WELCOME & OVERVIEW OF
ADVANCED PHOTON SOURCE (APS)

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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**
Basic Energy Science – DOE light sources
RADIATION FROM ACCELERATED CHARGES

From $\beta=0$ to $\beta \sim 1$

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

Jackson “Classical Electromagnetism”
X-RAY SYNCHROTRON - BASICS

LINAC

450 MeV

7 GeV

Storage ring

Booster
**SOURCES**

Anatoly Shabalin, PhD thesis

\[
\Phi = \frac{N_{\text{ph}}}{\Delta t \cdot \Delta \omega}
\]

Spectral brightness

\[
\mathcal{B} = \frac{\Phi}{4\pi^2 \Sigma_x \Sigma_x' \Sigma_y \Sigma_y'}
\]

- **1st/2nd generation Bending magnet**
- **3rd generation Undulator**
- **4th generation Flux Spectral brightness**
MAGNETIC LATTICE

Dipole

Quadrupole

Sextupole
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

(a): 24-bunch mode  154 ns
(b): 324-bunch mode  11.37 ns separation
Naturally polarized in the horizontal plane with a planar undulator.
Spatial coherence from ducks
https://www.youtube.com/watch?v=4o48J4strE
ADVANCED PHOTON SOURCE

- Highest Energy: 7 GeV
- High Brilliance
  - Small beams ($\lesssim \mu$m) & 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
Peer-reviewed APS journal articles

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<th>Other</th>
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200 PhDs
TRANSITION RATE AND CROSS SECTIONS

Transition rate

\[
\omega_{i \rightarrow f} = \frac{2\pi}{\hbar} \left| \langle f | H' | i \rangle + \sum_g \frac{\langle f | H' | g \rangle \langle g | H' | i \rangle}{E_i - E_g} \right|^2 \delta(E_i - E_f)
\]

| \langle i \rangle = |a; k_i \epsilon_i \rangle \quad E_i = E_a + \hbar \omega_i |
| \langle f \rangle = |b; k_f \epsilon_f \rangle \quad E_f = E_b + \hbar \omega_f |
HAMILTONIAN ELECTRON IN EMF

X-rays couple to charge, and to spin

\[ \mathcal{H} = \sum_j \left( \frac{(p_j + eA(r_j))^2}{2m} \right) \]  \hspace{1cm} \text{Kinetic}

\[ + \frac{e\hbar}{2m} \sigma_j \cdot \nabla \times A(r_j) \]  \hspace{1cm} \text{Zeeman}

\[ + \frac{e\hbar}{2(2mc)^2} \sigma_j \cdot [(p_j + eA(r_j)) \times \partial_t A_j - \partial_t A_j \times (p_j + eA(r_j))] \]  \hspace{1cm} \text{SO coupling}

\[ + \sum_n V_{jn} \]  \hspace{1cm} \text{Coulomb}

\[ + \sum_{k,\epsilon} \hbar \omega_k \left( a_{k,\epsilon}^\dagger a_{k,\epsilon} + \frac{1}{2} \right) \]  \hspace{1cm} \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)**

HEDM of material under thermomechanical load


XRD of \( \text{Nb}_{16}\text{W}_{5}\text{O}_{55} \) electrode


SAXS of colloids under shear


Bragg-CDI of diamond nanocrystals during annealing

Coherent crystal truncation Bragg rods
PROTEIN CRYSTALLOGRAPHY

PREPARE SAMPLE → CONDUCT EXPERIMENT → ANALYZE RESULTS

- Prepare sample
- Conduct experiment
- Analyze results

Diagram showing steps of protein crystallography:
- Prepare sample
- Conduct experiment
- Analyze results
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$_2$IrO$_4$

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

3D ptychography of an integrated circuit

Floures-Tomography of Zebra Fish

Rapid-Tomography of dendrite growth in aluminum

Cunningham et al., Science 363, 849 (2019)
NEXT GENERATION SYNCHROTRON

1st/2nd generation
Bending magnet

3rd generation
Undulator

4th generation

50 light-sources worldwide
22 synchrotrons planning 4th generation
APS will be the brightest hard X-ray synchrotron after APS-U delivery by 2024
Towards the diffraction limit
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 negligible 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 double bend lattice

APS Upgrade

APS-U 7-bend achromat lattice

\( \varepsilon_0 = 3100 \text{ pm.rad} \)

\( \varepsilon_0 = 42 \text{ pm.rad} \)
APS-U SECTOR
THE ADVANCED PHOTON SOURCE UPGRADE

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

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

Flux into 0.5 mm x 0.5 mm pinhole @ 30 m
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

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

A
Pinhole
Sample

B
Detector
Nanocrystal

C
Focusing optics
Order sorting aperture
Extended sample

D

E

F
Measured Fourier magnitude
Fourier transform
Modified image
Real-space image
Final output

Updated Fourier transform
FFT⁻¹

UNIQUE OPPORTUNITY: LENSLESS IMAGING OF EXTENDED 3D SAMPLES

With APS-U: coherent flux to image 1mm³ 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):

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

Credit: European XFEL
ALCF Systems Evolution

IBM BG/L 2004
Intrepid IBM BG/P 2007
Mira IBM BG/Q 2012
Theta Intel-Cray XC40 2017
ThetaGPU NVIDIA DGX A100 2020
Crux HPE-AMD + Polaris HPE 2021
Aurora Intel-HPE 2022
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"

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.


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