Update on APS upgrade science case and early experiments planning

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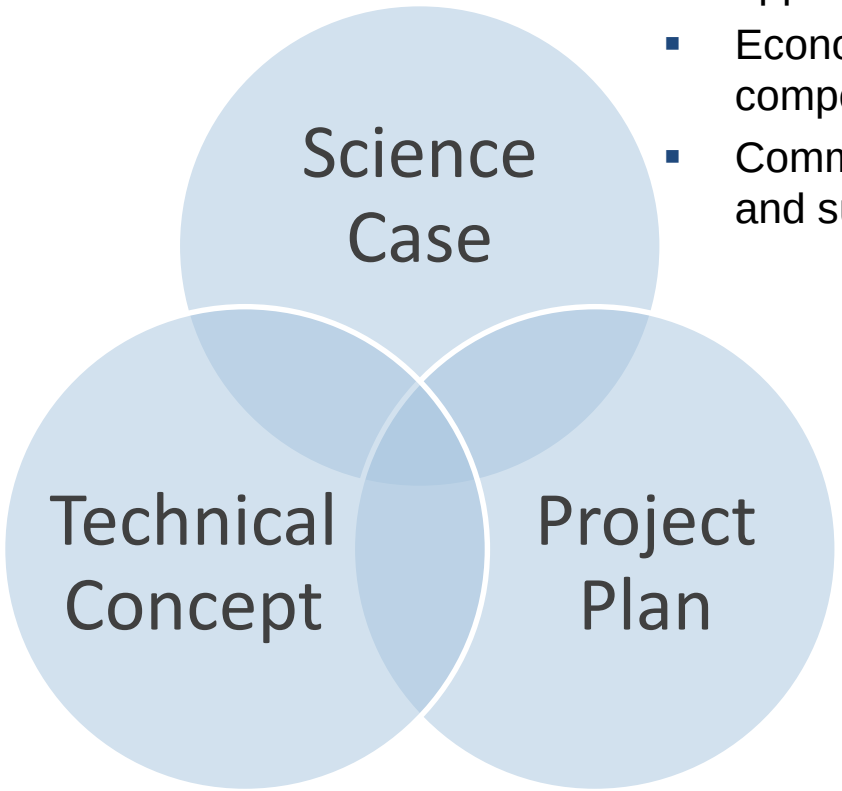
Moving the APS Upgrade Project forward

- Visionary scientific opportunities
- Economic and scientific competitiveness
- Community engagement and support

- Credible technical plan in place
- Plan maintains leadership capabilities in the face of international competition
- Can be built and made to work



- Project team ready to carry out a major DOE construction project
- Project scope, cost and schedule that is robust and credible
- Funding profile that is manageable

Science Case Development

Mission Need Presentation

- To establish Mission Need, a crisp storyline of the scientific capabilities and transformational opportunities enabled by APS-U is essential
- A large number of people contributed significantly to develop the strongest scientific case
- A tremendous amount of work was carried out to formulate the APS-U scientific mission need, which was presented to DOE mid-march, and received very very positively
- Affirmation on three major points:
  - Science case and its demonstration of mission need
  - Plan toward a CD-1 review by the end of the fiscal year
  - Additional beamline scope warranted by the science case and international competitiveness

Thanks to all who contributed to this really important task!

- *Need to develop with Community driven early science experiments*

APS-U: The ultimate 3D microscope

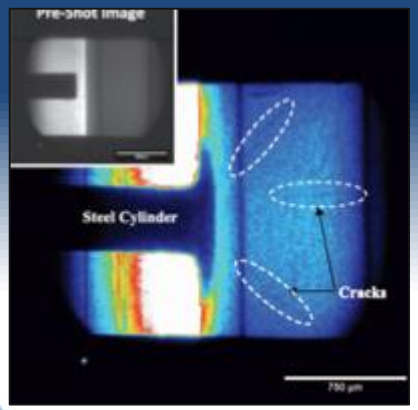
A new analytical tool to approach the supreme goal of measurement science:

To map any atom's position, identity and dynamics

High Energy

Penetrating bulk materials and operating systems

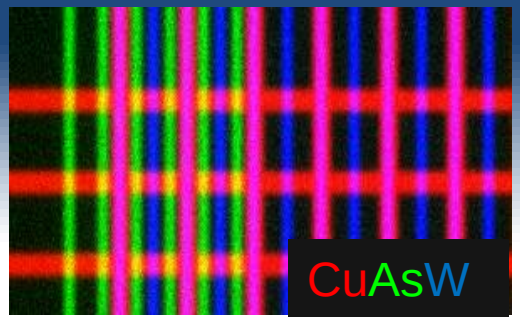
- World's brightest source of hard X-rays
- 3D mapping, deep inside samples
- X-ray cinematography in previously inaccessible regimes



Brightness

Providing macroscopic fields of view with nm-scale resolution

- Multi-scale imaging – connecting nanometer features across macroscopic dimensions
- Fast sampling with chemical, magnetic, electronic sensitivity

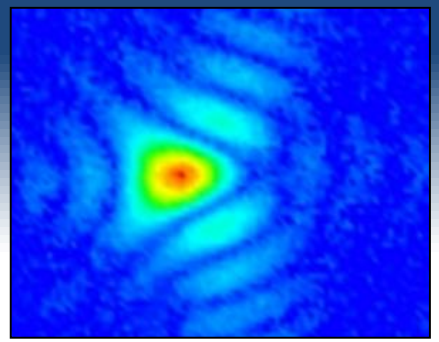


100 nm

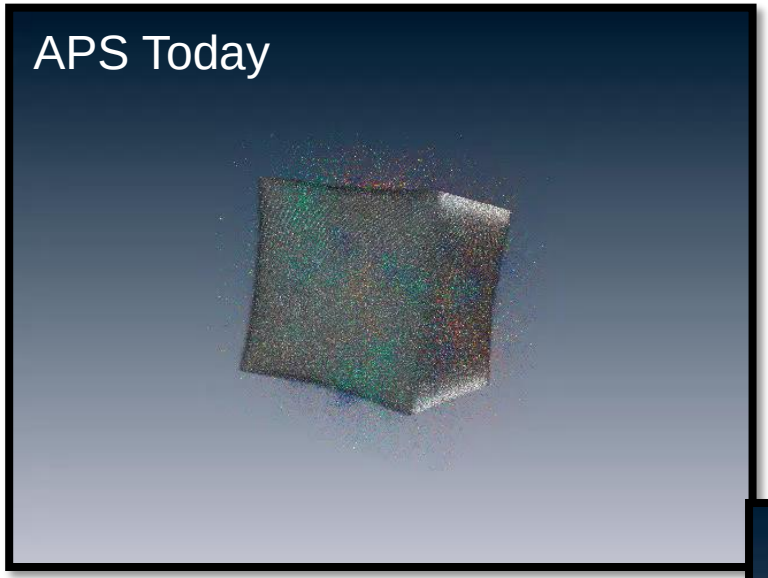
Coherence

Enabling highest spatial resolution even in non-periodic materials

- Extends lensless imaging to hard x-ray domain, with resolution down to <1 nm, localizing atoms
- Increases phase contrast for fast full field imaging
- Correlation methods improve by 10,000-1,000,000x



High brightness: Higher resolution, faster dynamics



1 nm Cu (green), Co (blue), Ni (yellow); only photon noise, $(1\mu m)^3$ alumina support visible

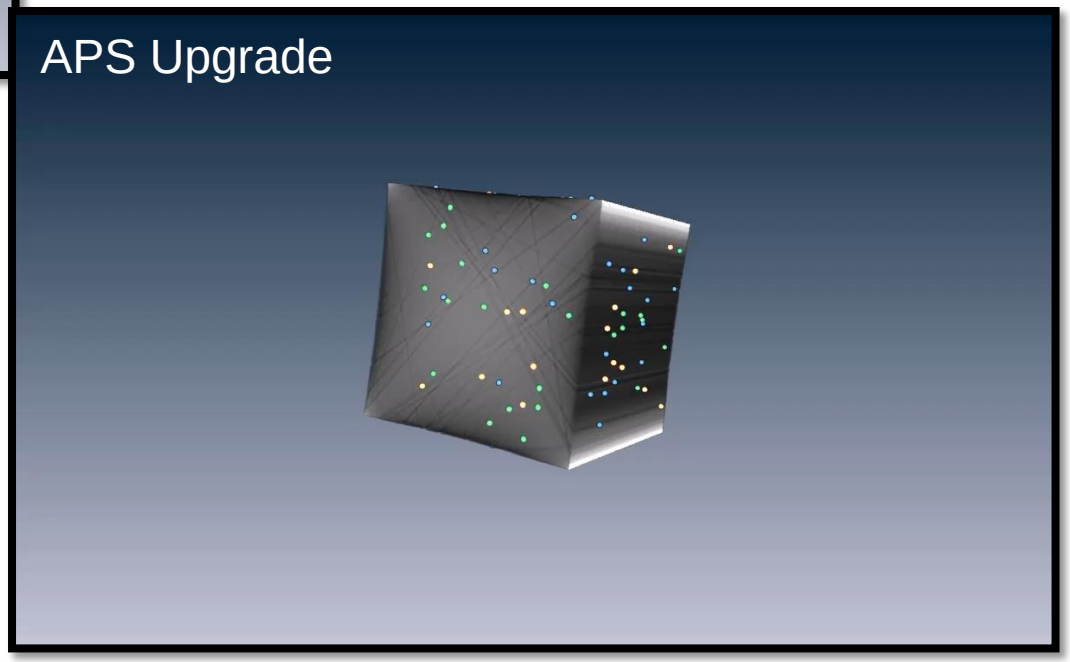
World's brightest storage ring light source above 4 keV

Brightness – increasing the number of photons that hit the target – is key to:

- Visualizing nanoscale structure across macroscopic fields of view
- Electronic/magnetic/chemical contrast

Only APS-U's extreme brightness at high energies enables exploration of individual nanostructures/defects

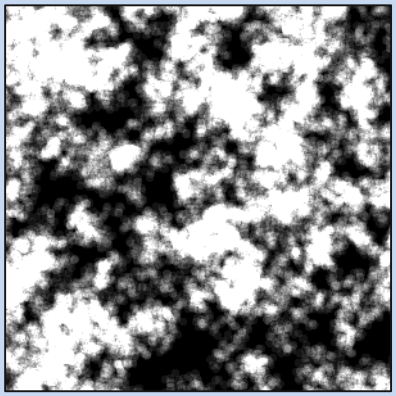
- Across length scales
- Deeply buried
- In real, complex environments
- Down to few-atom sensitivity

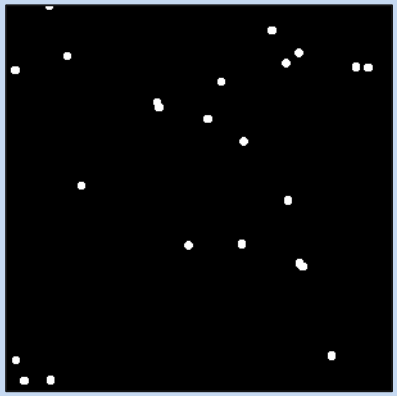


Catalytic nanoparticles clearly visible on alumina surface

APS-U's exceptional coherent flux opens new frontiers for study of dynamic processes

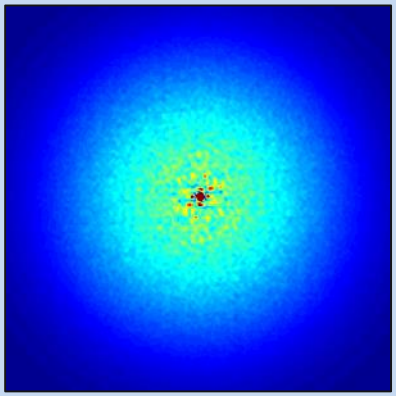
Ensemble (left) built up by fast particle dynamics (right)

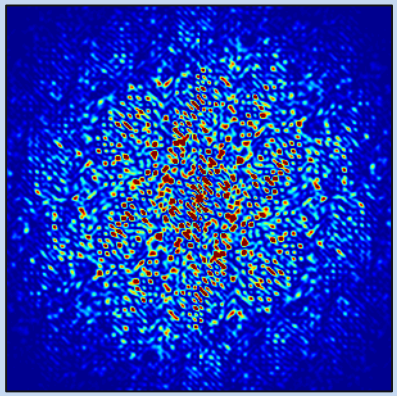




Today: X-ray photon correlation spectroscopy time-averages to ms, faster trajectories are lost

With APS-U: Speckle changes as sample evolves, dynamics are captured (simulation of 30x brightness)





Sensitivity ~ (Coherent flux)^2

APS-U: increases *up to 1,000,000x*

Allows us to probe:

- Continuous, atomic-scale dynamics down to nanoseconds
- Beyond standard pair correlations
  - Deterministic insight into growth mechanisms and stability of materials, deformation vs. diffusive motion, stick-slip in microfluidic flow

Argonne's leadership in HPC, computational science and data will propel and expand APS-U discoveries

New science at the upgraded APS will require:

- Real-time coupling of experimental data and modeling & simulation
- Real-time reconstructions (CDI, XPCS and movies, tomography)

APS today generates ~200 TB/month

- Current data flows ¼ of LCLS, exceed LHC
- With Upgrade, 1,000x more data

Argonne's leadership computing program addresses critical research needs for APS-U

- HPC and Mathematics and Computer Science expertise for new algorithms to understand data and for new approaches to data storage, manipulation and curation
- Pilot projects with ALCF on defect analysis, tomography, coherent imaging reconstruction, near-field high-energy diffraction microscopy

Experimental scattering

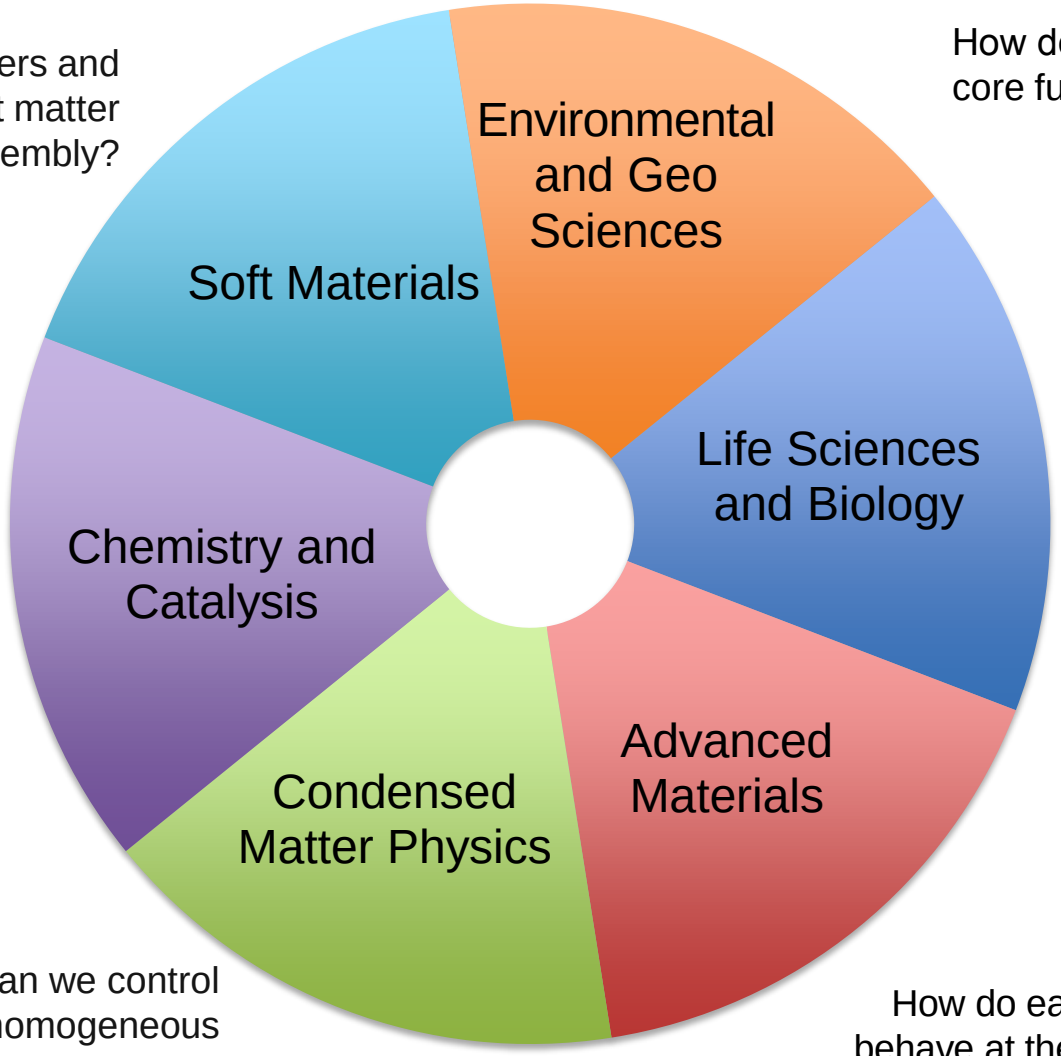
Structure

Simulated scattering

APS-U will revolutionize hard x-ray science, offer new approaches to answer critical scientific questions

What triggers and controls soft matter assembly?

How does the Earth's core function?



What roles do trace elements play in complex biological systems?

How can we engineer greener, advanced nanoscale catalysts?

Can we control inhomogeneous emergent states in quantum materials?

How do early-stage cracks behave at the sub-grain level in advanced structural materials?

Science Case Development

APS-U Science Planning Process

- We have launched the Science Planning process leading to an "Early Science"-type document, co-chaired by Stephen Streiffer and Paul Evans (U. Wisconsin)
- The goal of this process is to:
  - "…document the most exciting directions of scientific discovery for the upgraded facility and to map out the high-level technical requirements necessary to pursue these directions."
  - "…produce a highly selective, concise, and quantitative case describing the most exciting directions of research for the upgraded APS. "
- Working groups have formed, with WG leadership (confirmed):
  - **Biology and Life Sciences**: Gayle Woloschak (Northwestern), Bob Fischetti (ANL), Lee Makowski (Northeastern)
  - **Condensed Matter Physics**: Oleg Shpyrko (UCSD), John Freeland (ANL)
  - **Advanced Materials / Mesoscale Engineering**: Bob Suter (CMU), Dillon Fong (ANL), Peter Chupas (ANL)
  - **Chemistry and Catalysis**: A. Wilkinson (Ga. Tech), David Tiede (ANL), Karena Chapman (ANL)
  - **Soft Matter**: Bob Leheny (Johns Hopkins), Alec Sandy (ANL)
  - **Environmental Science and Geo Science**: John Parise (SBU), A. Lanzirotti (UC)

Science Case Development

APS-U Science Planning Process

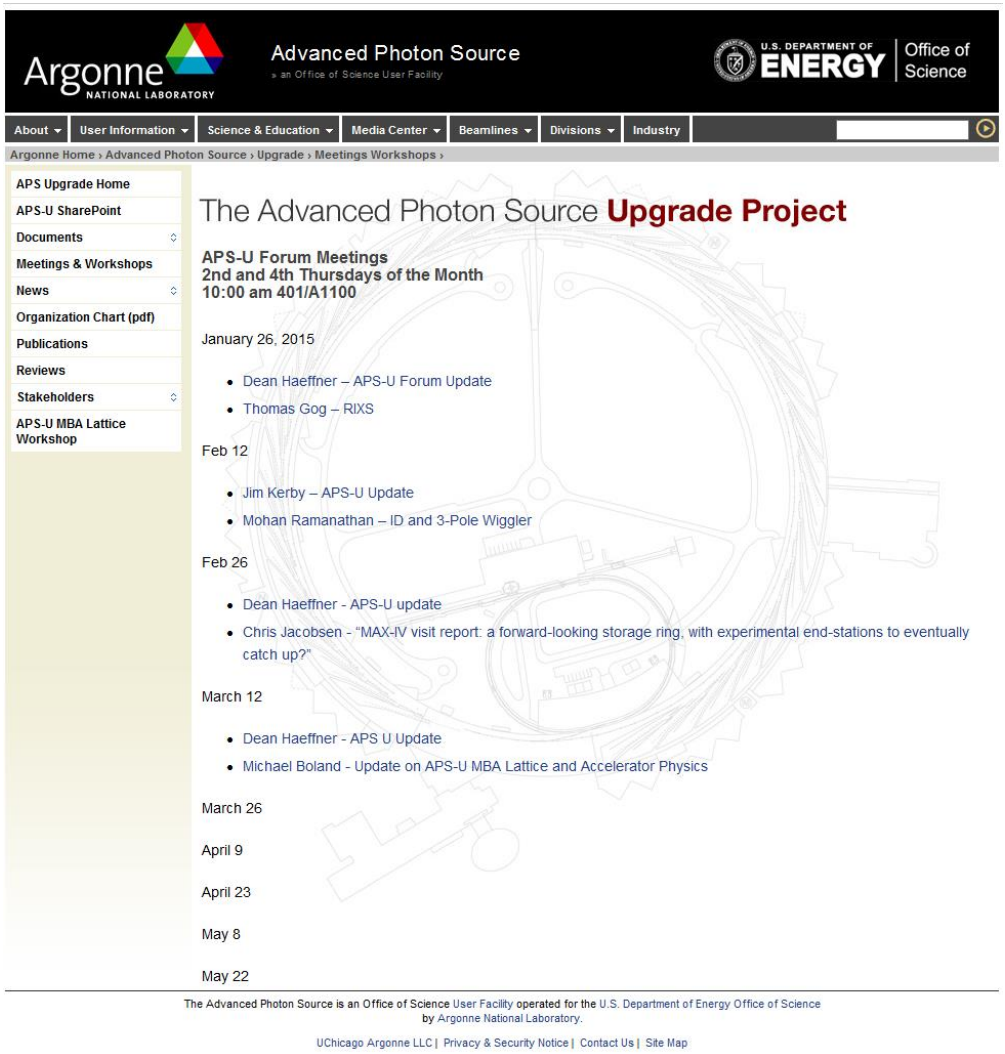
WE WANT YOU!

- Science Planning Workshops:
  - May 18-19: Chemistry and Catalysis
  - May 18-19: Biological and Life Sciences
  - May 19-20: Soft Matter
  - May 20-21: Condensed Matter Physics
  - May 21-22: Advanced Materials / Mesoscale Engineering
  - June 1-2: Environmental and Geosciences
  - (Plan to support remote participation via bluejeans)
- Builds upon the 2013 workshop series (more technical in nature)

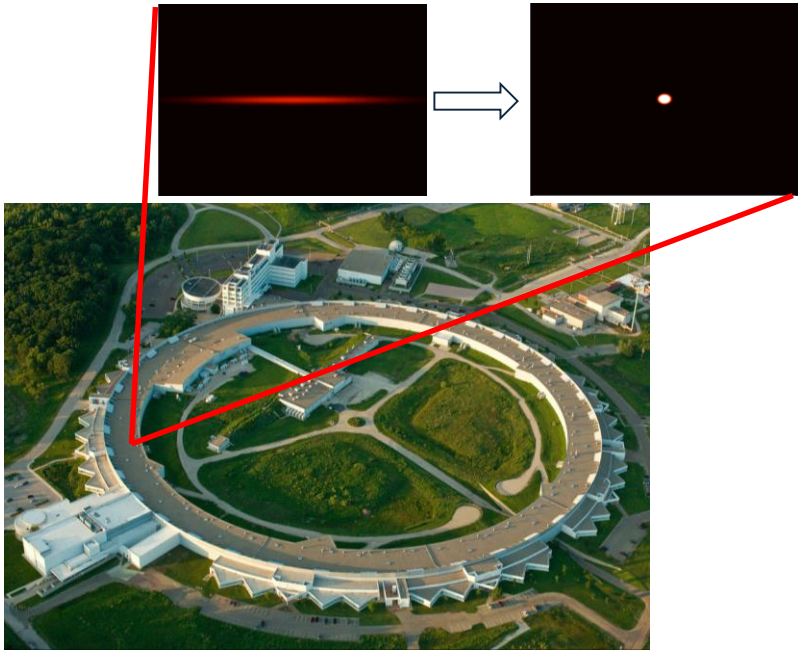
- Ultimately the success of the APS lies in its scientific excellence and creativity.
  - We would like to encourage you to contribute energetically and creatively to this process.
- Ways that you can contribute include:
  - articulating your ideas and bringing them to the working groups
  - participating in the planning workshops, and
  - using your time and energy to put the most promising ideas on a firm technical foundation.

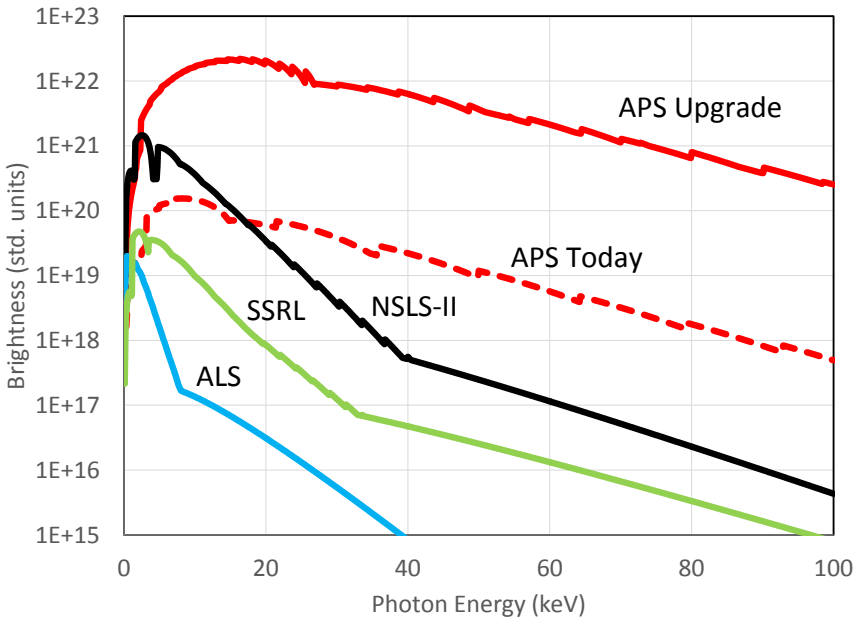
The Upgrade Forum

- We have launched the "Upgrade Forum"
  - This is a forum to fill a need for discussion, presentation, brain-storming around upgrade topics of mutual interest to the scientific community, beamline scientists, accelerator and project staff
  - It is the principal mechanism for communication and discussion with the resident scientific community
  - Dean Haeffner and Stefan Vogt are organizing
- Upcoming topics April 23:
  - T. Fornek, APS-U staging, removal and installation



The future is bright





Brightness vs. x-ray energy at top beamlines among BES synchrotron facilities

Thank you very much for your attention!!!