

# APS-U impact and perturbation for Structural Biology

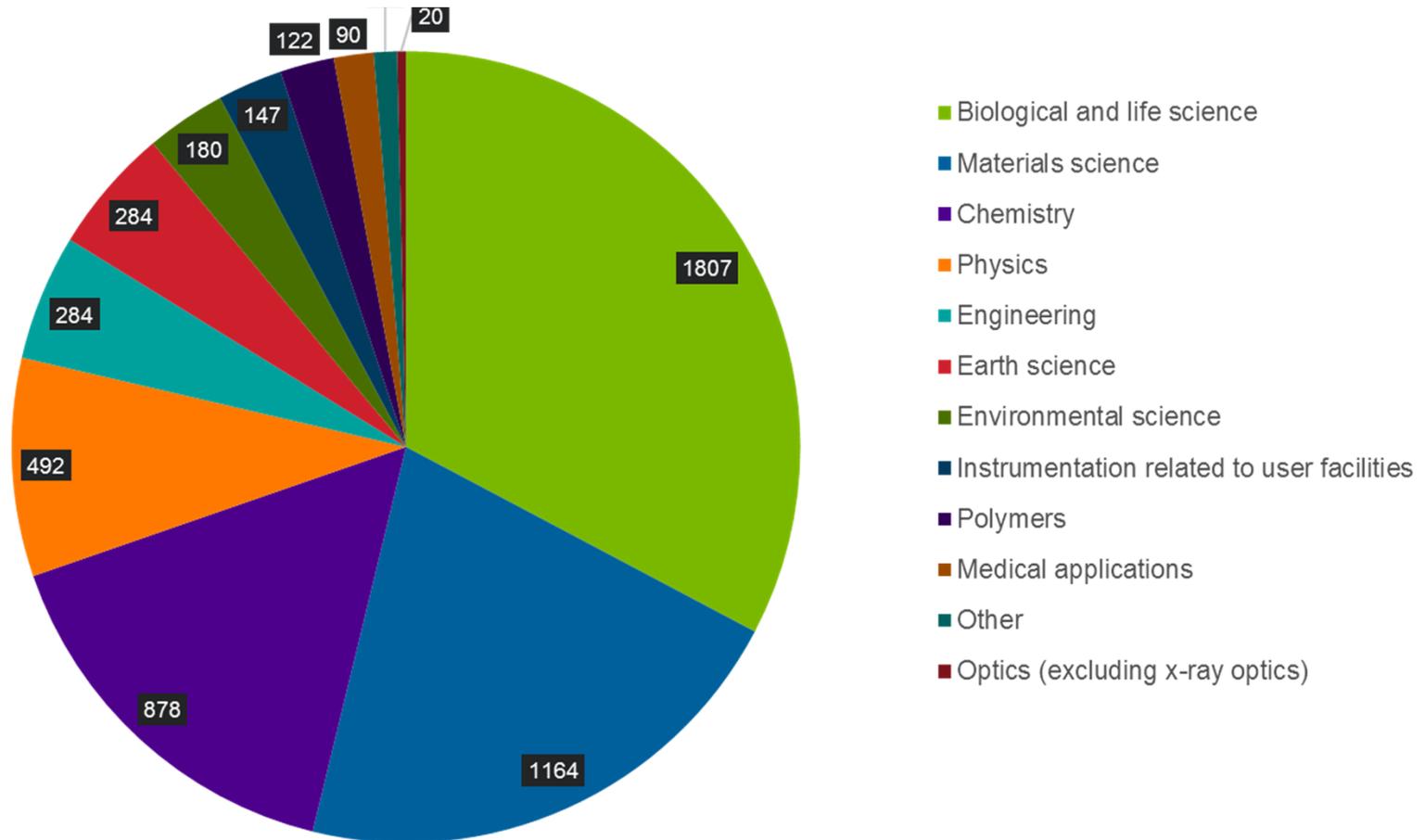
R. Fischetti, ANL

S. McSweeney, BNL

# Prepared with help an input from

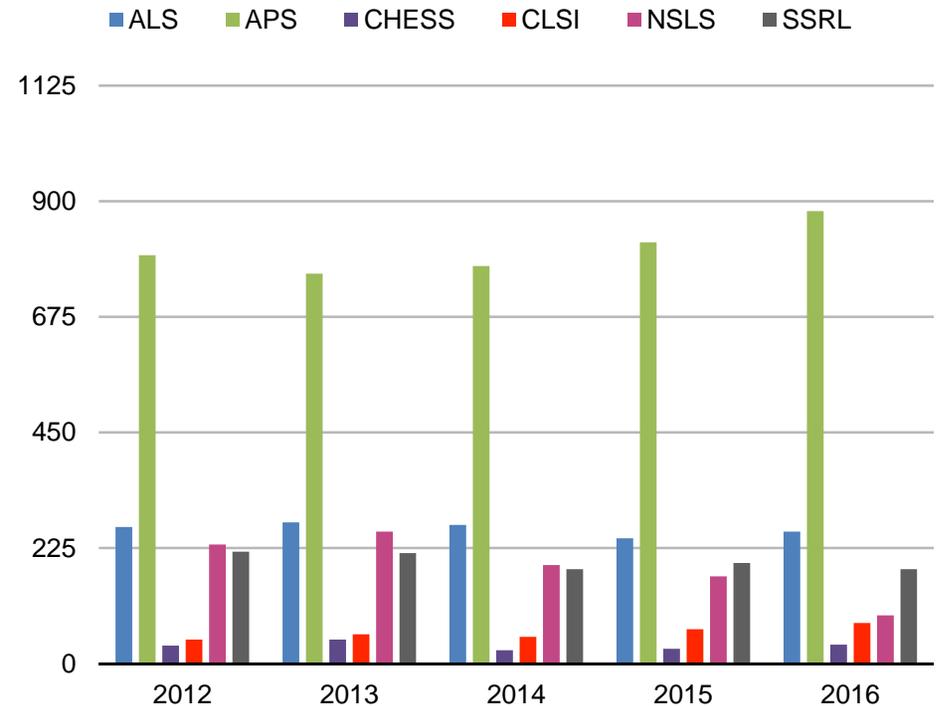
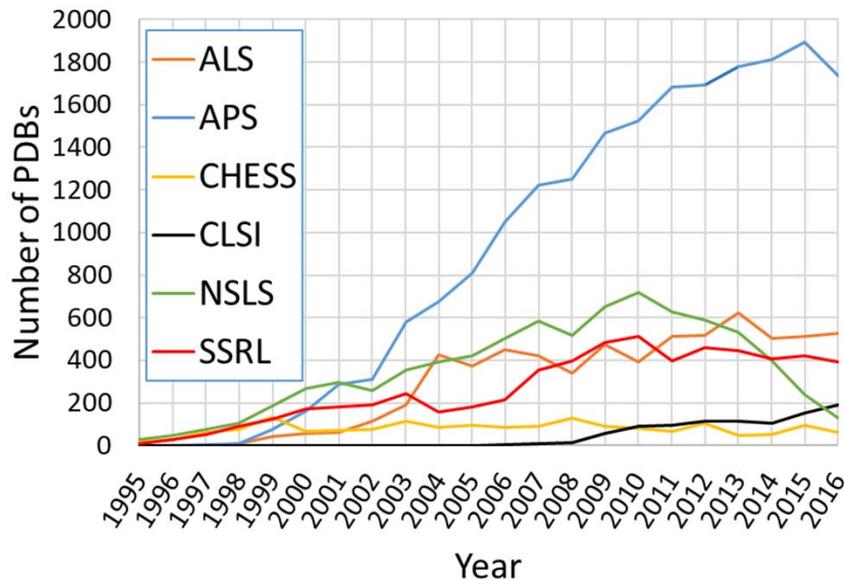
- ALS Paul Adams and Corie Ralston
- APS Bob Fischetti
- NSLS-II Sean McSweeney
- SSRL Britt Hedman and Keith Hodgson
- LCLS Soichi Wakatsuki
- CHESS Rick Cerione, Marian Szebenyi and Richard Gillian

# Bio & Life Sciences is the largest community at APS



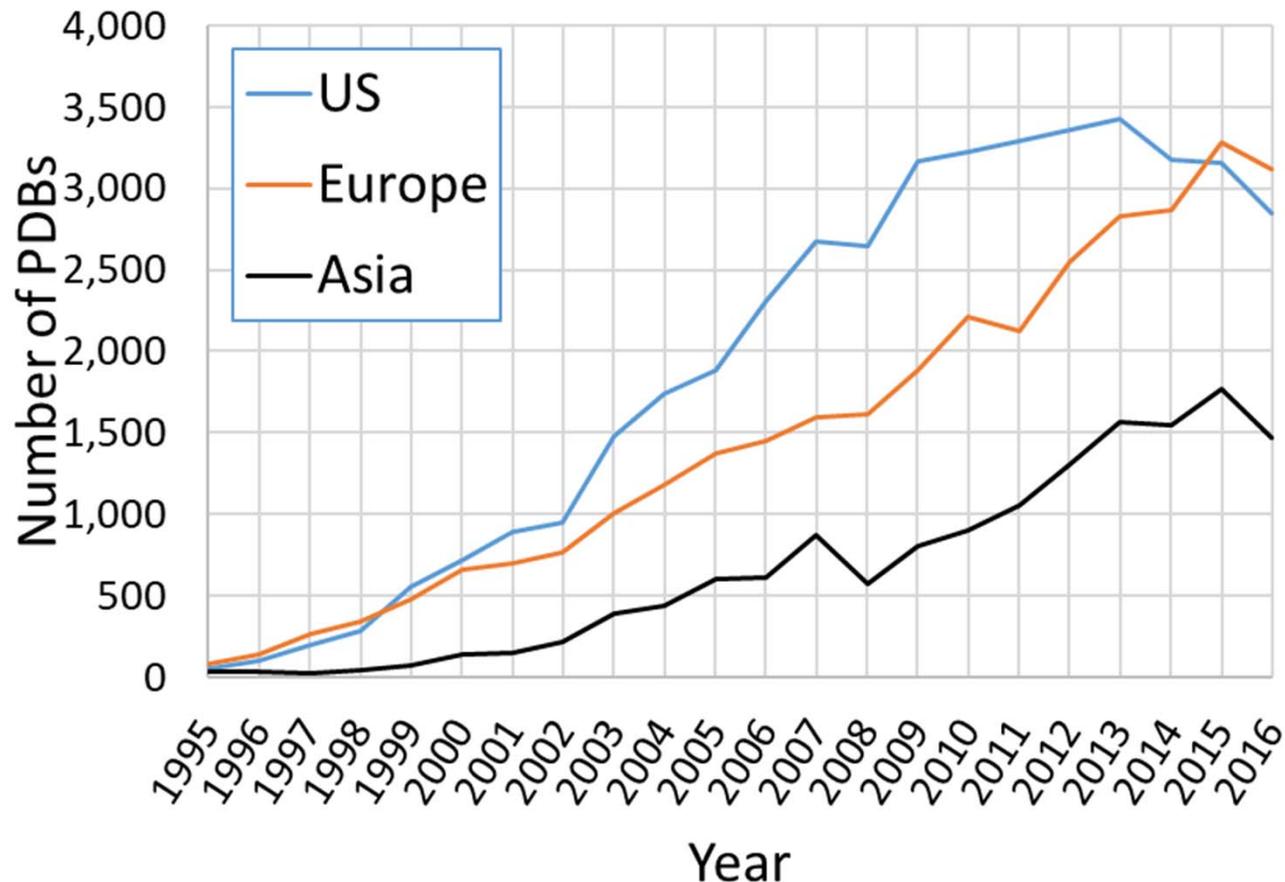
Unique Users

# APS plays a leading role in US structural biology.



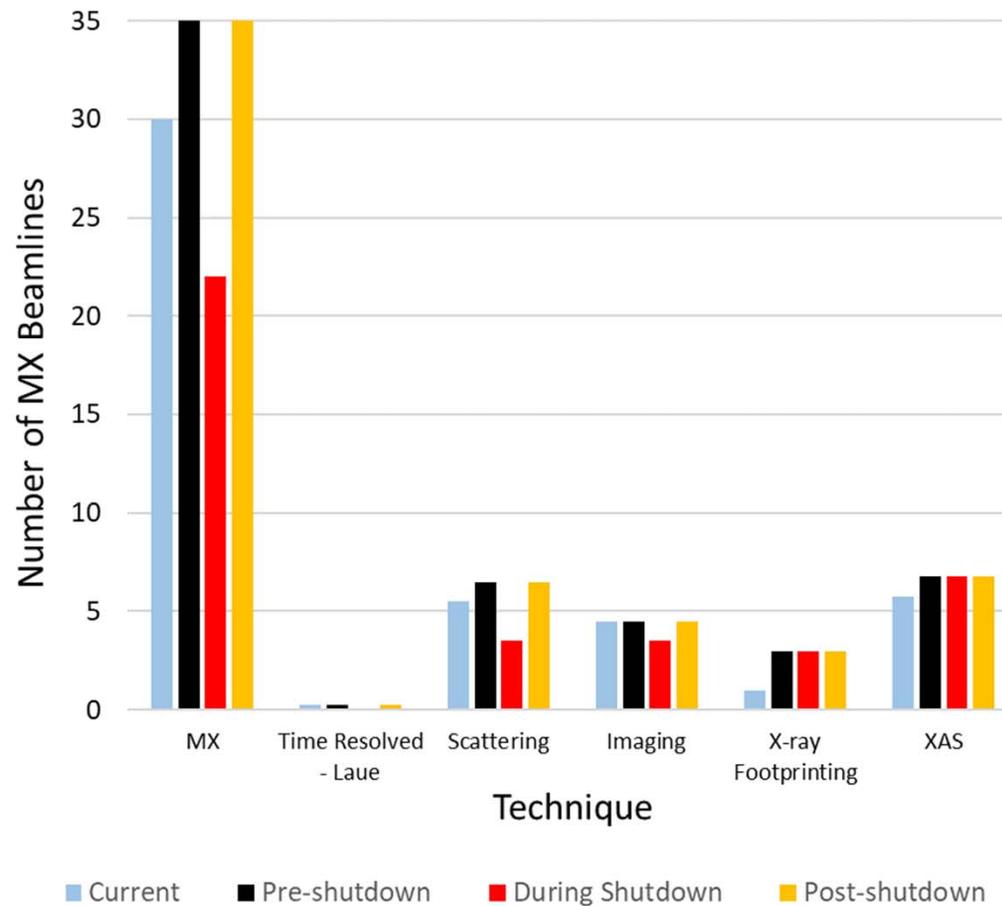
APS's leading role is clear both in terms of annual PDB depositions (l), and publications (r) (retrieved from biosync website, Oct 7<sup>th</sup> 2017)

# Europe has overtaken US as leader in productivity.



Europe and Asia continue to see strong growth in structural biology. New beamlines are coming on line and refurbishment of existing stimulates community interest - we need beamlines with characteristics that match the communities needs.

# Impact of APS-U on specific science areas.



The impact will be felt most strongly in MX & Laue. We estimate other techniques will be able to accommodate demand during APS-U

# Can the impact of APS-U for MX be mitigated by simple measures?

**Table 4:** Additional output per lightsource necessary to replace APS, and assuming NSLS-II is able to achieve the growth in capacity observed at other facilities.

	<u>AvePDB</u>	<u>AvePDB with NSLS-II</u>	<u>plus 20%</u>	<u>plus 50%</u>	<u>plus 100%</u>	<u>plus 200%</u>
ALS	473	473	567.6	709.5	946.	1419.
CHESS	65	65	78.	97.5	130.	195.
CLS	121	121	145.2	181.5	242.	363.
SSRL	383	383	459.6	574.5	766.	1149.
NSLS-II		250	250	250	250	250
Delta		-1701	-1492.6	-1180.	-659.	+383.

It seems impractical to assume that the effect of the APS-U shutdown can be mitigated by simple improvements in efficiency.

This is table 4 page 10 of the report

# The APS-U perturbation: duration.

Trying to understand the likely duration of the APS-U perturbation was not easy, and differences of opinion remain. The ease of transition from APS to APS-U will depend critically on the state of preparation of each beamline, thus we offer a range of possibilities based on our experience and the public data.

Duration of the perturbation to APS productivity after APS-U shutdown.

- Best case: 12 months to reach full operations + 6 months delay for PDBs to emerge= 18 months.
- Medium case: if resources are not available in a timely fashion: 18 – 36 months.
- Worst case: if the beamlines are “like new”: 36 – 48 months.

# Recomendations.

- Facilities should approach funding agencies with requests for funds to improve efficiency through a higher degree of automation.
- Facilities should approach funding agencies with requests for supplemental funding to provide funds for additional staffing to improve efficiency. This may include temporary reassignment of staff from APS beamlines.
- Although two new microfocus sources will come online in the next two years: one at SSRL, one at ALS, there still will be a significant shortage of beamlines providing microfocus capabilities for structural biology in the not too distant future. Therefore, one or more beamlines should be built, or upgraded, at the SR facilities to meet this growing need.

# More, perhaps APS specific, recommendations.

- APS management and APS CAT management initiate negotiation of interim agreements with lightsources that will be operations during the APS to APS-U transition period.
- APS management organize a “meeting of minds” bringing together APS-CATS, lightsource facilities and leaders & opinion formers in the structural biology community to evaluate the impact in a transparent fashion and as a consequence prioritized mitigations for the transition period.
- Consolidated action to stimulate the development of standardized higher density sample holders and mounts to allow for improvements of throughput in anticipation of greater demand at all facilities – this may be most effectively performed as a “stimulus package” associated with APS-U.
- Coordinated action, and communication by lightsource management with sponsors – national and CAT members at APS – to encourage big picture solutions to the problem facing us.



# Assumptions about APS Structural Biology beamlines

Assumptions about APS Structural Biology beamlines:

- Beamlines will be 20+ years old and need upgrading for reliability and to exploit the characteristics of the new source.
- Beamlines will be upgraded in place with the existing infrastructure. (However, SBC might be moved and rebuilt.)
- Beamlines are highly automated requiring extensive commissioning time to unsure reliability and robustness.
- Beamlines are well prepared for first light when the APS-U starts up, and can ramp up to full operations in 12 months. Do all CATs have sufficient staffing to accomplish this?
- Upgraded beamlines will return to the 100 PDB depositions/year output rate faster than new beamlines - typical 4-5 years as seen on the publicly available data on the Biosync web site.
- Users do not migrate away from the APS before the shut down (as they did with NSLS).
- The user community returns quickly after the beamlines are operational.