstrating the dimensionality and dynamics of the oxidation process.

APS BEAMLINES - IMAGING

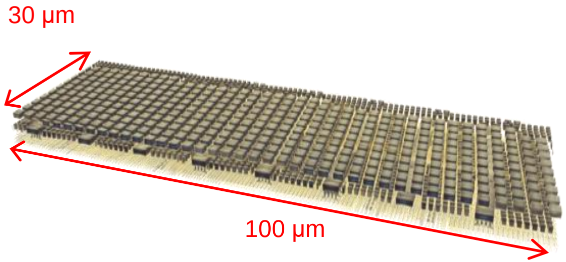
Dynamic (<ns to s) real space imaging with varying contrast (elemental, chemical, phase, …).

- Ultra-Fast Radiography (<1ns - ms)
- Rapid µ-Tomography (~1 µm)
- Transmission X-ray Microscope (~20 nm)
- Spectro-microscopy (20nm to µm)
- **Ptychography/Coherent Diffractive Imaging**

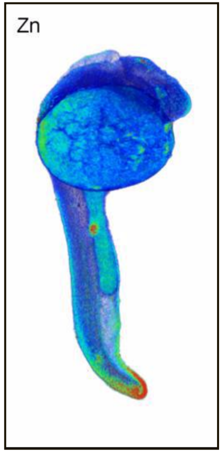


Cunningham *et al.*, *Science* **363**, 849 (2019)

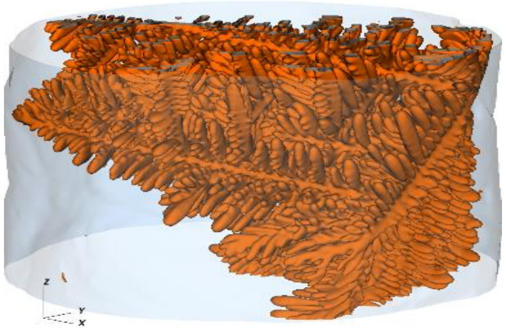
In-Situ Radiography of laser powder-bed additive manufacturing



3D ptychography of an integrated circuit

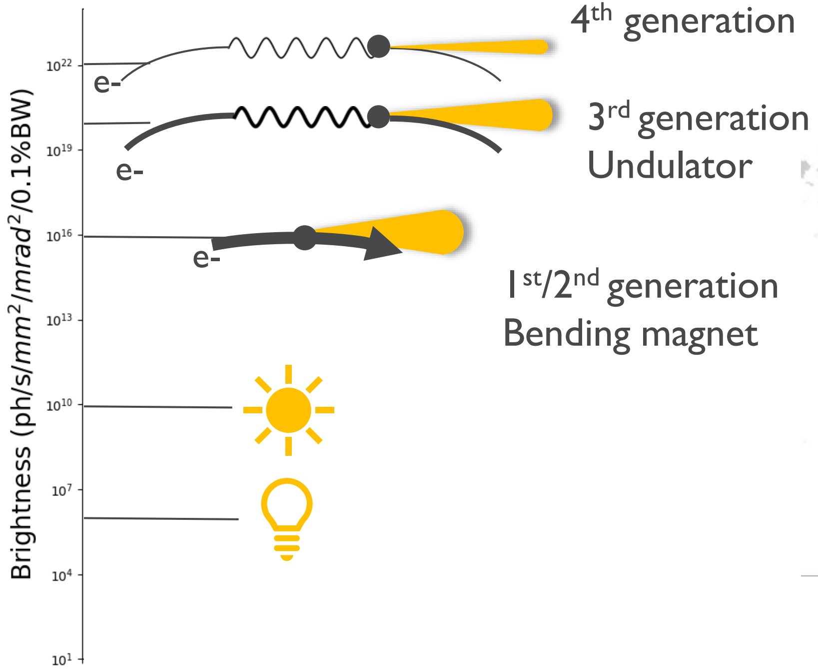


Floures-Tomography of Zebra Fish



Rapid-Tomography of dendrite growth in aluminum

NEXT GENERATION SYNCHROTRON



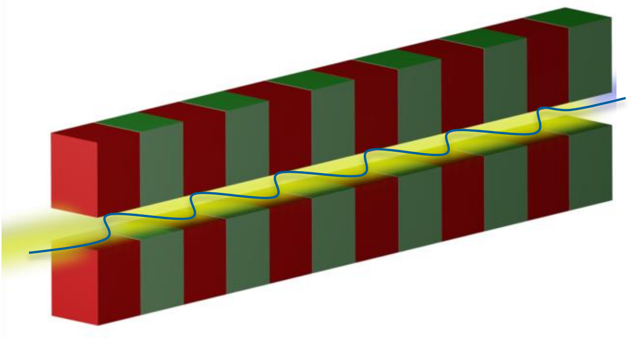
50 light-sources worldwide

4^{TH} GENERATION PROJECTS

- 22 synchrotrons planning 4th generation
- APS will be the brightest hard X-ray synchrotron after APS-U delivery by 2024
- Towards the diffraction limit

- Brownfield projects
- Greenfield projects

DIFFRACTION LIMITED STORAGE RING



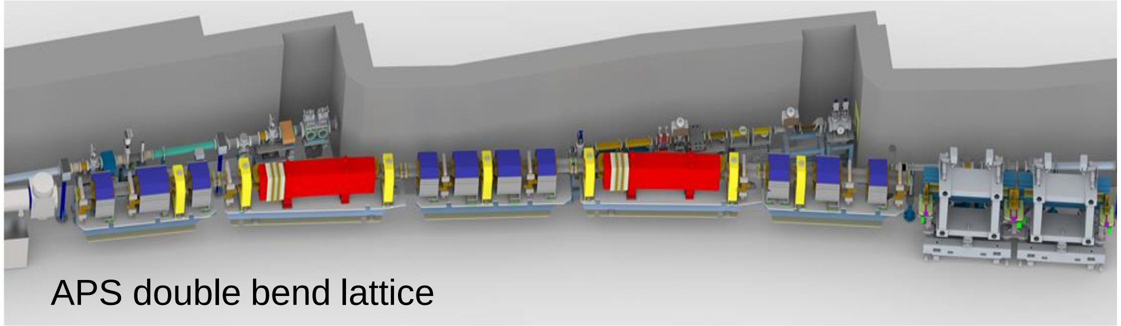
- Phase space distribution of an undulator is far from Gaussian
- However, fully coherent in the limit of zero electron beam emittance and zero energy spread
- Lower the electron emittance to make it negligeable compared to the natural emittance. Diffraction limited if :

$$\varepsilon_{x,y} \ll \frac{\lambda}{4\pi} \text{ (rms)}$$

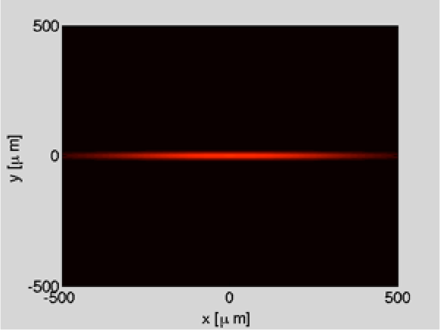
$$\varepsilon_{x,y} \ll \frac{\lambda}{2} \text{ (FHWM)}$$

APS-U – HIGH BRIGHTNESS STORAGE RING LATTICE

APS Today

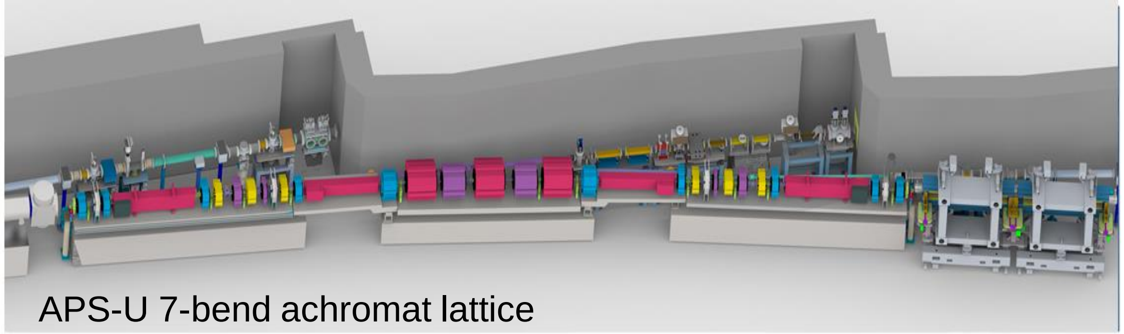


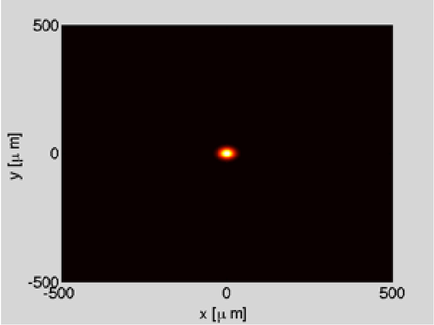
APS Today



ε_o = 3100 pm.rad

APS Upgrade





ε_o = 42 pm.rad

APS-U SECTOR


3



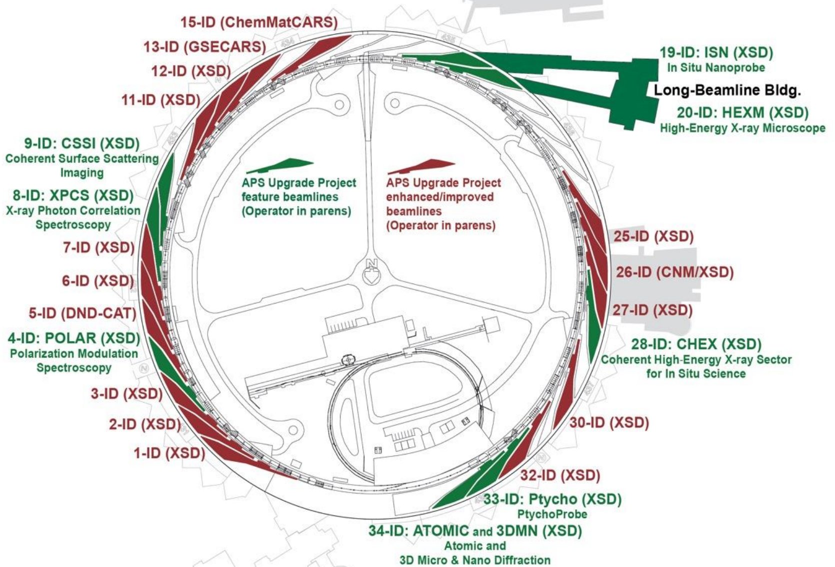

THE ADVANCED PHOTON SOURCE UPGRADE

x 500

$815M

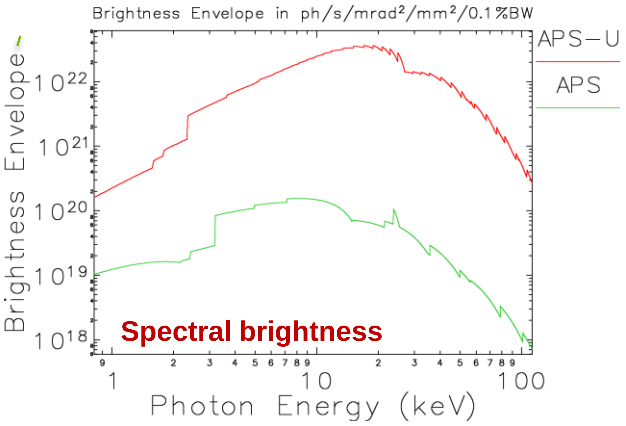
$ 1.5B

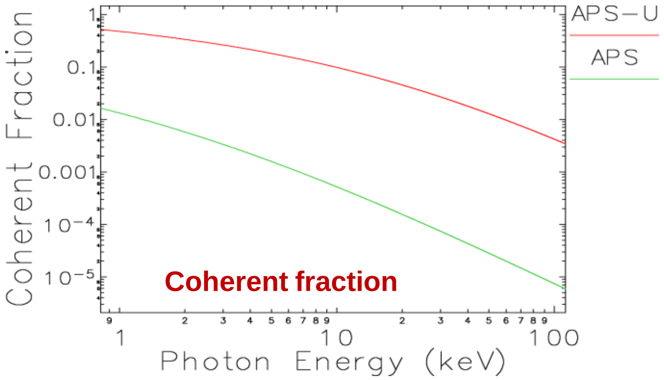
- New storage ring
- New and upgraded beamlines
- New infrastructure

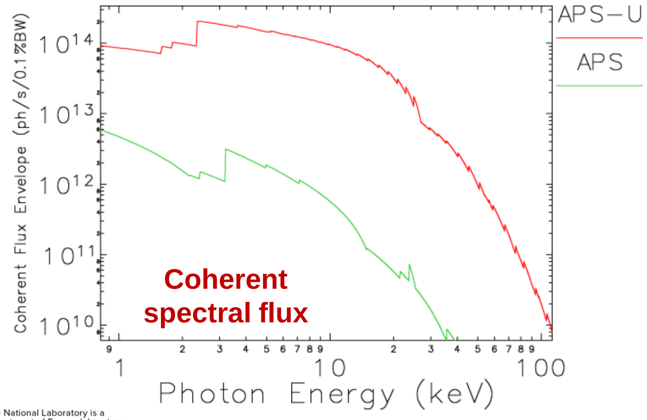


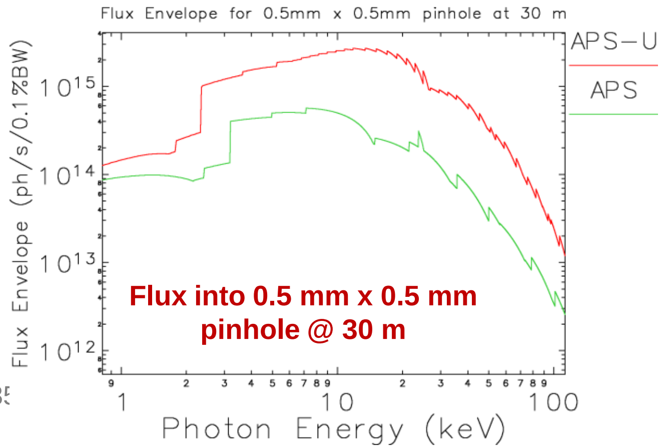
Long Beamline Building, which will house two of the nine feature beamlines.

APS-U – HIGH BRIGHTNESS STORAGE RING LATTICE



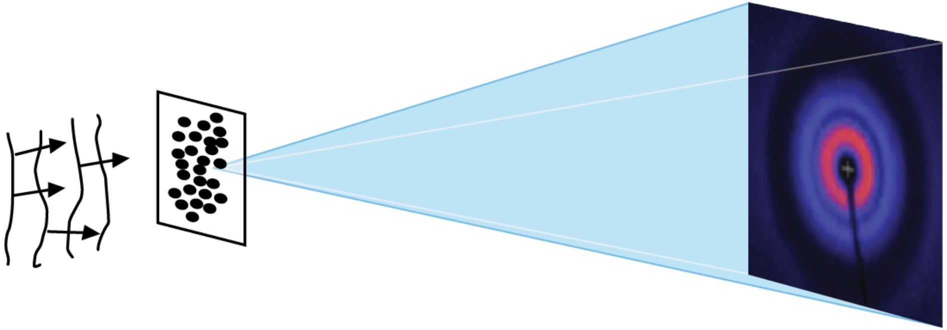




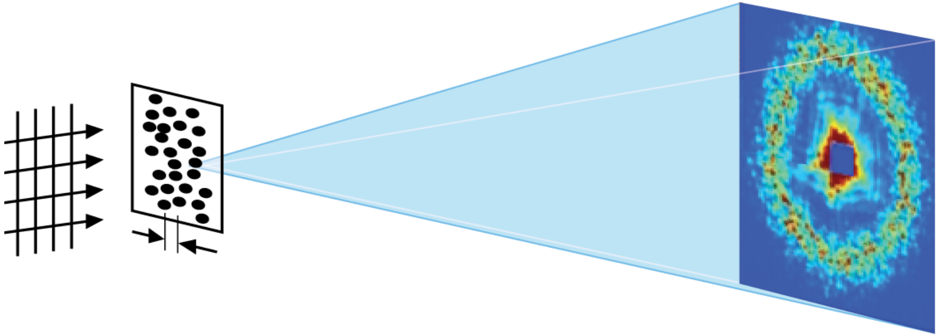


Coherent x-ray studies

Game-changing leap from average to local time/space information



Incoherent beam carries average information; resolution limited by optics

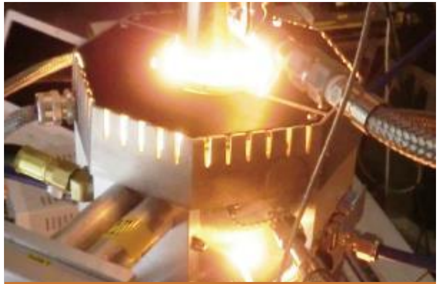


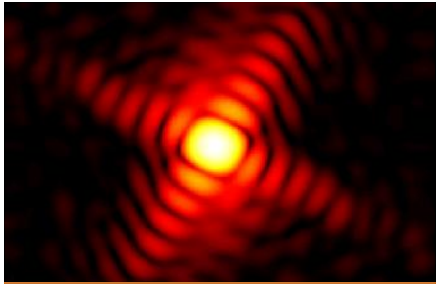
Scattering of coherent beam carries all microscopic, local information

non-periodic arrangements, correlations, dynamics

Spatial resolution limited only by x-ray wavelength, coherent flux

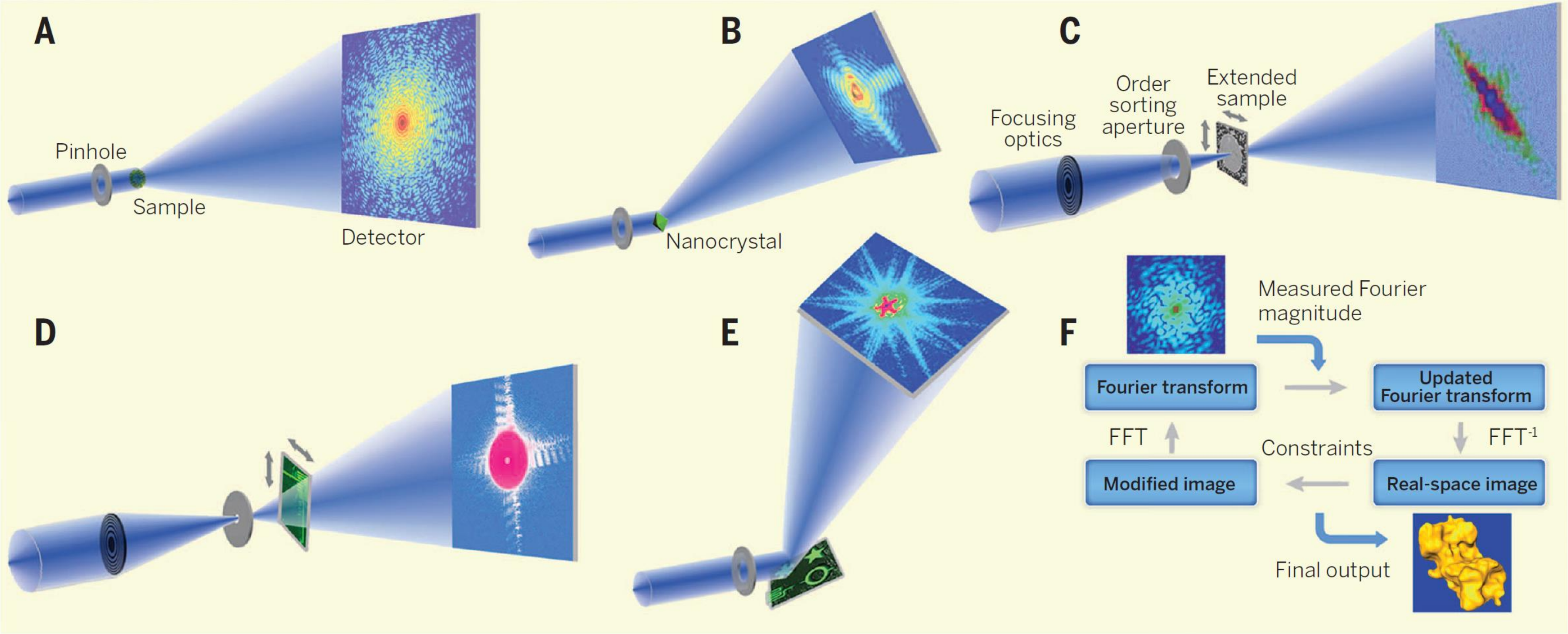
DRIVERS





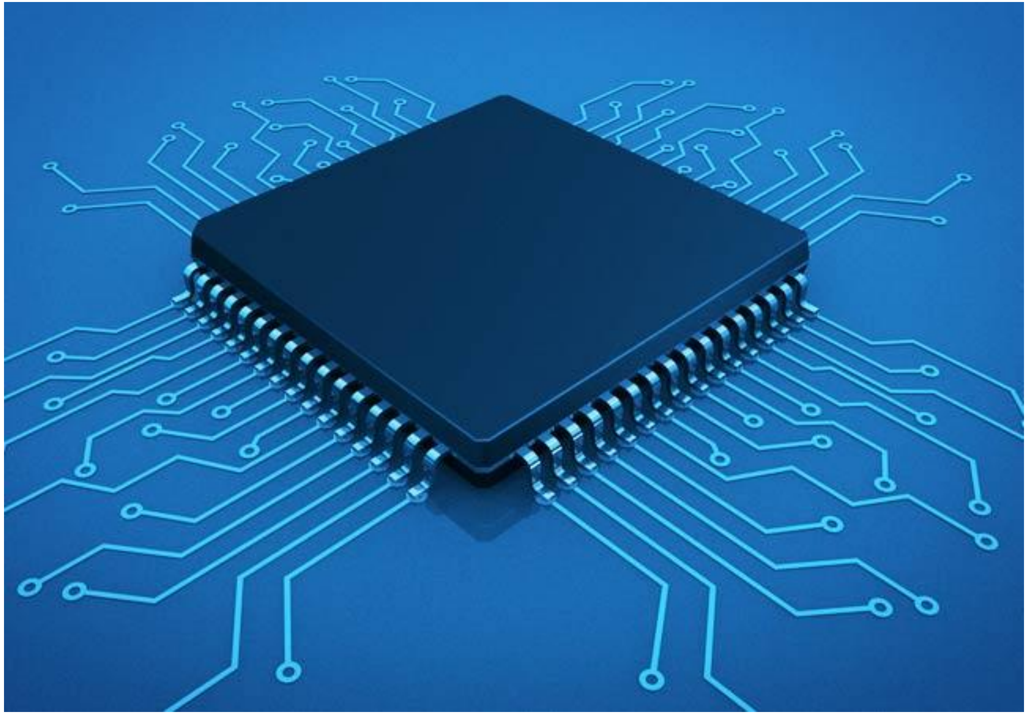
HIGH ENERGY	BRIGHTNESS	COHERENCE	DATA SCIENCES
Penetrate bulk materials and operating systems	Provide 3D fields of view, at a scale visible to the naked eye, with resolution at the nanometer scale	Enable highest spatial resolution even in materials that do not have a fixed, repeating structure	Enable real-time data analysis and decision making at the beamline

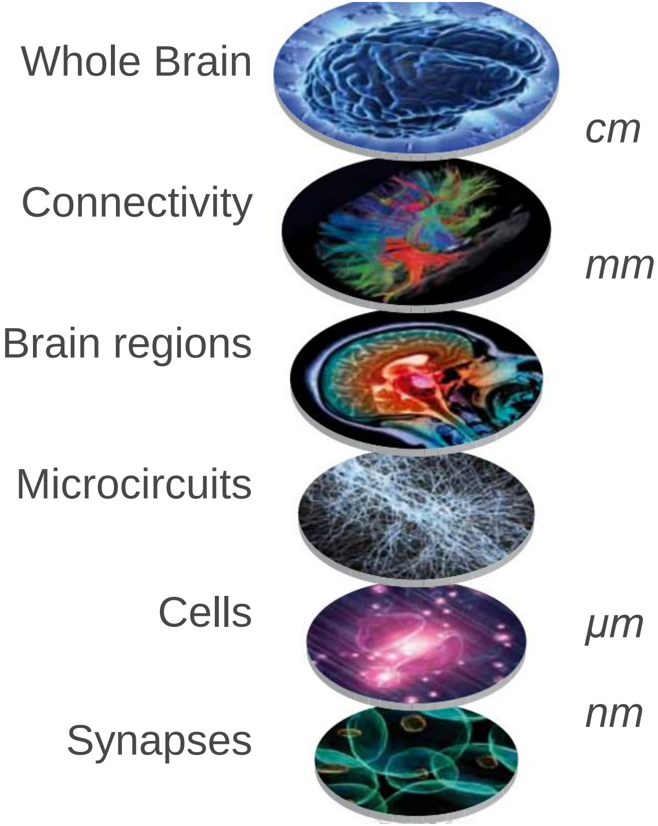
COHERENT DIFFRACTION IMAGING



Miao, Science, VOL 348 ISSUE 6234, (2015)

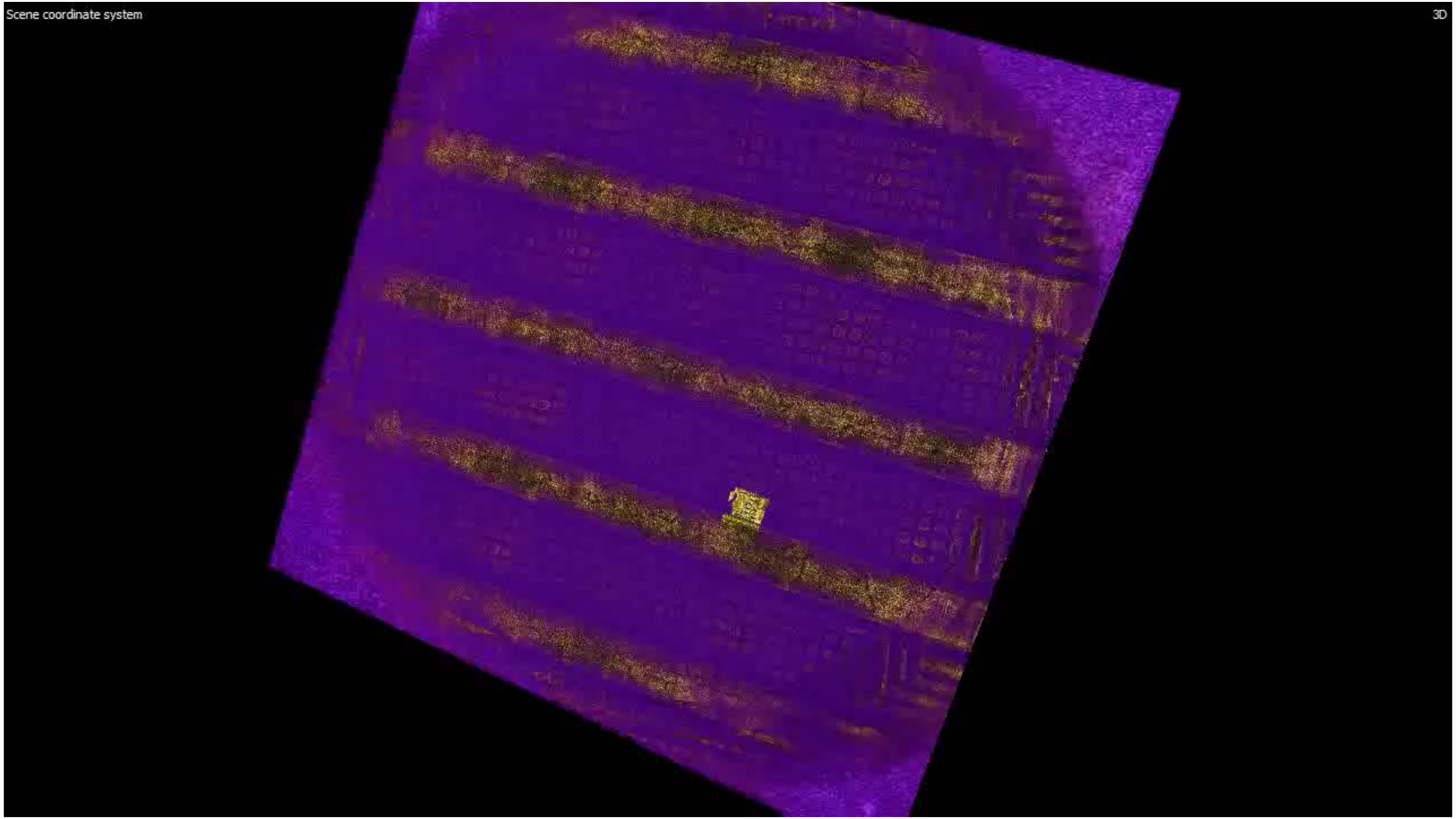
UNIQUE OPPORTUNITY: LENSLESS IMAGING OF EXTENDED 3D SAMPLES





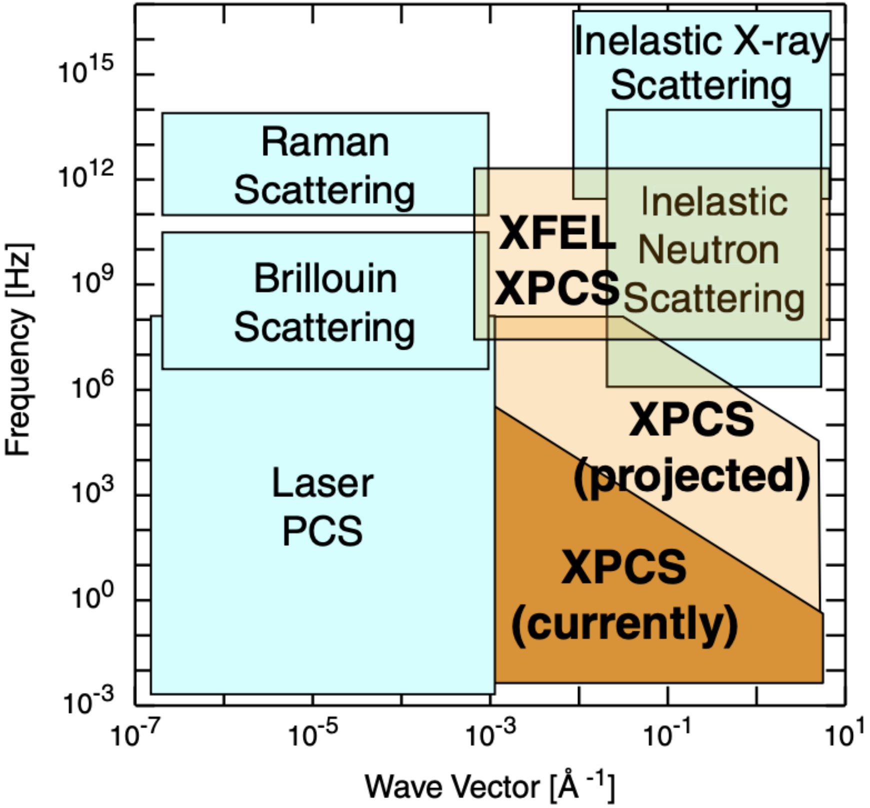
With APS-U: coherent flux to image 1mm^3 at 10 nm 3D resolution in ~1 day

LAMINOGRAPHY OF 16 NM IC



Scan FOV: 50 µm diameter

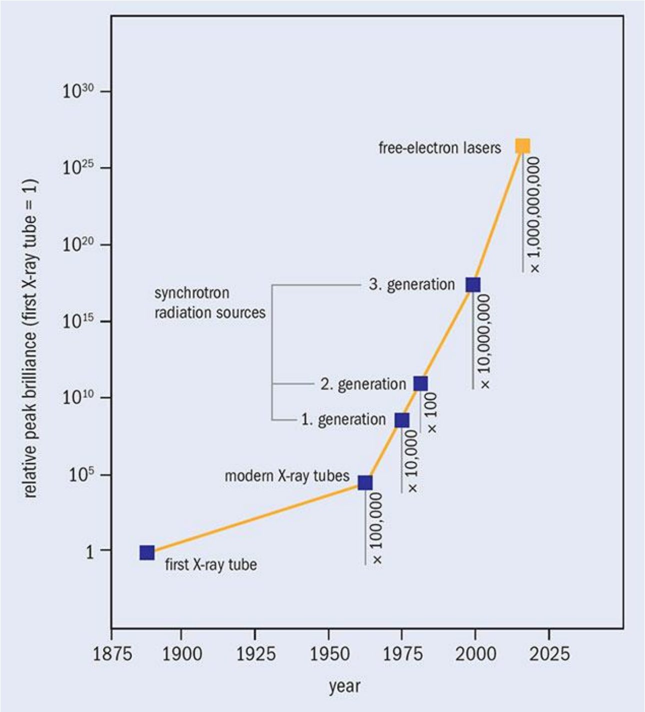
X-RAY PHOTON CORRELATION SPECTROSCOPY



- Dynamic structure factor probed in the time domain.
- Measuring speckle patterns at different time.
- Computing the intensity-intensity correlation function.

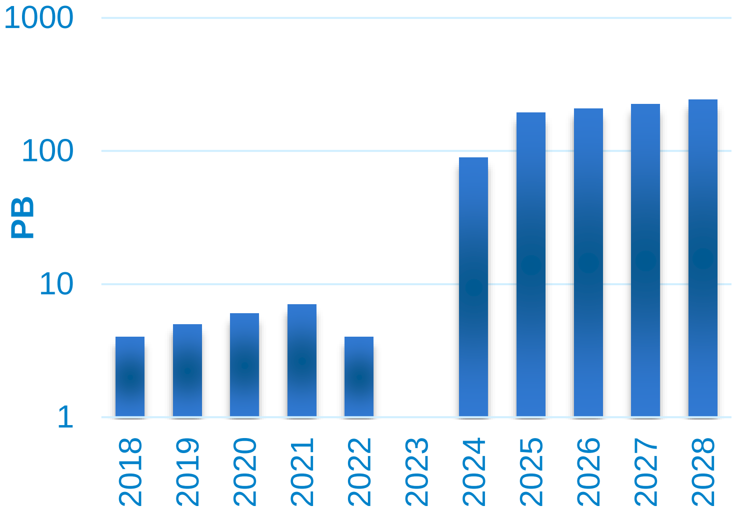
$$g_2(q,\tau) = \frac{\langle I(q,t)I(q,t+\tau)\rangle_t}{\langle I(q,t)\rangle_t}$$

THE BIG-DATA PROBLEM (AND OPPORTUNITY):

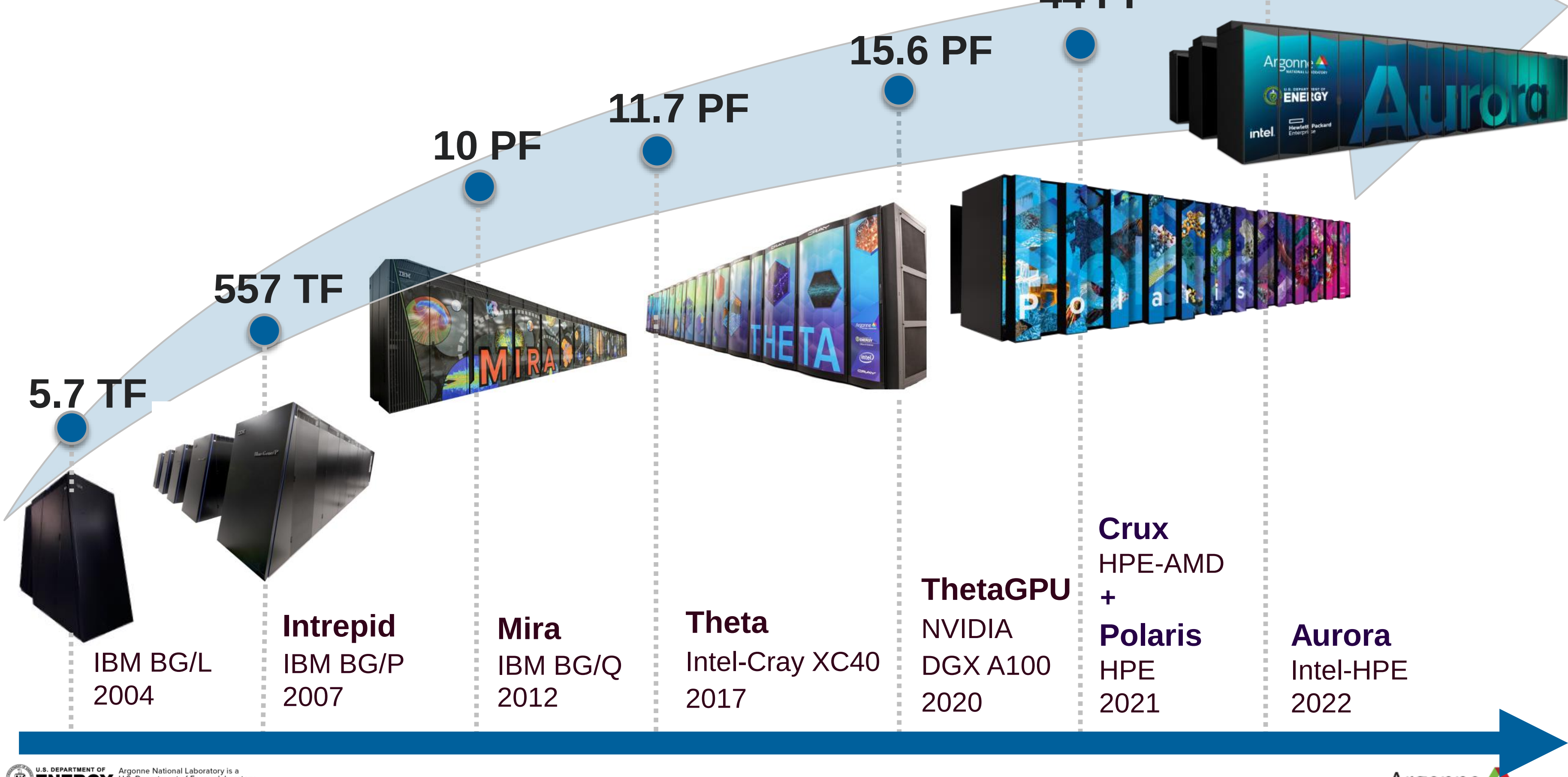


Credit: European XFEL

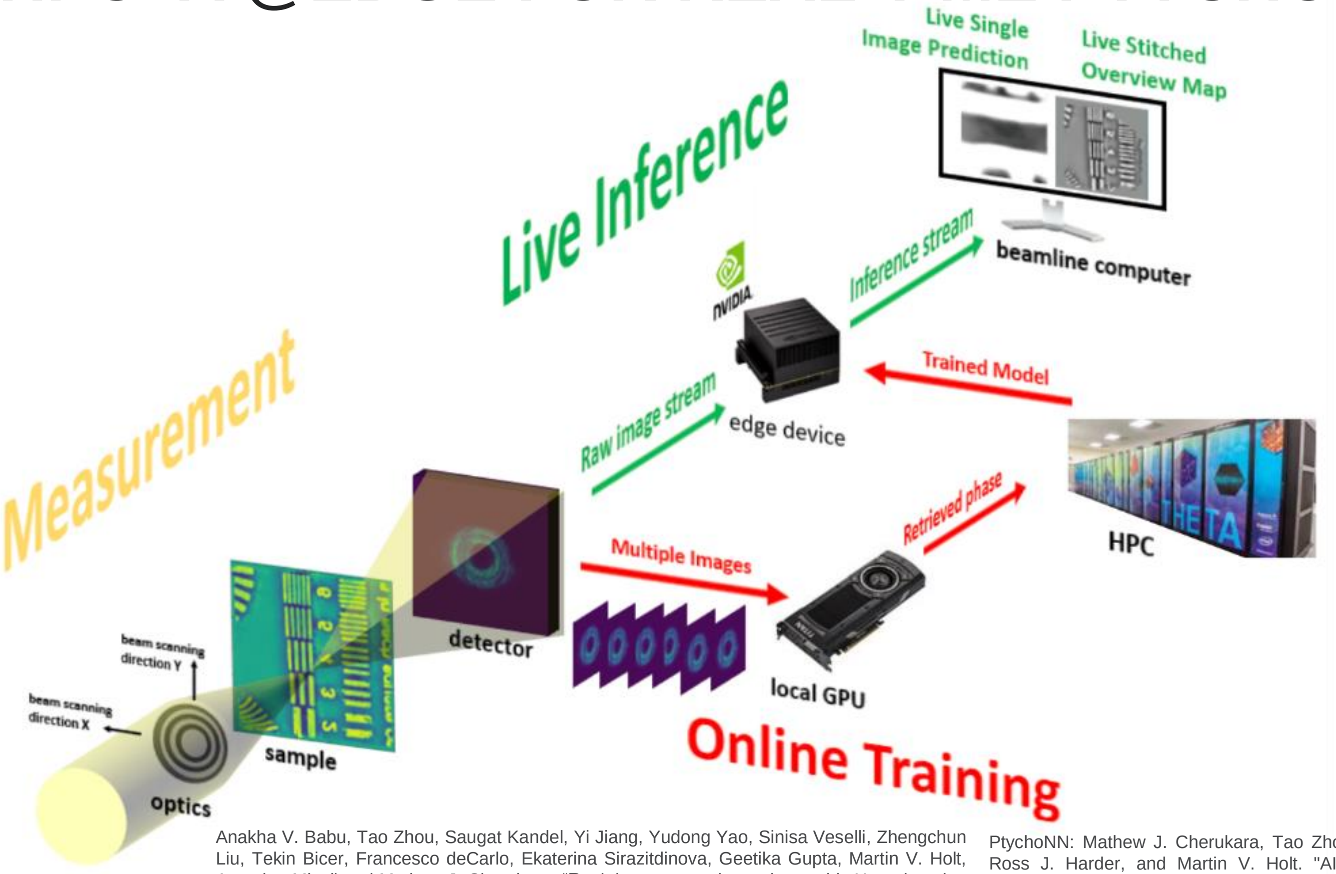
Cumulative data generation at the APS over the next decade by fiscal year.



ALCF Systems Evolution



HPC+AI@EDGE FOR REAL-TIME PTYCHOGRAPHY

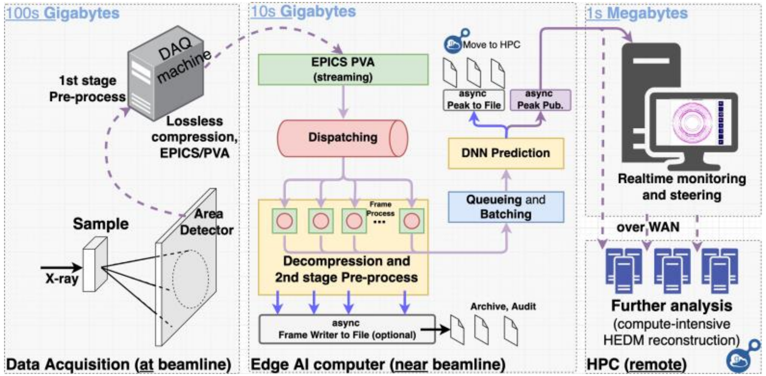


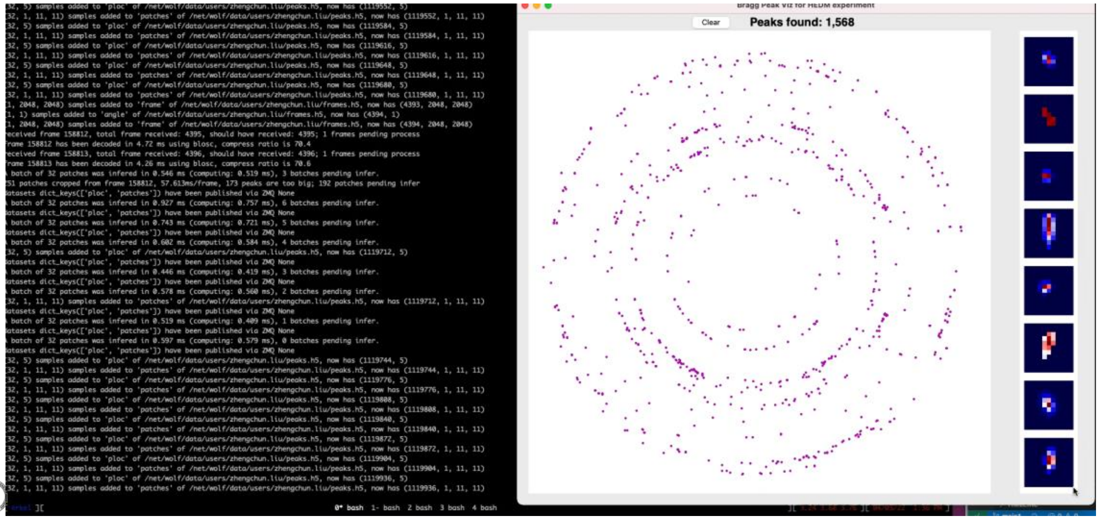
- >100X faster
- Live inference @ 100 Hz on 512x512 images
- <25 X lower-dose imaging:

Anakha V. Babu, Tao Zhou, Saugat Kandel, Yi Jiang, Yudong Yao, Sinisa Veselli, Zhengchun Liu, Tekin Bicer, Francesco deCarlo, Ekaterina Sirazitdinova, Geetika Gupta, Martin V. Holt, Antonino Miceli and Mathew J. Cherukara, "Real-time nanoscale ptychographic X-ray imaging using deep learning at the edge"

PtychoNN: Mathew J. Cherukara, Tao Zhou, Youssef Nashed, Pablo Enfedaque, Alex Hexemer, Ross J. Harder, and Martin V. Holt. "AI-enabled high-resolution scanning coherent diffraction imaging." *Applied Physics Letters* 117, no. 4 (2020): 044103.

REAL-TIME STREAMING ANALYSIS OF DIFFRACTION DATA





Data volume reduced by > 100,000 without losing information for final HEDM reconstruction.

- **A trained neural network (BraggNN) running on an edge computing device (NVIDIA Jetson) performs the Bragg peak analysis.**
- **EPICS/PVA streams data directly to our pipeline, all data only sits in memory for the full lifetime, thus mitigating stress to storage system.**

Liu, Z, Sharma, H, Park, J-S, Kenesei, P, Miceli, A, Almer, J, Kettimuthu, R, Foster, I, IUCrJ, 9 (1) 2022.

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