Argonne NATIONAL LABORATORY

… for a brighter future

U.S. Department of Energy

THE UNIVERSITY OF CHICAGO

Office of Science
U.S. DEPARTMENT OF ENERGY

A U.S. Department of Energy laboratory managed by The University of Chicago

Charge to the participants in the APS Renewal Workshop

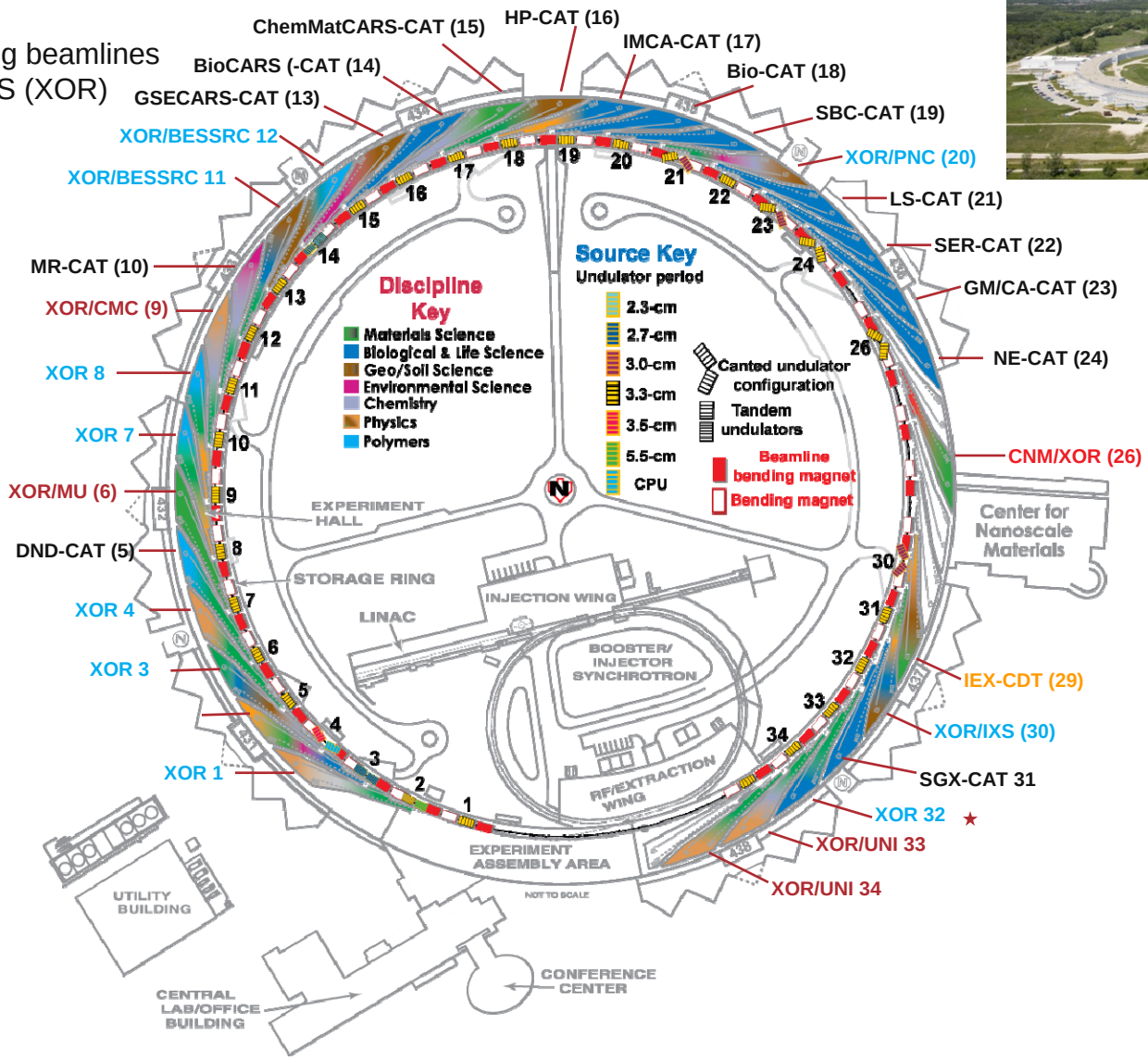
J. Murray Gibson

October 20th 2008

Thank-you all for coming!

APS today

FY '08: 54 operating beamlines
30 operated by APS (XOR)

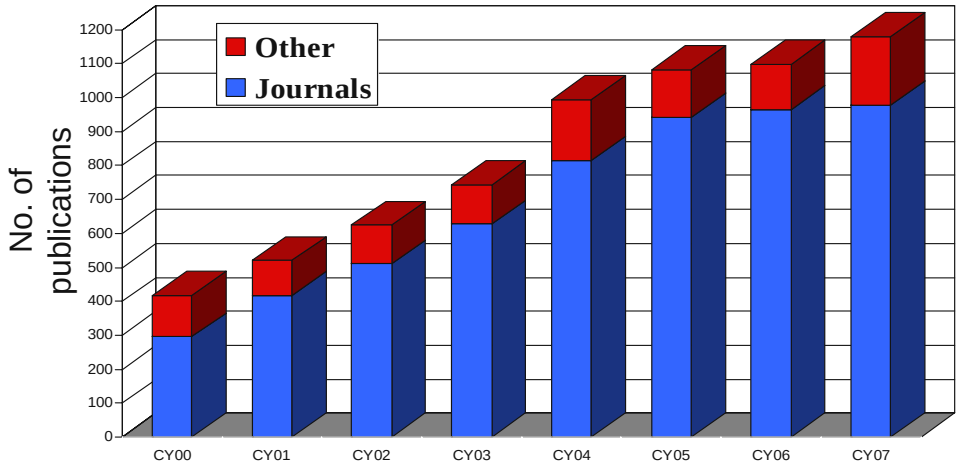


Key

CAT sectors
Current XOR sectors
Transitioning to XOR sector
CDT sector
Operated jointly (APS, CNM)

Annual published output from APS users

Journal Papers

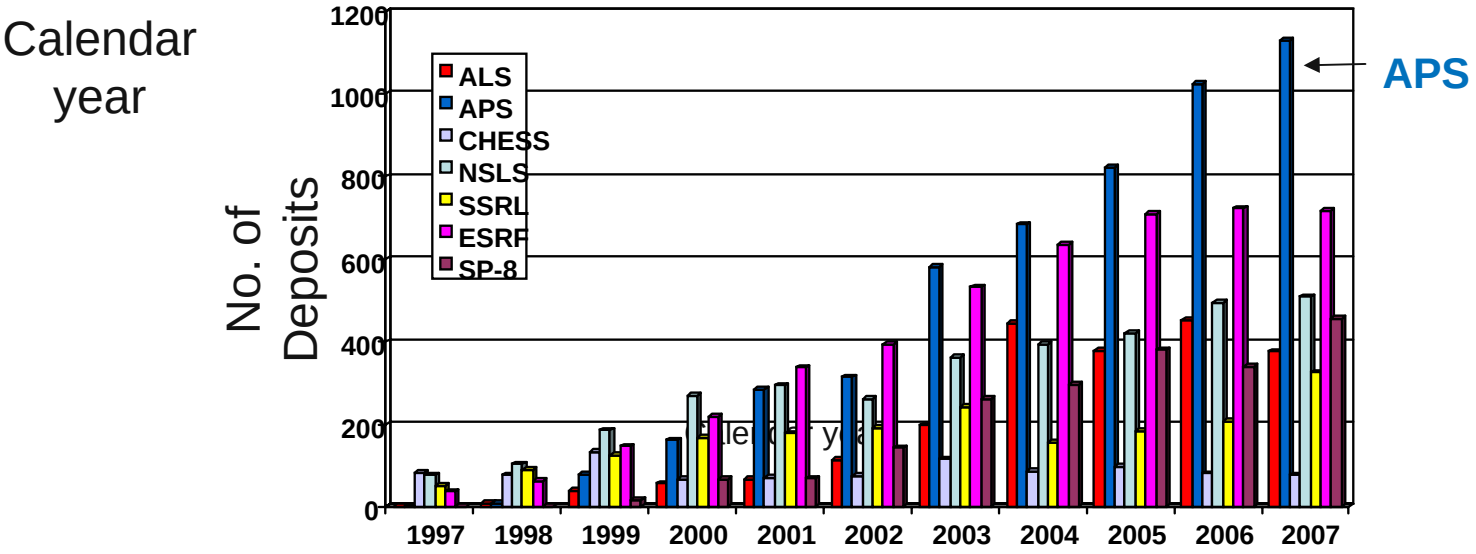


151 papers in *Cell*, *Nature*, *Science*, *PNAS*, *PRL* in 2006

60% of 2007 APS journal papers had impact factor >3.5 (c.f. 53% in 2001)

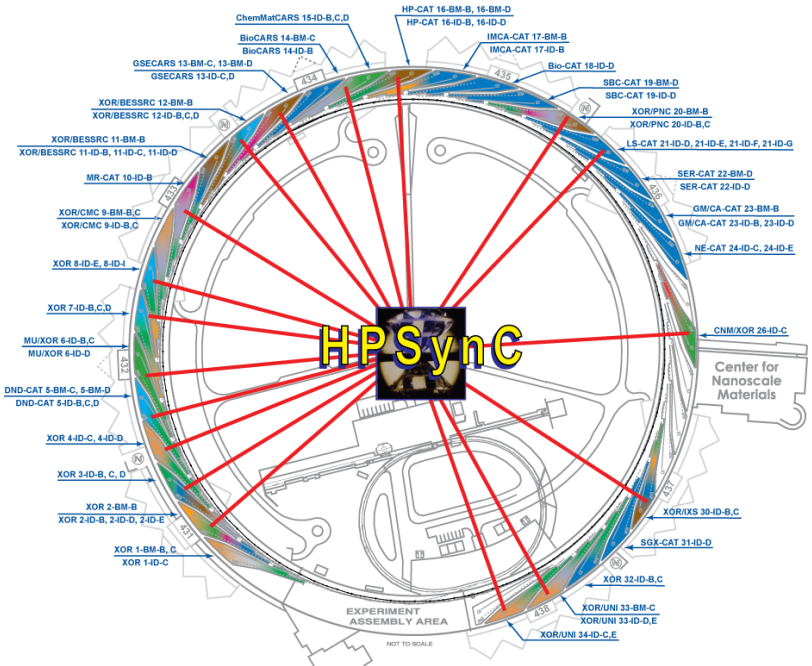
***as of 4.30.08**

PDB Deposits

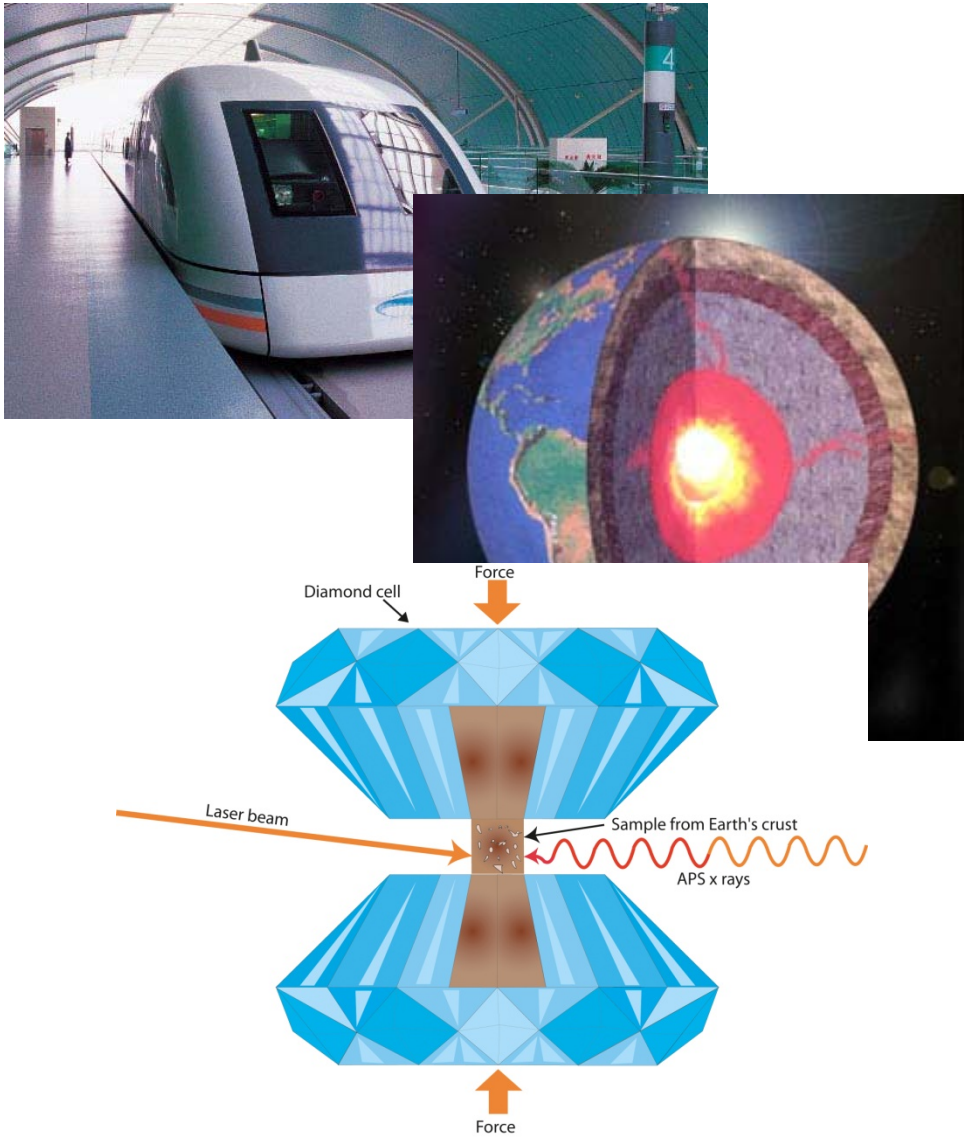


APS research under extreme conditions flourishes

- High-pressure science
  - A foundry for new materials
- Planetary science
- In-situ science, e.g. surface/interface

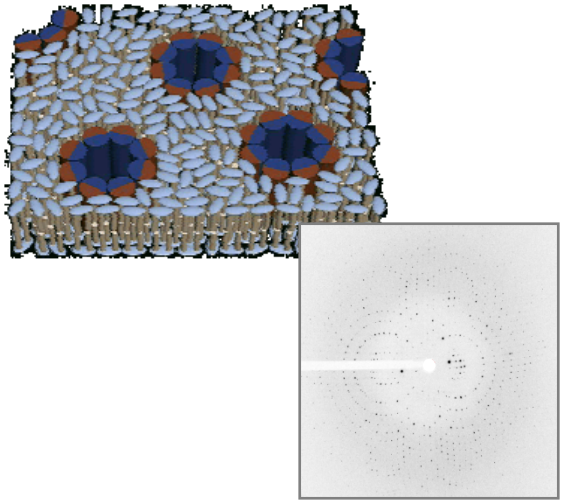


75 papers in *Nature*, *Science*, *PRL* and *PNAS* from APS high pressure science in 2003-2007

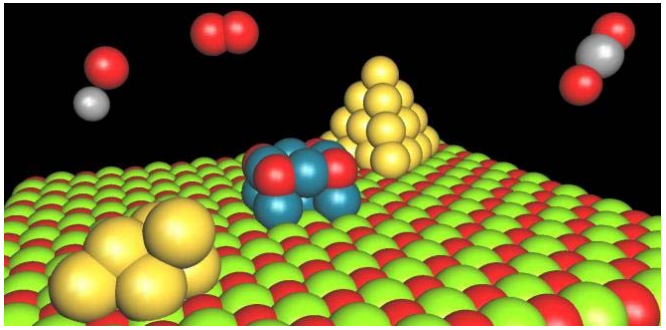


Where is APS science impact growing most rapidly?

- Protein crystallography
- Science under extreme conditions
- Biological applications of imaging
- Nanoscience
- Catalysis
- …..

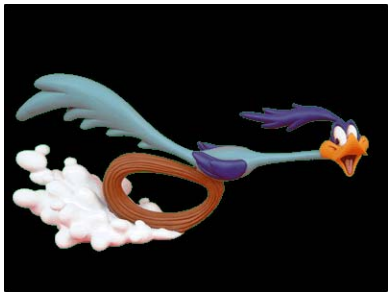


The future will be



ultrasmall

ultrafast

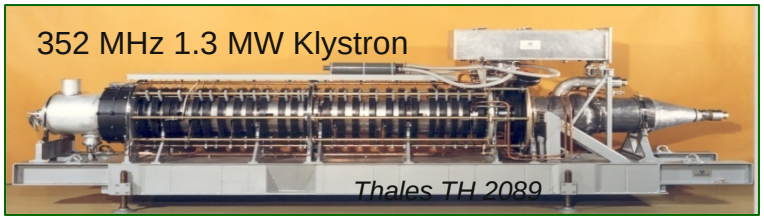


But many components (on accelerator and beamlines) are becoming obsolete

- An RF coupler to the booster failed this winter and led to a 40 hour downtime – this component had never failed in 11 years of operation

- We plan for obsolescence, but our resources to cope with it are inadequate

- Take nothing for granted – e.g. water brought down the Roman Empire (Gibbons)



What is the opportunity for an APS Renewal project?

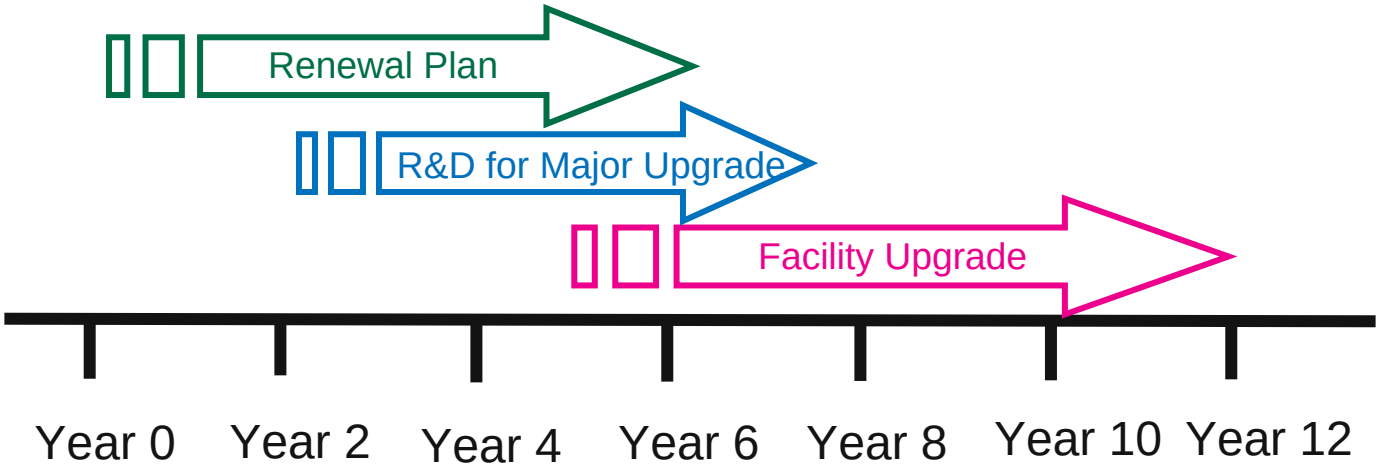
- Users demand new capabilities
- New possibilities in instrumentation
- In many cases, capacity is inadequate
- Obsolescence is a major problem

- These issues were identified in DOE and UC reviews of APS in 2007
  - DOE requested the development of a renewal plan

  - Covering five years, addressing renewed beamlines and supporting techniques
    - *And encompassing obsolescence issues*

The renewal plan dovetails with Argonne's strategic planning

- The APS 2020 Plan is an high-priority component of the ANL Business Plan, recently submitted to DOE, that (among other things) describes the Laboratory's major activities over the next 5-10 years.
- Hard x-ray science is a major feature of the ANL business plan
- The APS 2020 Plan has several components to keep APS at state-of-the-art for hard x-rays:
  - APS Renewal Plan - a 5 year science-driven investment plan that will focus on beamlines, optics, detectors, and source improvements
  - R&D for Major Upgrade - a plan that focused on the R&D required for a major facility upgrade that will build on the Renewal Plan that will take SR sources to the next level
  - Facility Upgrade - a project that, once defined and approved by funding agencies, would keep the synchrotron radiation facilities at ANL at the state-of-the-art to 2020 and beyond.



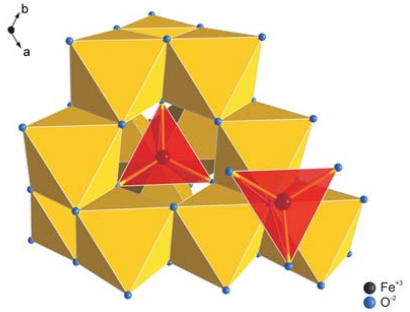
How does would an APS renewal fit the national picture for third generation and new sources?

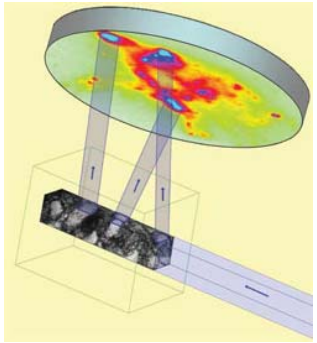
Source Name	Location	Type	1st Year of Operation	Characteristic Energy	No. of Beamlines	No. of Users (2007)
Advanced Photon Source	Illinois	Third-generation storage ring	1996	19.5 keV	60	3420
Advanced Light Source	California	Third-generation storage ring	1993	3.2 keV (12 keV super-bend)	43	1784
Stanford Synchrotron Radiation Laboratory	California	Upgraded second-generation storage ring	1973 (upgraded to third-generation in 2003-2004)	7.5 keV	34	1151
National Synchrotron Light Source	New York	Second-generation storage ring	1982	7.1 keV	65	2219
Cornell High Energy Synchrotron Source	New York	Partly dedicated (CESR: 3.5-12 GeV)	1980	10.4 keV	13	507
Linac Coherent Light Source	California	Free-electron laser	2009	N/A	4 (instmnts)	N/A
National Synchrotron Light Source II	New York	Upgraded second-generation storage ring	2015	2.4 keV	~58 possible	N/A

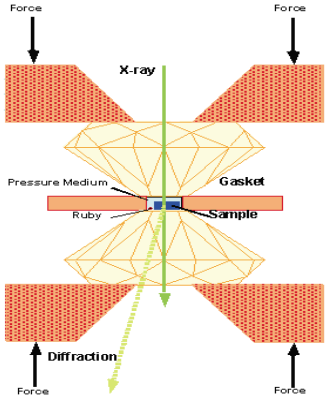
APS is the brightest source of hard x-rays with the largest user community in the USA - renewal will complement NSLS-II and LCLS

How would an APS renewal fit the international picture for hard x-ray sources?

Source Name	Location	Type	1st Year of Operation	Characteristic Energy	No. of Beamlines	No. of User VISITS (06)
Advanced Photon Source	U.S.	Third-generation storage ring	1996	19.5 keV	60	10,800
ESRF	France	Third-generation storage ring	1994	9.6 and 20.3 keV	49	6,090
SPring-8	Japan	Third-generation storage ring	1997	28.9 keV	48	11,640
PETRA III	Germany	Third-generation storage ring	2009	20.8 keV	14 (15-20 possible)	N/A

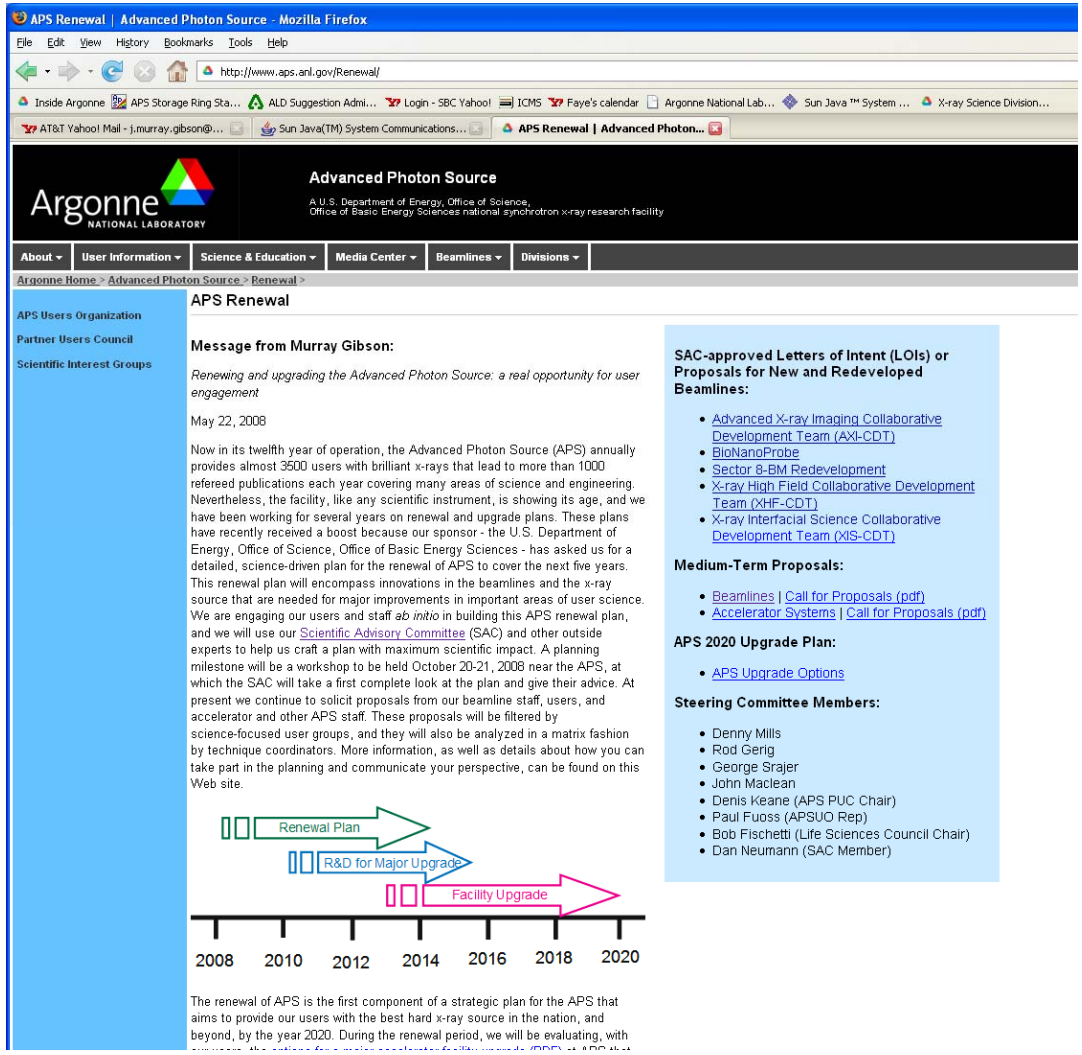






Each facility is planning for upgrade and renewal

APS Renewal – what have we done so far?

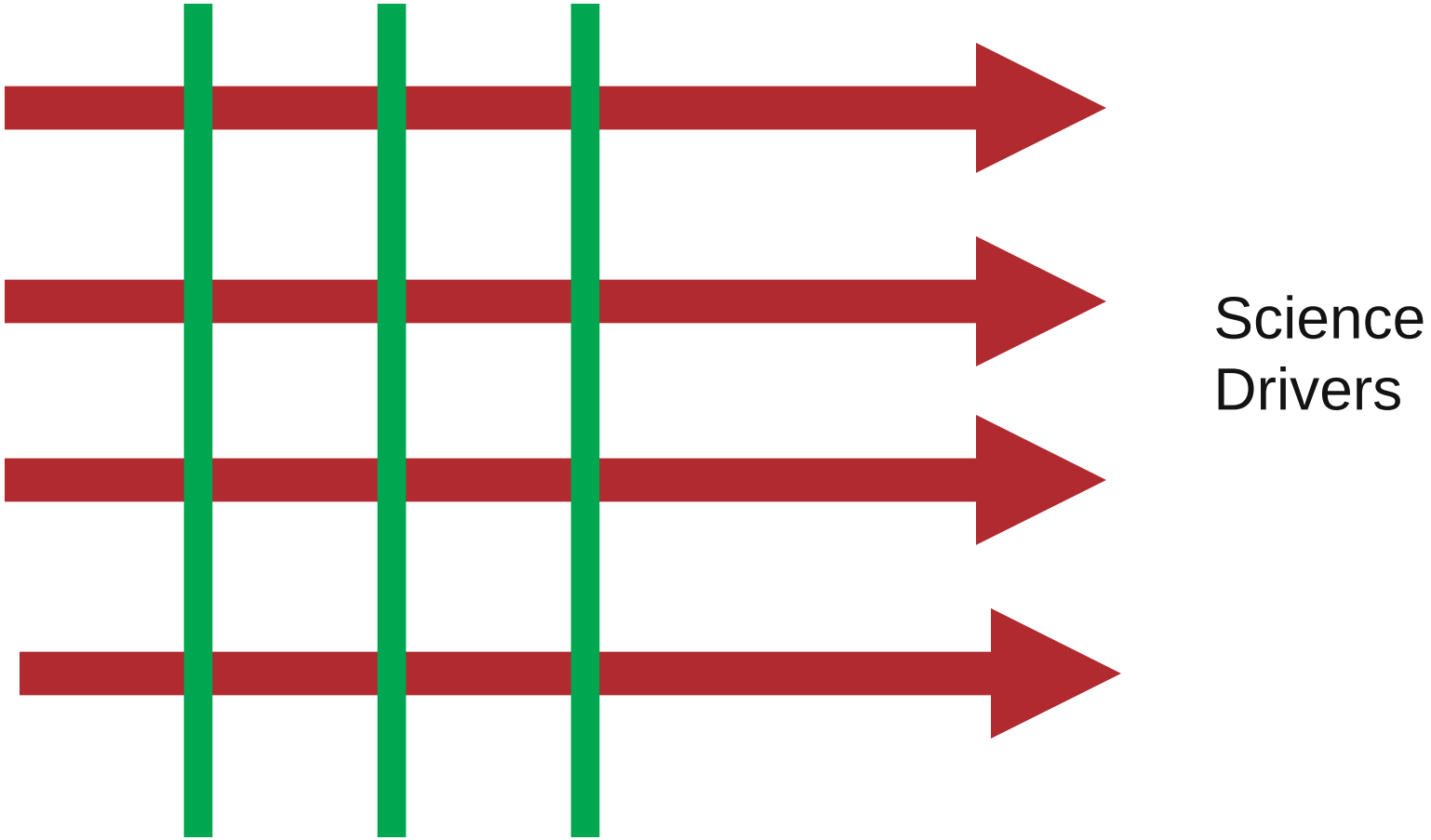


Steering Committee Members

- **APS Renewal Steering Committee**
  - Dennis Mills, Chair (SUF)
  - Rod Gerig (SUF)
  - George Srajer (XSD)
  - John Maclean (AES)
  - Paul Fuoss, APSUO representative (MSD)
  - Denis Keane, APS PUC representative (DND CAT/Northwestern)
  - Bob Fischetti, Life Sciences representative (GM/CA CAT)
  - Dan Neumann, SAC representative (NIST)
  - Diane Wilkinson, Administrative Support (ASD)

Thanks for all the time and effort you put in this!

A matrixed approach to the renewal



Call for Beamline- & Accelerator-Related Renewal Proposals

- In February 2008 we got things rolling by sending out an e-mail to:
  - CAT Directors,
  - XOR Group Leaders, and
  - Beamline Managers and/or Lead Scientists

  requesting that they develop ***beamline renewal proposals*** for the medium term (next 5 years). Beamline Advisory Committees (BACs) for the XOR beamlines were asked to help out here too.

42 Beamline-related renewal proposals were submitted

- We have ***7 letters of intent/proposals*** for entirely new beamlines
- At the same time, we requested ***source renewal proposals*** from the accelerator side that address obsolescence, reliability/spares, improved performance, and facility infrastructure.

69 Accelerator-related Proposals were submitted

Technical coordinators

- **Beamline Techniques**
  - **Coherence**: Ian McNulty (XSD)
  - **Full field imaging**: Wah-Keat Lee (XSD)
  - **General Diffraction (Bulk and Interfaces)**: Jon Tischler (ORNL)
  - **High Pressure**: Guoyin Shen (HP CAT)
  - **High Energy**: Dean Haeffner (XSD)
  - **Inelastic Scattering**: Thomas Gog (XSD)
  - **Nuclear Resonant Scattering**: Ercan Alp (XSD)
  - **Magnetic scattering**: Jonathan Lang (XSD)
  - **Microprobe**: Jorg Maser (CNM/XSD)
  - **Macromolecular Crystallography**: Craig Ogata (Bioscience ANL)
  - **Powder Diffraction**: Brian Toby (XSD)
  - **SAXS**: Byeongdu Lee (XSD)
  - **Spectroscopy (EXAFS, XANES)**: Matt Newville (GSE CARS)
  - **Time-resolved**: Eric Dufresne (XSD)
- **Technical Support**
  - **Beamline controls**: Mark Rivers (GSE CARS)
  - **Detectors**: Steve Ross (XSD)
  - **Nanopositioning**: Deming Shu (XSD)
  - **Optics**: Tom Toellner (XSD)
  - **Scientific software:** Peter Jemian (AES)
- **Behind the Shield Wall**
  - **Accelerator Operations**: Michael Borland (ASD)
  - **Beam Stability**: Glenn Decker (ASD)
  - **Front Ends**: Patrick den Hartog (AES)
  - **IDs**: Liz Moog (ASD)
- **Facility Infrastructure** John Maclean (AES)

Building the Science Case - FOCUS OF THIS MEETING

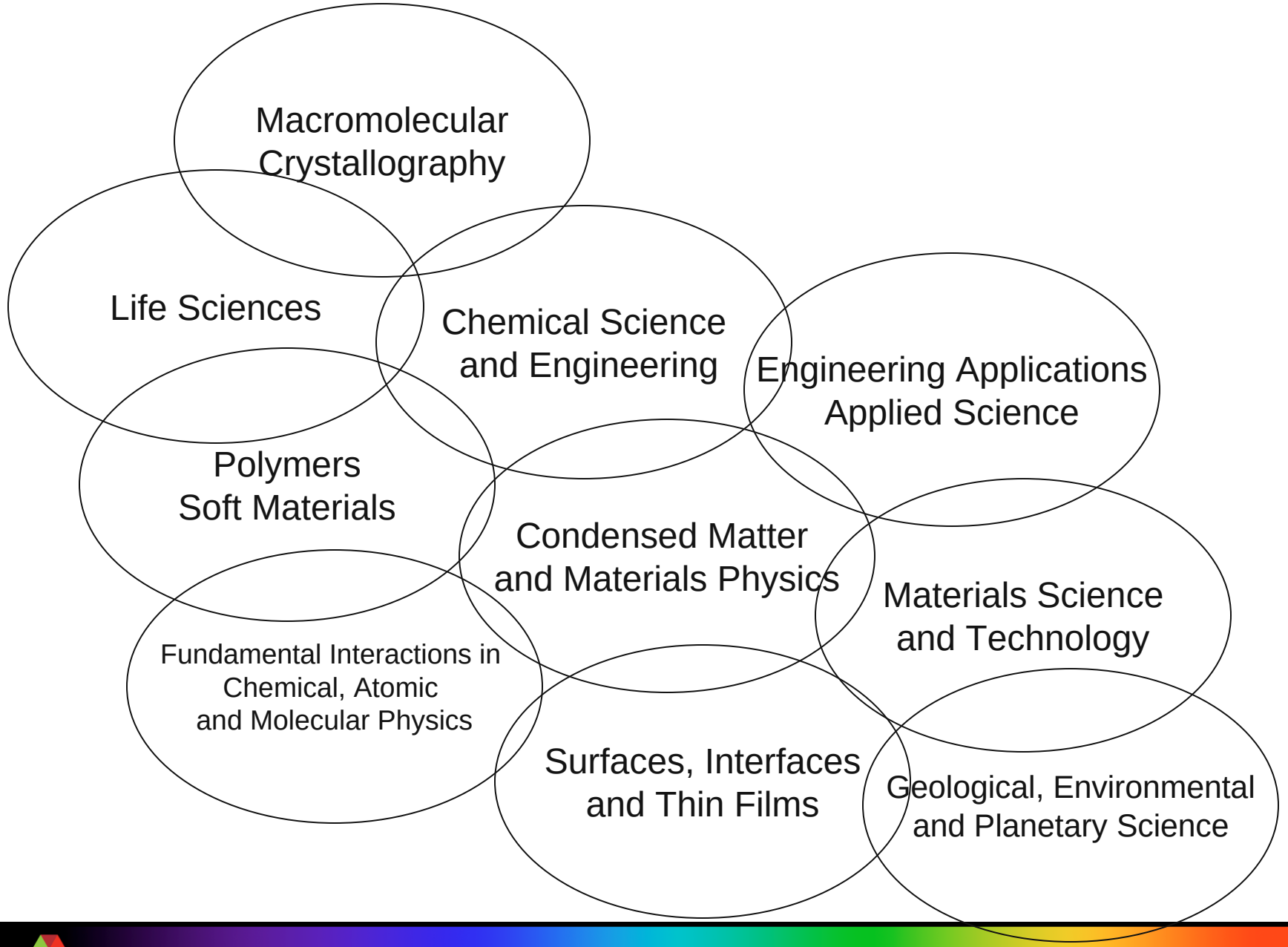
- It is essential that we build a strong ***science case*** for the renewal plan and use this to prioirtize our choices

- 10 Science areas/disciplines were identified by the Renewal Steering Committee

– Chemical Science and Engineering	J. Miller, ANL
– Condensed Matter and Materials Physics	S. Bader, ANL
– Engineering Applications/Applied Science	G. Ice, ORNL
– Fundamental Interactions in Chemical, Atomic and Molecular Physics	S. Rice, U of Chicago
– Geological, Environmental, and Planetary Sciences	N. Sturchio, UIC
– Life Sciences (excluding MX)	L. Makowski, ANL
– Macromolecular Crystallography (MX)	T. Kossiakoff, U of Chicago
– Materials Science and Technology	P. Evans, U of Wisconsin
– Polymers, Soft Materials	K. Shull, Northwestern
– Surfaces, Interfaces, and Thin Films	P. Fenter, ANL

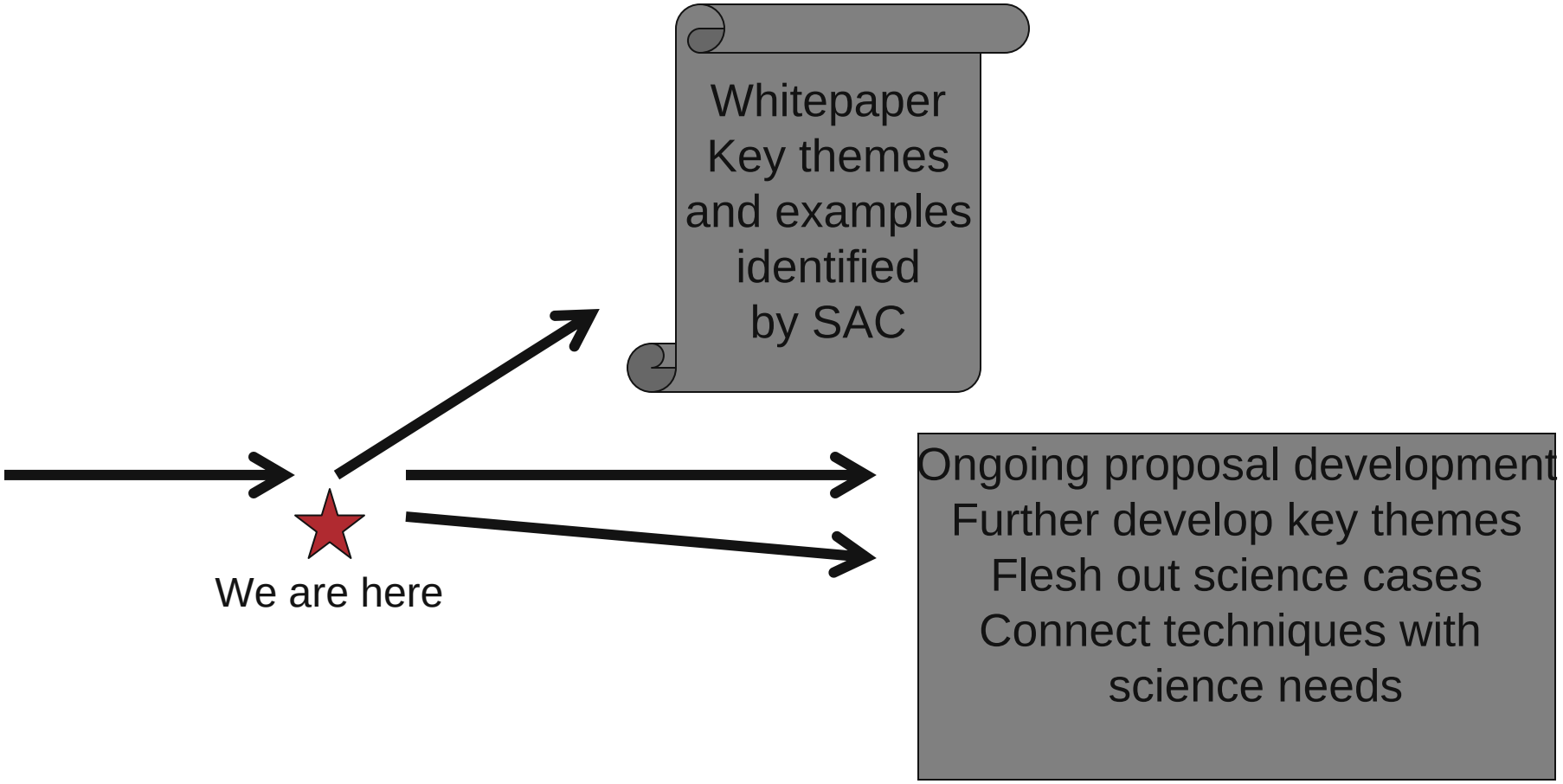
- A total of 56 scientists served on the Science Teams representing 28 different institutions that covered universities, industry, DOE facilities, and other government laboratories.

Thanks to all of you!


Macromolecular Crystallography
Life Sciences
Chemical Science and Engineering
Engineering Applications Applied Science
Polymers Soft Materials
Condensed Matter and Materials Physics
Materials Science and Technology
Fundamental Interactions in Chemical, Atomic and Molecular Physics
Surfaces, Interfaces and Thin Films
Geological, Environmental and Planetary Science

Short term roadmap

Due early Nov!



Whitepaper “bones” already prepared

What must we accomplish at this meeting?

- Critically flesh out the science cases
- Make the connection between techniques for science needs
- Identify key scientific themes and questions of most importance for a renewal
  - For whitepaper and to guide proposal development

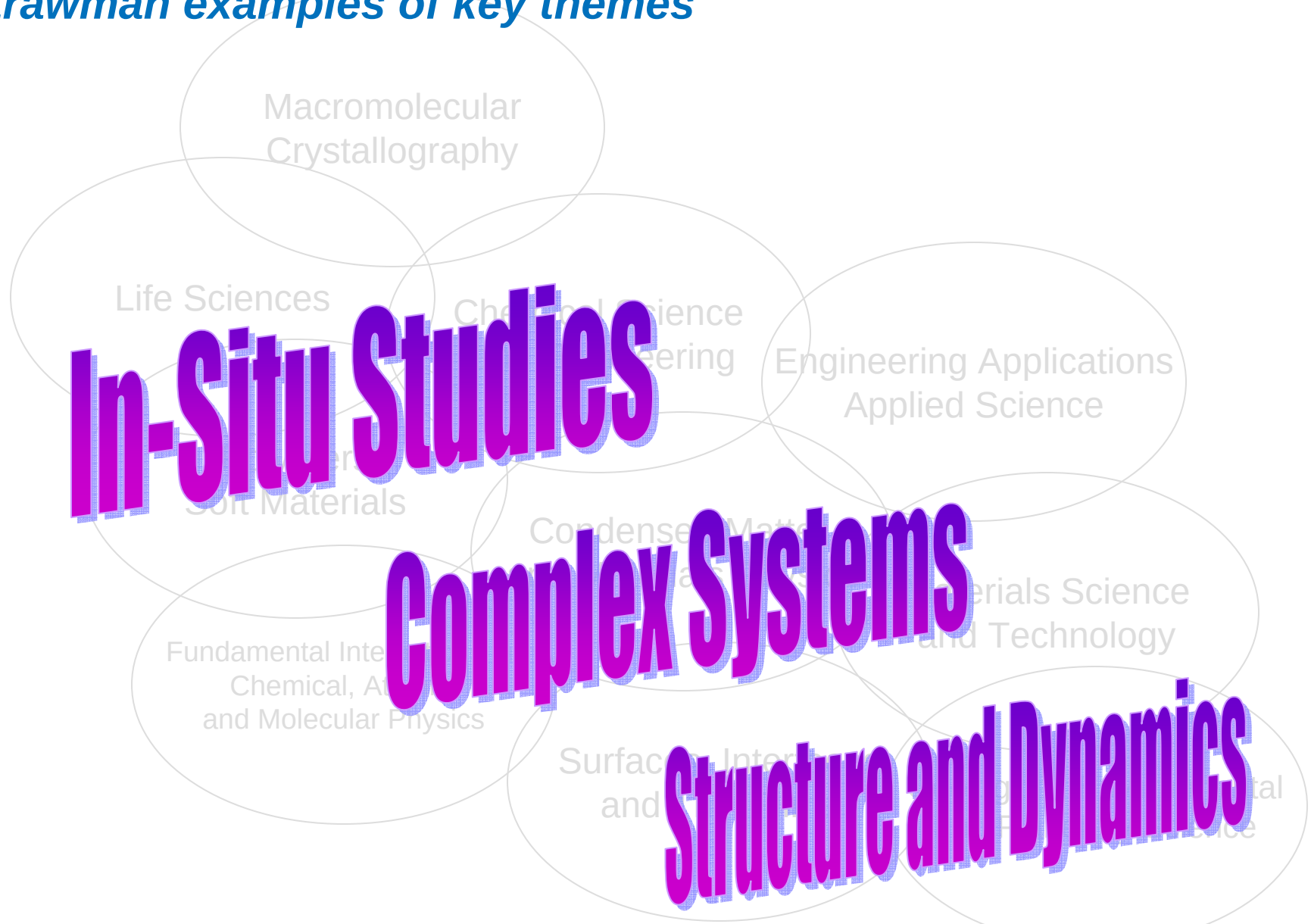
- Keep momentum going after the meeting in fleshing out science cases, identifying priority components of the renewal, and developing more detailed plans - we would like strengthened science cases with clear technique connections for our initial proposal as an outcome of this meeting (completed in several months).

Key needs for white paper from this meeting

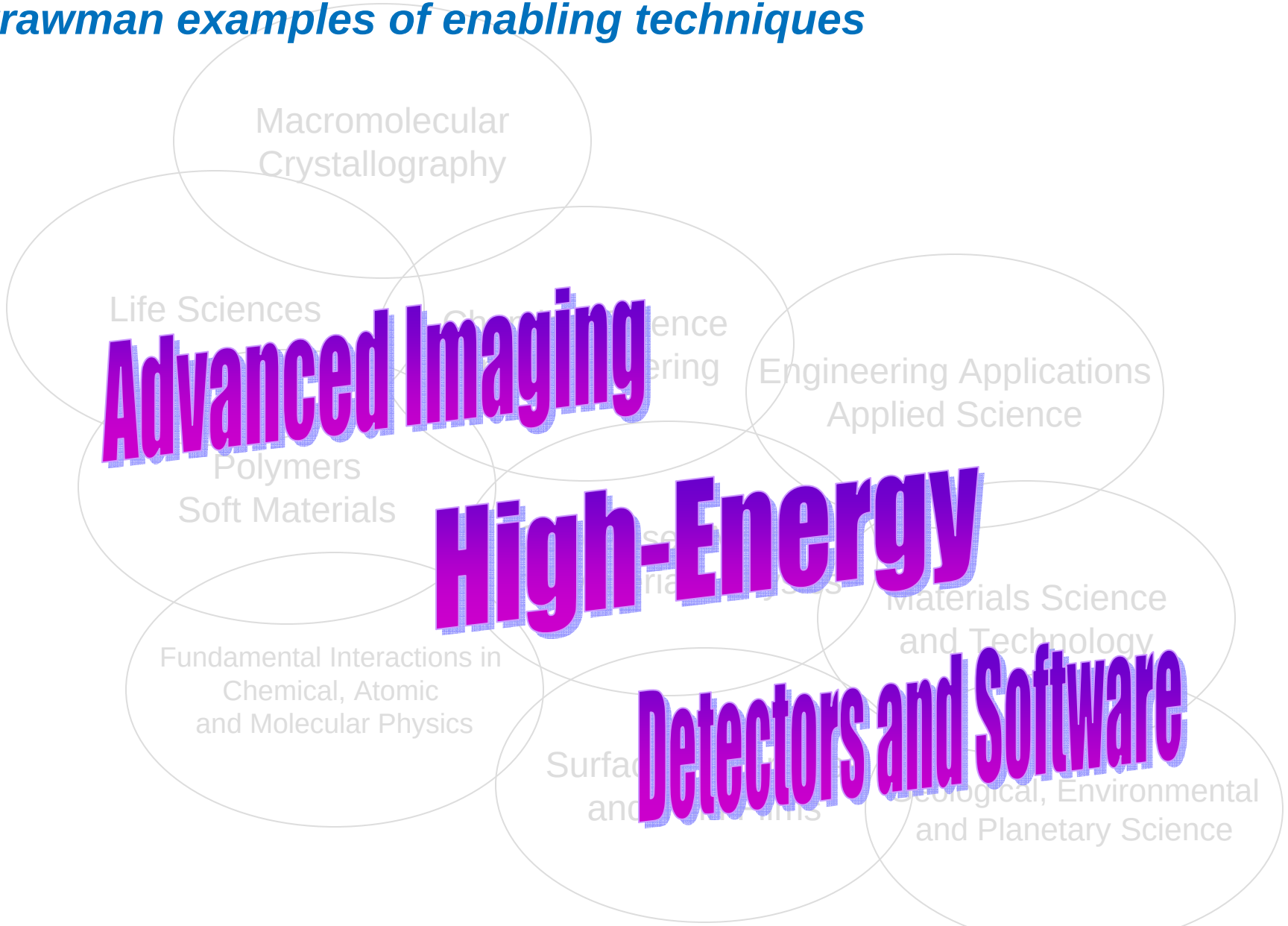
- Identify key science themes (no more than 5)
  - These may not map directly with science cases but could be cross-cutting
  - Energy should be a major focus, if not a theme
- For each theme list some high-priority science questions (from science cases)
  - And explain briefly how the renewal will accomplish these

- The SAC representatives here will have this as their main responsibility
  - The list is not meant to be exclusive, but to pick the highest priority ideas
  - All science cases and broader plan will move forward in parallel
    - *Expect a book like ESRF's laying our preconceptual design as precursor for CD-0*
    - *Major focus at next user meeting in May - workshops on key themes*

Strawman examples of key themes



Strawman examples of enabling techniques



Longer term roadmap for renewal project

CD-0

Table 1. SS/MS Critical Decision (CD) Points.

Pre-conceptual	Conceptual Design Phase	Execution Phase	Operations Phase
Approve:	CD-1 Mission Need	CD-2 Baseline	CD-3 Start Construction or Remedial Action	CD-4 Start Operations or Complete Cleanup

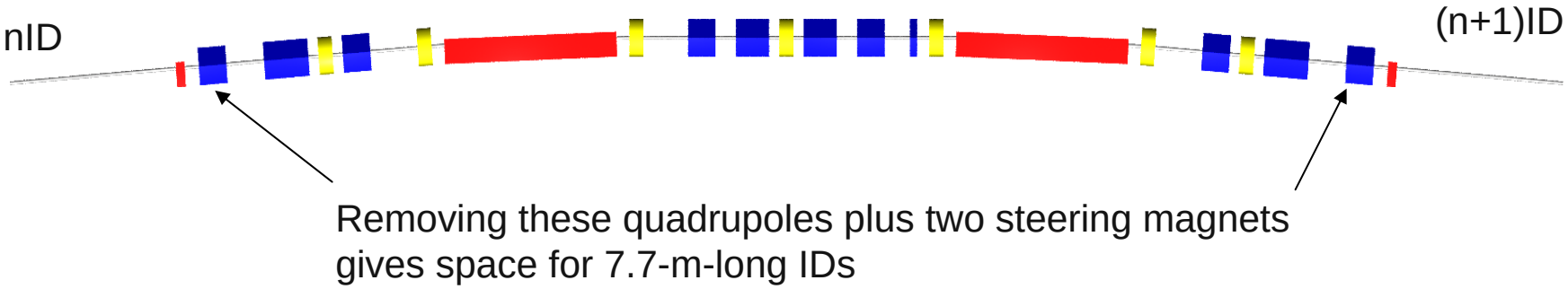
- Whitepaper -> Proposal for CD-0
- Develop a Pre-conceptual design (2009) and full proposal -> CD-1
- After CD-1 develop a full conceptual design, allow some R&D if required
- CD-2 beginning of project

- Note that obsolescence issues will not be funded through the renewal project, but through normal AIP funds. But it is important to plan together.

And after the renewal – a machine upgrade to keep APS at state-of-the-art beyond 2020?

Option	Flux (relative)	Max. Ave. Brightness (relative)	Time Required	Approximate Dark Time	Cost	Technical Risk
APS today	1	1 (2.4m U33)	N/A	N/A	N/A	N/A
ERL@APS	0.5	140 (4.8m U33)	10 years, including R&D	6 months	$$$	Very high
APS 1nm	7	40 (8m U33)	5 years, including R&D	1 year	$	Moderate
APSx3	7	18 (8m U33)	5 years, including R&D	1 year	$	Moderate
cAPS	3	2 (8m U33)	5 years, including R&D	none (use periodic shutdowns)	$	Moderate
APS-LSS	3~7	4~10 (8m U33~special ID)	6 years	none (use periodic shutdowns)	$	Very low to low
USR7	7	400 (8m U33)	5 years, including R&D	none	$$$$	Moderate
XPS	7	75 (8m U33)	7 years, including R&D	2 years	$$	Very high
XFEL-O	1 to 100	10^7 to 10^9	7 years, including R&D	none	$$	High

APS-LSS: Ring with all Long Straight Sections

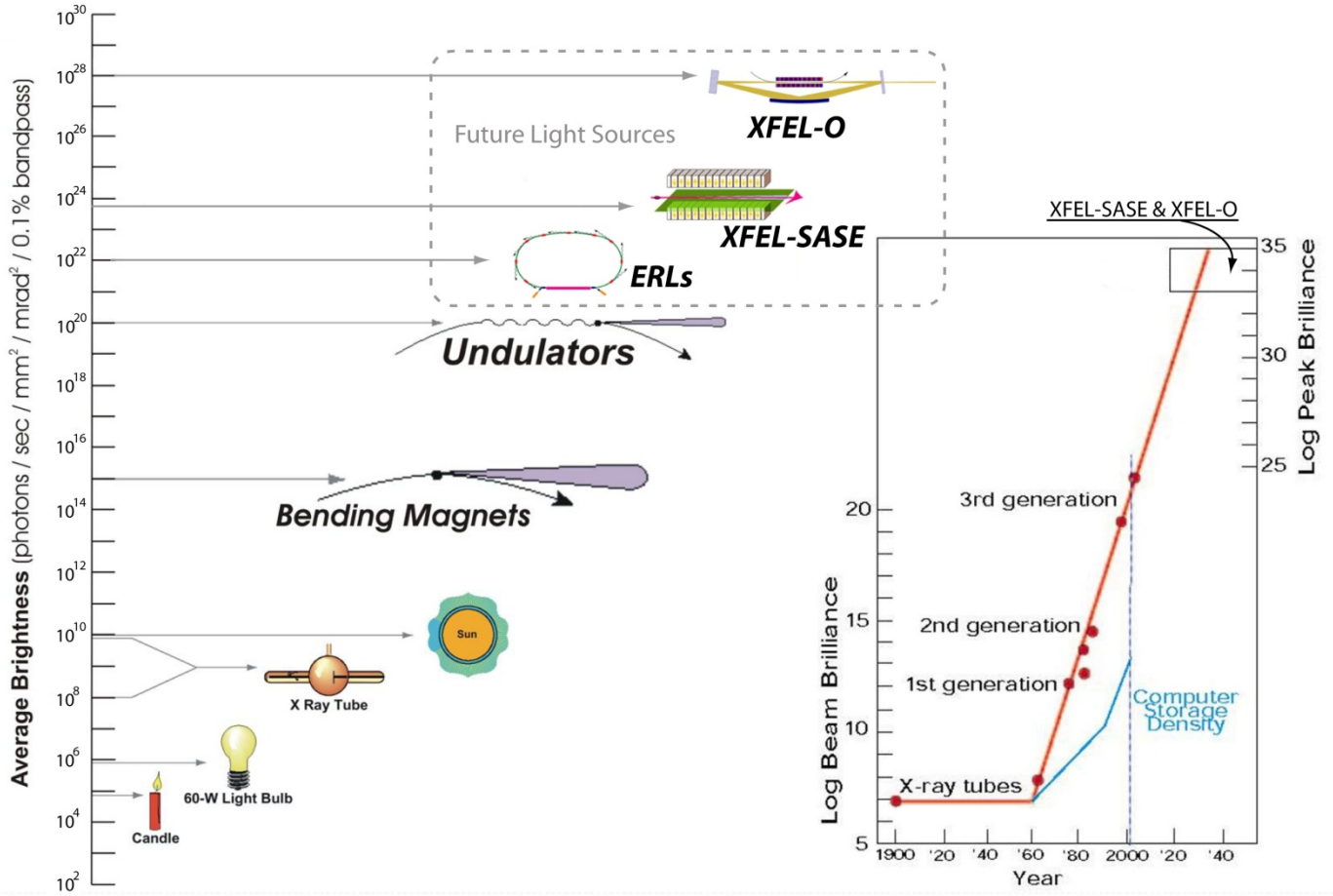


- In this option, we lengthen every straight section by 2.9m
  - Allows more and longer insertion devices
- Modest emittance increase from 3.1 to 3.3 nm[1]
- Drawbacks
  - Reduced flexibility for lattice functions
    - *May choose to leave a few sectors unaltered*
- Technical risk is very low
  - Can be mocked up prior to any hardware changes by just turning off the Q1 quadrupoles
  - Actual mechanical changes can be staged

[1]V. Sajaev, "Post ERL Ring Lattice," ASD/APG/2007-06.

Revolutionary possibilities for futures sources/upgrades?

K.J. Kim and Y. Shvydko, PRL in press



Both the ERL and the XFEL-O look promising as hard x-ray sources with revolutionary properties

Considering a machine upgrade after the renewal

- Should look at needed photon source characteristics
  - This is theme of BESAC photon workshop next week
    - *Energy - hard x-rays*
    - *Coherence*
    - *Brightness Ave, Peak*
    - *Flux*
    - *Spatial Resolution*
    - *Time Resolution*
    - *Energy Resolution*
    - *Polarization*

- Decisions not needed now, but important we show that renewal will leverage capabilities of an upgrade
  - LSS option is a shorter term possibility that could be considered and not preclude a longer term upgrade (similar to ESRF choice)

Conclusion and actions for this meeting

- We have a real opportunity here to make the case for APS renewal
- We must
  - Identify a few key science themes and examples (SAC)
  - Critically develop science cases and connect with needed techniques
  - Remain involved after the workshop

  - Think beyond the beamline renewal and consider possible machine upgrades

- Thank-you - I trust it will be a stimulating couple of days

Extras

Five Grand Challenges for Science and the Imagination – *how APS makes an impact*

- **How do we control materials and processes at the level of electrons?**
  - *e.g., imaging spins at interfaces (XMCD)*
- **How do we design and perfect atom-and energy-efficient synthesis of new forms of matter with tailored properties?**
  - *e.g., catalysis (NEXAFS), photosynthesis (time resolved)*
- **How do remarkable properties of matter emerge from complex correlations of atomic and electronic constituents and how can we control these properties?**
  - *Colossal magnetoresistance, quantum phase transitions*
- **Can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living systems?**
  - *Self-assembly (SAXS), imaging for hierarchical systems*
- **How do we characterize and control matter away—especially very far away—from equilibrium?**
  - In situ *studies (surface/interface, extreme conditions), suited to hard X-rays*

From the BESAC report on "Controlling Matter and Energy: Five Challenges for Science and the Imagination," Fleming and Ratner (9/2007)

Draft Structure for the APS Renewal White Paper (already have bones)

- The body of the White Paper should be 8-12 pages and contain:
  - Scientific Vision for a Renewed APS
    - *With the help of the SAC, identify a limited number of important problems and provide example solutions that a renewed APS could provide.*
  - APS in the National and International Context
    - *Stress the unique capabilities of the APS*
    - *Need to renew to remain competitive internationally*
  - Explanation of the process for developing the plan
  - Cost and Schedule
  - Beyond the renewal - the possibility of a major accelerator upgrade
- Appendix
  - Scientific Cases (Executive Summary and list of Team Members?)