Framing the Renewal Proposal

Paul Fuoss, APSUO Representative

Define the context and the goals of the Renewal proposal

- How it supports the DOE mission?
- Why it is good for users?
- Why it is scientifically compelling?

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Developing the overall framework that will support the structure of the APS Renewal

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Define the context and the goals of the Renewal proposal

- How it supports the DOE mission
- Why it is good for users
- Why it is scientifically compelling

Challenging because it must take into account the existing user programs and infrastructure.

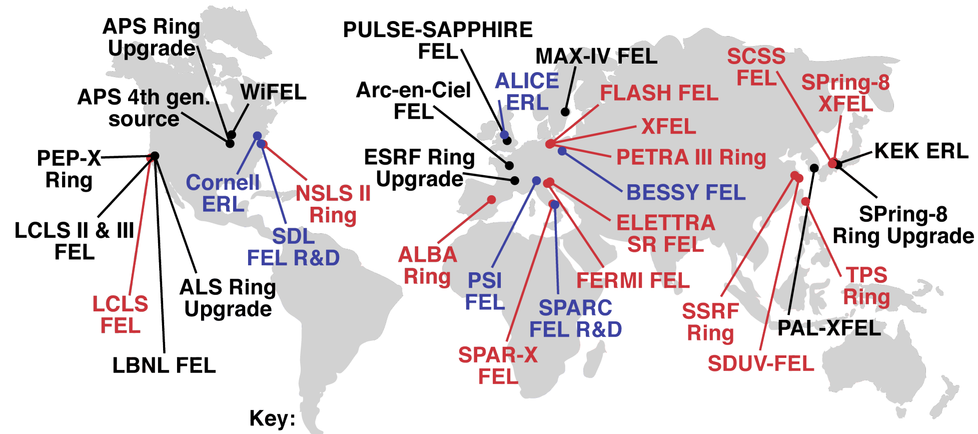
Overview

- **Strategic Context for the APS Renewal**
- Summary of Science Case Reports
- Mapping of Instrumentation Proposals onto Science Thrusts
- Going beyond the Instrumentation Proposals
- Summary - The Next Steps

Strategic Context - Competing Facilities

There are at least 10 third generation synchrotron sources in the world. All compete with APS in some aspect.

But the primary competition from other high energy machines and U.S. facilities.



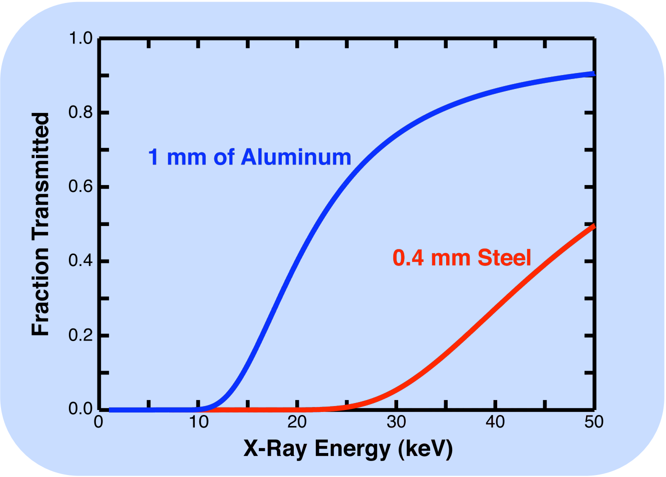
Key:
Red - funded (operational or under construction)
Blue - funded R&D program
Black - concepts and proposals

Source	Type	Critical Energy	Beamlines
ALS	3rd	3.2 keV	43
		Super-Bend 12 keV	
APS	3rd	19.5 keV	60
ESRF	3rd	20.3 keV	49
LCLS		N/A	6
NSLS	2nd	7.1 keV	65
NSLS II	3rd	2.4 keV	<58
PETRA III	3rd	20.8 keV	14
SPring 8	3rd	28.9 keV	48
SSRL	++2nd	7.5 keV	34

Strategic Context - Weaknesses of the APS

- **Complex physical and organizational arrangement of beamlines and science programs.**
- **Many beamlines were initially configured with marginal optics and instruments (usually because better technology wasn't available or affordable).**
- **Most beamlines are >10 years old and have not been updated to take advantage of the capabilities of the storage ring.**
- **Accelerator infrastructure is fifteen years old.**
- **Programs are constrained by the physical infrastructure**
  - Size of the experimental floor limits length of beamlines
  - Availability of office space is limited
  - Laboratory facilities are often inadequate for current programs

Strategic Context - Strengths of the APS



- **An exceptional accelerator complex**
  - best storage ring reliability in the world
  - very good electron brightness and current
  - large ring offers great flexibility for rearranging electron optics
- **High energy x-rays offer great flexibility**
  - penetrate through thick samples and environmental chambers
  - simplified scattering geometries because of the large Ewald sphere associated with high energy x-rays.
- **Some experimental facilities are best in class**
- **World leading scientific programs in some disciplines**

Overview

- *Strategic Context for the APS Renewal*
- **Summary of Science Case Reports**
  - **Interfacial Sciences**
  - **Materials Science and Technology**
  - **Chemical Science and Engineering**
  - **Condensed Matter and Materials Physics**
  - **Interactions in Chemical, Atomic and Molecular Physics**

  ^{R}Materials^{R}Conditions^{R}Time

  - **Macromolecular Crystallography**
  - **Geological, Environmental and Planetary**
  - **Polymers and Soft Materials**
  - **Life Sciences**
  - **Engineering Applications and Applied Research**

  Mastering Hierarchy

- Mapping of Instrumentation Proposals onto Science Thrusts
- Going beyond the Instrumentation Proposals
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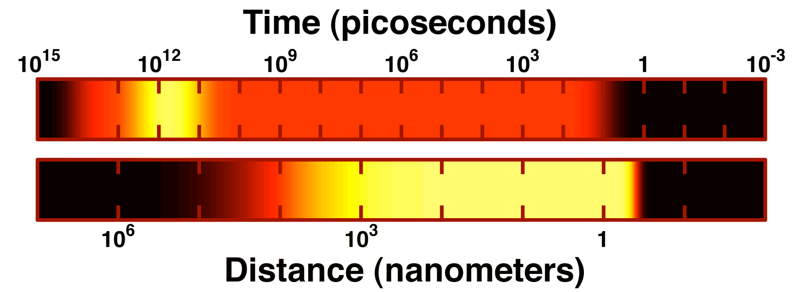
Workshop - Interfacial Sciences

Opportunities

- Explore the spatial and temporal behavior of interfacial reactivity in complex environments (i.e. Belousov-Zhabotinsky reactions).
- Construct and characterize complex materials with emergent interface properties such as $LaAlO_3$-$SrTiO_3$.
- Develop detailed models of the atomic level processes occurring during growth of materials using techniques such as PLD, MOCVD and ALD.
- Examine the mechanisms at buried interfaces that limit the performance and lead to degradation and failure of devices such as fuel cells.
- Use XPCS to examine the intrinsic fluctuations and phase transitions at surfaces and buried interfaces.



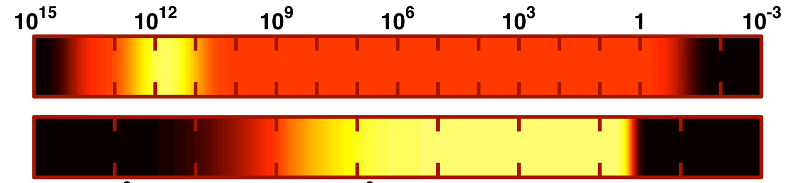
Needed Capabilities

- Development of the X-Ray Interfacial Science facility with facilities for large, complex experiments.
- Fast readout, high dynamic range x-ray area detectors and associated data collection and visualization software.
- Optics and infrastructure to support x-ray microscopies such as XRIM.
- Coherent x-ray beams and sample manipulation technology to enable coherent x-ray microscopy.

Workshop - Materials Science and Technology

Opportunities

- Identification and control of phases and processes relevant to crystal growth.
- Determination of the properties of materials under transient compression.
- Understanding rare, stochastic events behind nucleation, crack initiation and other seemingly random events using time-reversal imaging.
- Measuring strain in nanometer scale devices such as semiconductor devices.
- Time-resolved structural response of materials to applied electric and magnetic fields.
- Characterization and control of interfaces between engineered materials an biological systems.



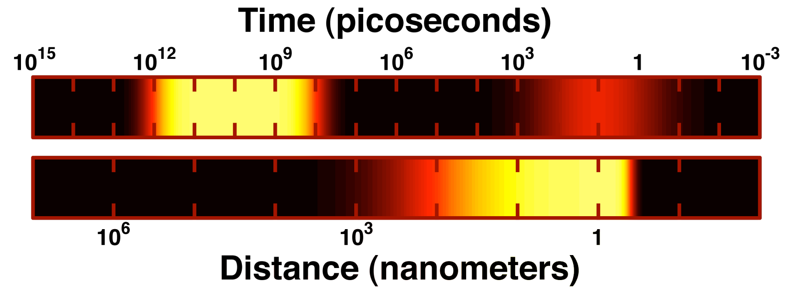
Needed Capabilities

- Full-field microscopy and topography
- Nanodiffraction with beam spots smaller than 10 nm.
- Fast readout, high dynamic range x-ray area detectors.
- Improved energy dispersive detectors.
- Short pulse x-ray source for time-resolved studies.

Workshop - Chemical Science and Engineering

Opportunities

- Improved understanding of metal-ion speciation in solution including coordination, ligation and oligomerization.
- Determining the time-dependent structure of complex catalytic nanoparticles under differing reaction conditions.
- Developing catalysts with selectivity approaching that of biological systems.
- Relationship of solution-electrode interface to the stability and efficiency of fuel cells.
- Developing compositions and synthesis methods for non-noble nanoparticle materials for high efficiency fuel cells.



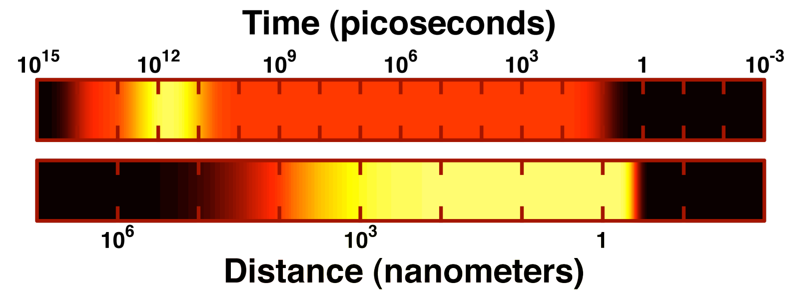
Needed Capabilities

- Powder diffraction with an emphasis on in situ analysis for determining the structure of nanometer sized clusters.
- EXAFS and XANES with differential, spatial and time-resolved capabilities.
- SAXS and GISAXS including resonant (anomalous) scattering.
- New spectroscopies incorporating high energy resolution fluorescence analysis (HERF) and resonant inelastic x-ray scattering (RIXS).

Workshop - Condensed Matter and Materials Physics

Opportunities

- Developing fundamental insights into:
  - emergence of complex phenomena from simple ingredients.
  - correlated electron/atom systems.
  - integration of materials with competing properties (i.e. ferromagnetic and superconducting).
  - “design rules” governing 3D structure and properties of soft materials.
  - the physics of the nanoworld.
  - phase transitions and self-assembly.
- Use insights to develop:
  - high efficiency, low cost photovoltaic devices.
  - improved thermoelectric materials.
  - materials for advanced semiconductor devices including spintronics, optical computing, opto-electronics and quantum computing.



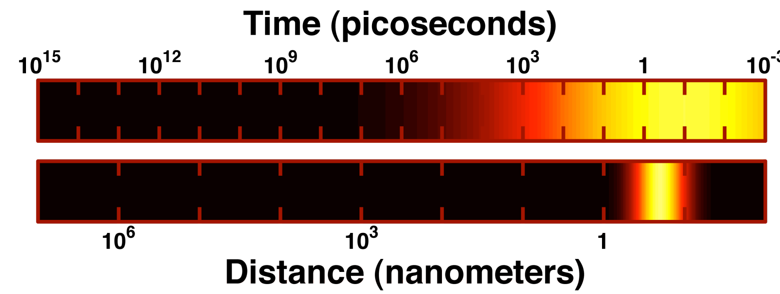
Needed Capabilities

- Broad range of specialized, high performance techniques including inelastic, magnetic, ultra-fast and coherent x-ray scattering.
- Combinations of extreme environments including high and low temperature, magnetic fields, ultra -short EM pulses and shock waves.
- In situ processing and synthesis, ideally in portable systems to take advantage of specialized beamlines.

Workshop - Fundamental Interactions in CAM Physics*

Opportunities

- Control dynamic processes at the atomic and molecular level, particularly electron and atomic motion.
- Develop x-ray phenomena such as electromagnetically induced transparency for novel x-ray devices.
- Determine the structure of chemical transition states.
- Follow energy flows and molecular reconfigurations through multi-step processes (e.g. photosynthesis)
- Use field-free molecular alignment to improve angle resolved photoelectron and Auger spectroscopy of molecules.
- Measure the dynamic responses of nanomagnetic materials, nonlinear optical materials, ferroelectric and multiferroic devices, and metamaterials to applied fields.



Needed Capabilities

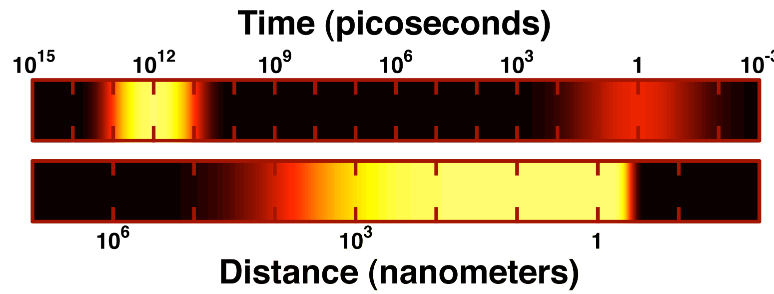
- Development of SPX source, a high flux picosecond x-ray source based on Zholents rf-deflection cavity approach.
- High repetition rate, high intensity laser facility.
- Suitable sample and environmental chambers to perform gas phase spectroscopy.
- X-ray optics to make efficient use of the much different x-ray phase space of the SPX source

**Chemical, Atomic and Molecular*

Workshop - Macromolecular Crystallography

Opportunities

- Greatly expand the range of proteins and protein complexes whose structure can be determined using microbeams to study
  - micron sized crystals
  - highly ordered regions in non-uniform crystals
- Understand the interplay between structure, dynamics and function through the use of time-resolved x-ray crystallography



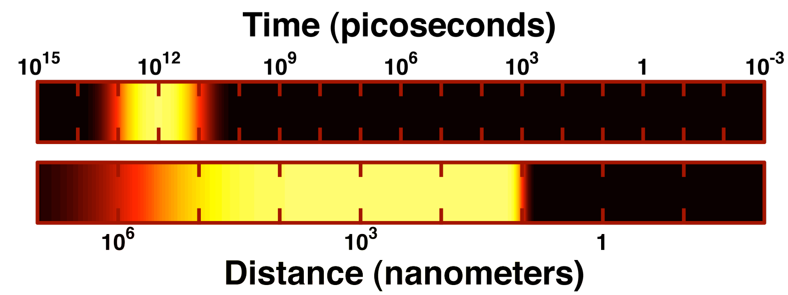
Needed Capabilities

- Fast readout, high dynamic range x-ray area detectors
- Optics and beam stability improvements to support micro-x-ray crystallography.
- Micro-mechanical systems for high stability and precise alignment of crystals.
- Advanced Protein Crystallization Facility

Workshop - Geological, Environmental and Planetary

Opportunities

- Improving knowledge of the complex mineral-fluid interface to make efficient and intelligent use of natural resources.
- Determining the composition, reactivity and transport of geologically and environmentally formed nanoparticles.
- Improved detection capability for trace elements will aid in understanding 3D transport in porous media.
- Determining the microenvironment (the few cubic microns adjacent to actively metabolizing cell surfaces) is crucial to predicting the fates of contaminants.
- Synchrotron radiation provides a crucial tool in understanding interplanetary dust and comet particles, and thus the evolution of our solar system and the universe.



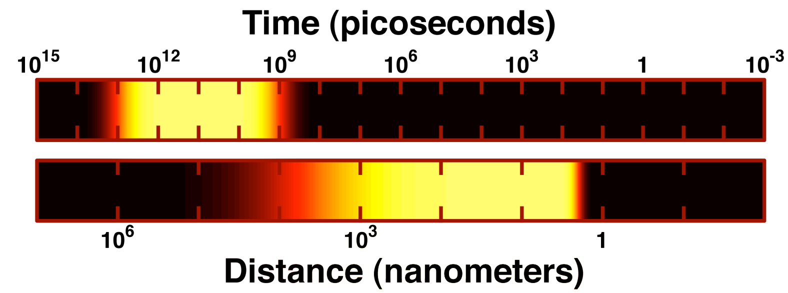
Needed Capabilities

- Higher intensity x-ray microprobes and nanoprobes.
- High performance spectroscopic detectors.
- Improved high pressure capabilities for simulating planetary interior conditions.
- Tomographic x-ray diffraction and spectroscopy imaging.

Workshop - Polymers and Soft Materials

Opportunities

- Understand the structure and dynamics of emulsified heterogeneous fuels in order to improve extraction and combustion technologies.
- Explore structure-property correlations in organic electronics, control those correlations and improve device performance.
- Measure the dynamics of polymer systems, including ‘beta’ processes near glass transitions using XPCS.
- Elucidate the mechanisms and interactions of molecular self-assembly at interfaces and create better ordered organic thin films.
- Understand the distribution of ions near liquid-liquid and liquid-vapor interfaces.



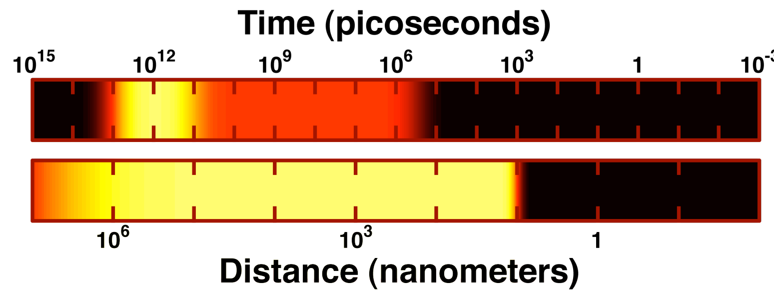
Needed Capabilities

- Liquid interface instrument optimized for 30 keV - 80 keV photons
- Area detectors with improved spatial resolution.
- SAXS, GISAXS, XSW, SXRF microscopy, XPCS and TXM instruments.
- Capability to perform measurements with sample cooled to cryogenic temperatures.

Workshop - Life Sciences

Opportunities

- Use solution scattering to determine the molecular dynamics of membrane proteins, enzymes undergoing catalysis, and structure evolution during protein folding.
- Large field, x-ray phase contrast imaging has great potential such as:
  – determining the flow of fluids (e.g. respiration or blood) through small organisms.
  – exploring evolution of organisms through the fossil record.
  – seeing the impact of drugs (e.g. asthma medications) on biological structures.
- Use x-ray nanoprobes to determine the structure and mechanisms of metal atoms in cells.
- Use x-ray imaging and x-ray scattering to determine the response (e.g. internal strain) of biomaterials under load.



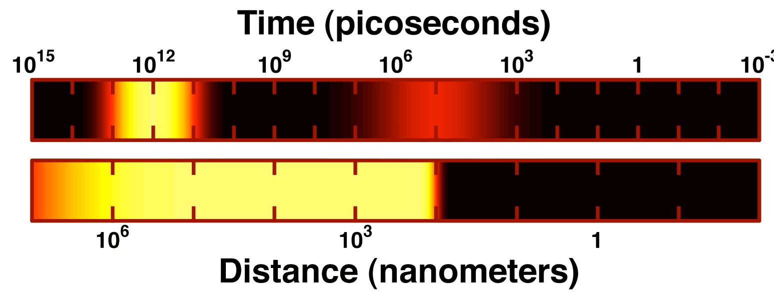
Needed Capabilities

- Bionanoprobe capable of microscopy, micro-spectroscopy, spectro -microscopy and nano-CT
- Wide field x-ray phase imaging
- Coherent diffraction imaging.
- SAXS/WAXS/fiber diffraction.
- Cryopreservation infrastructure
- Improved detectors with high dynamic range and high spatial resolution
- Advanced Protein Crystallization Facility

Workshop - Engineering Applications and Applied Research

Opportunities

- High brightness, high energy x-ray beams offer unique advantages for non-destructive imaging.
- Detection of minor phases at interfaces of real materials will provide important insight into the performance of materials in extreme environments.
- In situ studies of dislocation behavior near surfaces and interfaces will provide crucial data for multiscale modeling of materials.
- Transient phase detection during materials processing (e.g. heat treating) will test theories and clarify pathways towards ideal microstructures.
- Performance of materials under dynamic deformation is fundamentally different and is important for national security.



Needed Capabilities

- Complete upgrade of 1-ID
- Polychromatic nanoprobe
- High-energy, energy-dispersive beamline
- Dedicated high-energy tomography station with phase contrast sensitivity
- Additional capacity for high-energy x-ray measurement of aggregate stress/strain/texture

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Summary of the Proposal Mapping

- **16** proposals strongly support ***Hierarchical Imaging.***
- **19** proposals strongly support ***RMaterialsRConditionsRTime***
- **17** proposals were judged to only weakly or indirectly support the whitepaper thrusts.

- Note that the instrument proposals were requested from the beamline staff **six months before** the Renewal Workshops were held and the science thrusts developed.
- ***It is remarkable that two thirds of the instrument proposals map directly onto the whitepaper science thrusts.***

Remember, mapping is subjective. The current mapping doesn't imply anything about the scientific or technical merit of any proposal.

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- **Going beyond the Instrumentation Proposals**
  - **Instrumentation proposals were developed in the context of specific beamlines.**
  - **Significant opportunities are created by making the problem bigger.**
  - **Need a vision that is greater than the sum of its parts.**
- Summary - The Next Steps

Sum of Parts - Detectors

- A large effort on detectors can yield breakthroughs that extend beyond the APS to the entire synchrotron community.
- Most detectors efforts need to target a significant market to reach economies of scale.
- Large effort can only be afforded by spreading the cost across the entire facility (entire synchrotron community?).
- Don’t let the best be the enemy of the ~~good~~ much better.

Sum of Parts - New Optics, Nanomechanics and Detectors

- A broadband source like the APS needs achromatic optics to fully use the available photons.
- State of the art optics can produce 20 nm spot sizes but before they can be used for routine experiments, improvements are needed in:
  - electron source stability
  - optics mounts and control
  - sample manipulation
  - post sample x-ray optics
  - detectors
- A breakthrough effort spanning such diverse areas will not be accomplished by a single scientific group or a small team.

Sum of Parts - Time Resolved Studies

- Half of the Science teams reported a need for ultra-fast x-ray beams.
- These efforts span a large number of techniques, more than can be accommodated on one or two sectors.
- The SPX facility would feed more sectors but those need to be contiguous.
- Optimal use of the SPX facility requires the relocation of several beamlines.

Sum of Parts - From Beamlines to Instruments

- Current synchrotron practice requires a staff scientist to be available full time to help users.
- Many synchrotron experiments are no more complex than an atomic force microscope (AFM). At most laboratories, AFM's are routinely operated by students and post-docs after a short training session.
- Effective automation and controls would allow APS beamlines to be operated in a similar manner, freeing both staff and users to be more productive.
- Making this leap requires significant investment from a diverse set of groups to create
  - stable, reproducible optics
  - sophisticated interfaces with good user retention
  - diagnostics to determine when experts must be called
  - effective documentation and training
- Instruments produce **Better Science** through **Reproducible Performance**.

Sum of Parts - Breaking Through the Wall

- There is a very large cost associated with the first beamline that breaches the walkway and out of the APS experimental hall.
- There are numerous efforts that would benefit by this expansion
  - Long imaging beamline
  - Interface sciences facility
  - High magnetic field laboratory
- APS site constraints mean that there are only certain areas suitable for exterior expansion.
- Clustering these efforts (which implies moving existing beamline programs) can spread the cost and make all of them more affordable.

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Summary - Next Steps for the APS Renewal

- Create a report from the Science Workshop
- Form study team to create documentation for CD-0
  - Focus on what beamlines are required for a world class programs in Hierarchical Imaging and ^{R}Materials^{R}Conditions^{R}Time.
  - Instrumentation proposals address “what upgrades would make my beamline world-class”.
- Work with the users to generate additional concepts
  - Renewal will be focus of the Users Meeting