# NSLS-II Scientific Computing Workshop

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Workshop on Scientific Computing at Modern Synchrotron Facilities
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# NSLS-II Project Timeline

| | | |
|---|---|---|
| Aug 2005 | CD-0, Approve Mission Need | (Complete) |
| Jul 2007 | CD-1, Approve Alternative Selection and Cost Range | (Complete) |
| Jan 2008 | CD-2, Approve Performance Baseline | (Complete) |
| Dec 2008 | CD-3, Approve Start of Construction | (Complete) |
| Feb 2009 | Contract Award for Ring Building | (Complete) |
| Aug 2009 | Contract Award for Storage Ring Magnets | (Complete) |
| Feb 2011 | 1st Pentant of Ring Building Ready for Accelerator Installation | |
| Feb 2012 | Beneficial Occupancy of Experimental Floor | |
| Oct 2013 | Start Accelerator Commissioning | |
| Jun 2014 | Early Project Completion; 1st Beam to Beamlines soon afterwards | |
| Jun 2015 | CD-4, Approve Start of Operations | |

← June 15, 2009: Start of Construction Celebration

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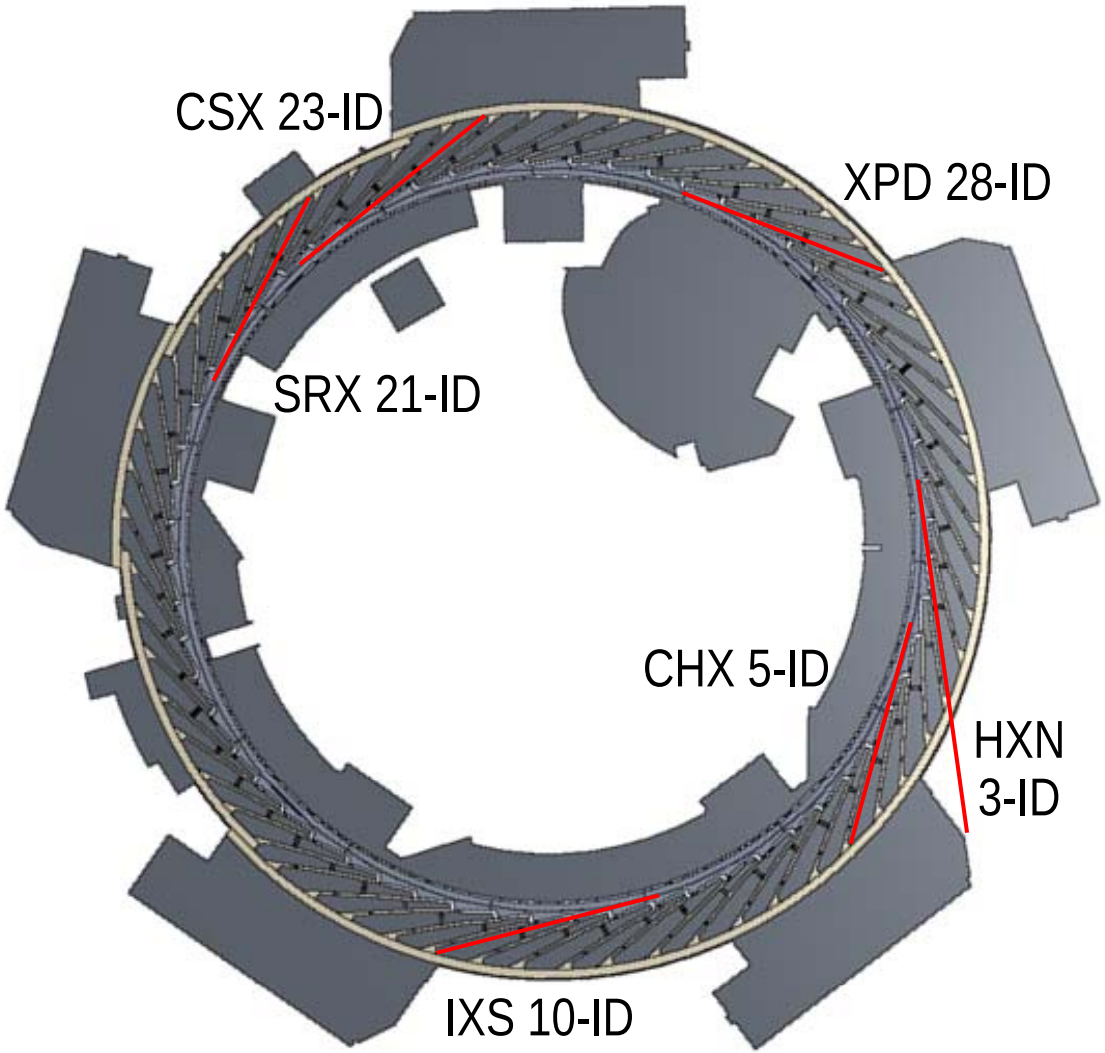
# Six Beamlines in NSLS-II Construction Project

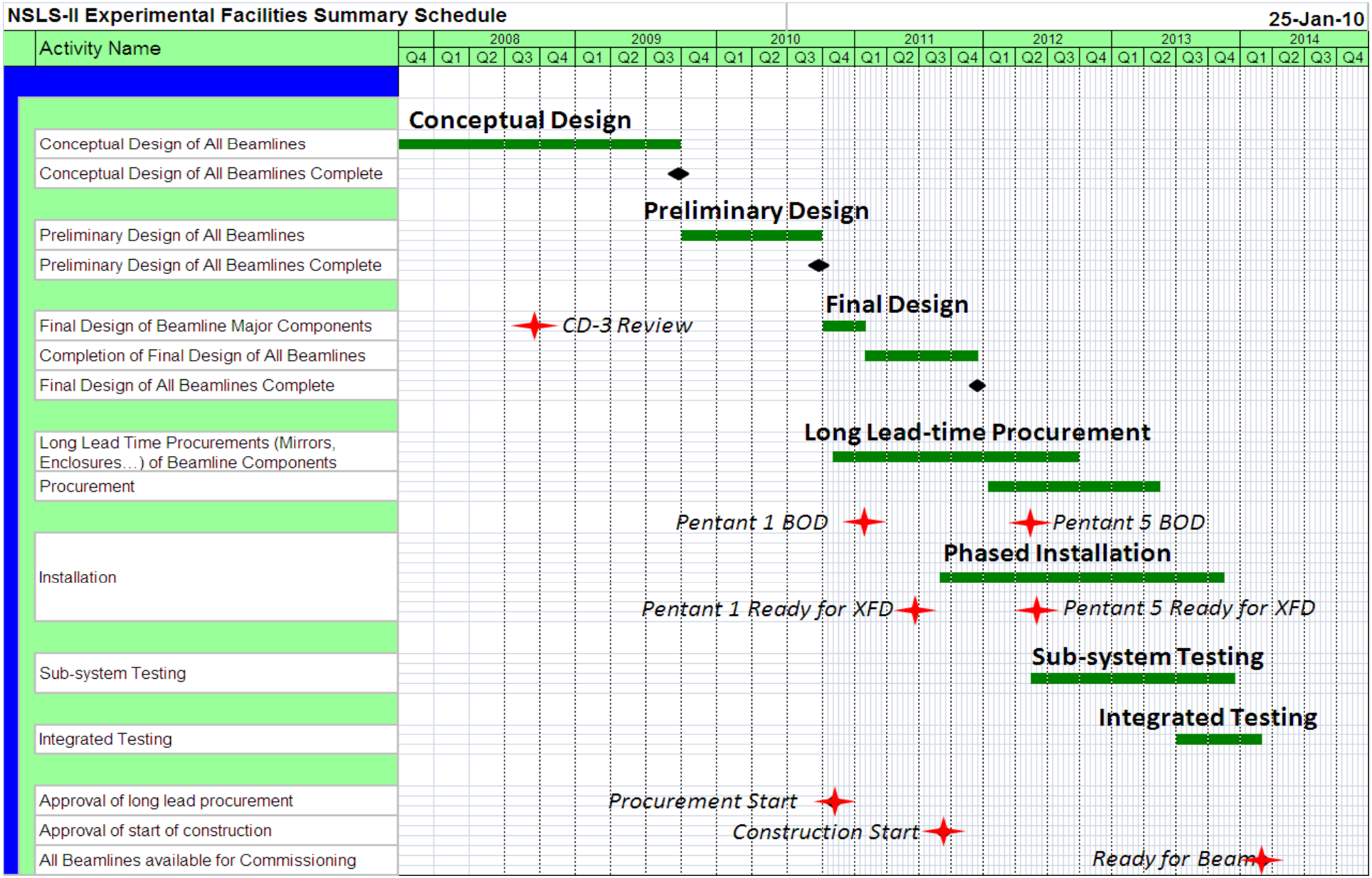



- Inelastic X-ray Scattering (IXS)
- Hard X-ray Nanoprobe (HXN)
- Coherent Hard X-ray Scattering (CHX)
- Coherent Soft X-ray Scattering & Polarization (CSX)
- Sub-micron Resolution X-ray Spectroscopy (SRX)
- X-ray Powder Diffraction (XPD)

*Note: beamline location assignments preliminary*

*Conceptual design report posted at http://www.bnl.gov/nsls2/docs/PDF/CDRs_SixProjectBeamlines_NSLS-II.pdf*

# NSLS-II Project Beamline Schedule

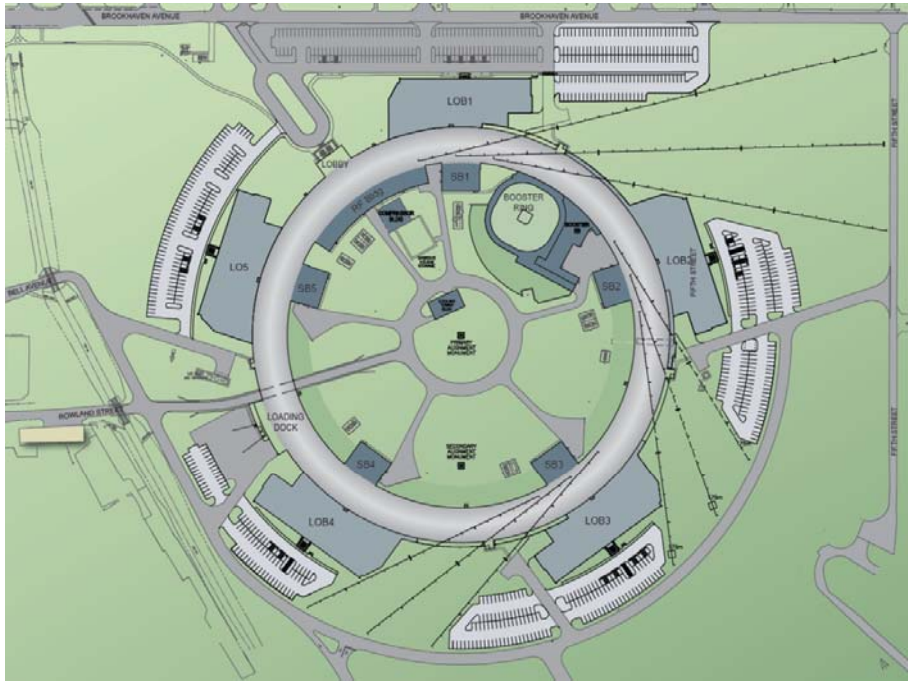


# NSLS-II Beamline Build-out Strategy

| FUNDING | BEAMLINES |
|---|---|
| BES – Project | 6 insertion device beamlines in base project scope (1st beam in 2014) |
| BES – Early Operations | ~ 20 bending magnet beamlines transferred from NSLS to NSLS-II, using NSLS-II early operations funding (~2015) |
| BES – MIE | ~ 12 insertion device beamlines |
| Non-BES | Life Science beamlines and other non-BES missions |

- 27 insertion device beamlines
- 31 BM / 3PW / IR beamlines
- at least 58 beamlines, plus canted IDs
- current estimate of fully built-out facility: 75-80 full-time equivalent beamlines

~ 37 beamlines operating by 2016-17
→ 60% of capacity



# Future Beamlines

**2010 Call for Beamline Development Proposals**
**National Synchrotron Light Source II**

March 26, 2010

- Open to all areas of science, including both physical and life sciences
- Independent of the funding source and the type of beamlines
- Several anticipated funding opportunities — from Department of Energy, National Institutes of Health, and other sources

## Critical Dates

Call for proposal issued
March 26, 2010

Informational session Wednesday, April 14, 2010

Letter of Intent due Monday, April 26, 2010

Beamline proposal due Monday, June 21, 2010

SAC review
Summer 2010

## Related Materials

Proposal template

NSLS-II Beamline Development Policy

NSLS-II Source Properties

NSLS & NSLS-II User Access Policy (draft)

Conceptual Design Report for Six Project Beamlines

Background Beamline Information

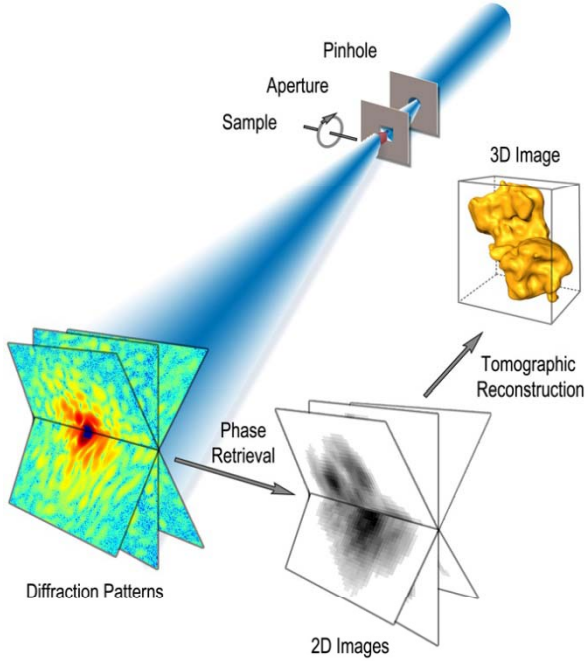
# Expected Data Rates at NSLS-II

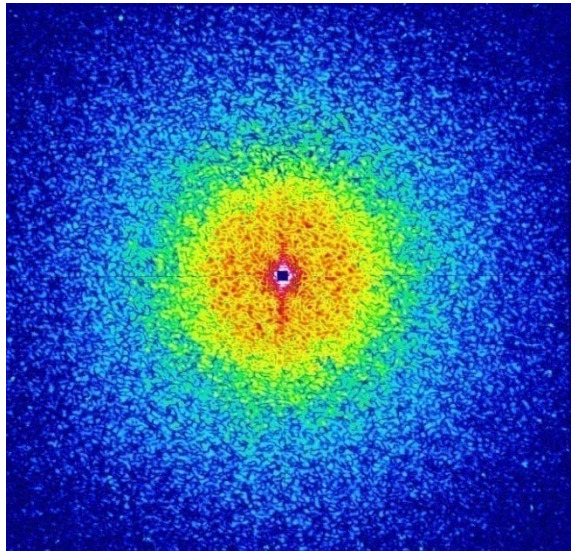
- High spectral brightness and spectral photon flux at NSLS-II will lead to unprecedented data collection and accumulation rates
- Most demanding experiments will be in the areas of x-ray imaging and high-throughput crystallography
- Typical data rates at each of these beamlines are estimated below:

| Experiments at NSLS-II | Peak data rate (Gb/s) | Typical dataset (TB) | Daily data rate (TB) |
|---|---|---|---|
| Coherent diffraction imaging (3x3 6M 16-bit @ 1 kHz x6000) | 800 | 1 | 2 |
| X-ray fluorescence microscopy (400x 12-bit 1K A/D @ 10 kHz x$10^9$ pxl) | 50 | 1.5 | 1 |
| High-speed x-ray tomography (2K x 2K 12-bit @ 4 kHz x3000) | 240 | 0.02 | 3 |
| Macromolecular crystallography (2x2 6M 16-bit @ 10 Hz x360 3 λ's) | 5 | 0.05 | 10 |

# Coherent X-ray Diffraction Imaging

- Coherent X-ray Diffraction Imaging has the potential to open up structural science from mostly crystal-based today to noncrystalline materials;
- Optimized experiment on a 2 μm object at ~ 2 nm resolution will require a 2D area detector array with 3x3 area detectors of 6M pixel each ➔ 54M pixels per one frame of diffraction pattern;
- Assuming 16 bit dynamic range in intensity, this leads to 0.86 Gb/frame; At 1 kHz frame rate, the peak data rate is 860 Gb/sec.; Many thousand frames are summed together to accumulate statistics;
- 3D dataset requires 6000 frames, leading to 1.2 TB per dataset (32-bit dynamic range); Such dataset is expected to be collected in ~12 hours at NSLS-II;
- Data analysis include FFT and inverse FFT with many thousands of iterations, requiring 4x as much data during analysis.



Coherent diffraction pattern from a nanoporous Au microparticle (data obtained at APS by Xiao & Shen)

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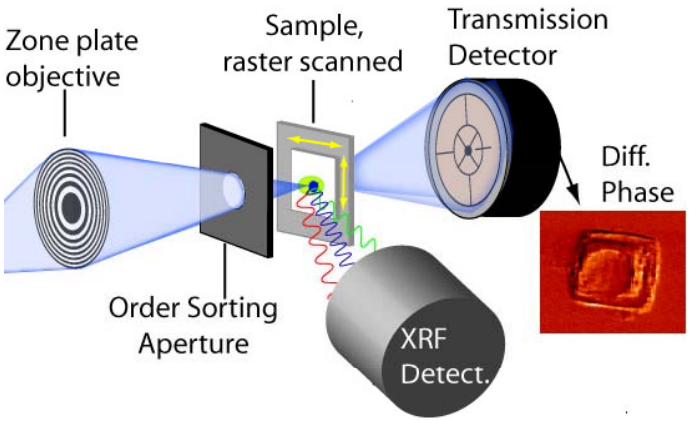
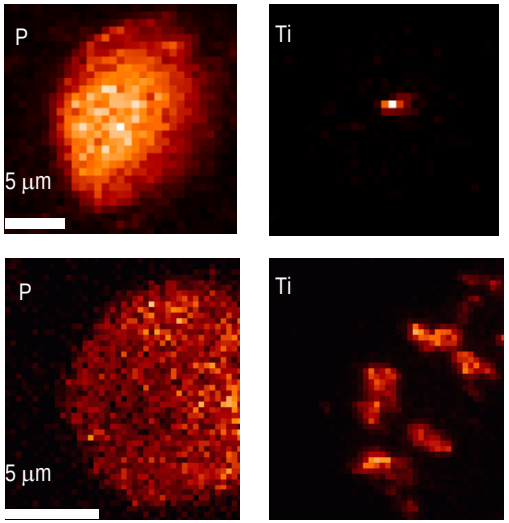
# Scanning XRF Microscopy & Tomography

- X-ray fluorescence microscopy offers high elemental sensitivity (<$10^{-21}$gm at NSLS-II), easy quantification, chemical state mapping, & 3D tomographic imaging;
- Optimized experiment on a 5 μm biological cell at 5 nm resolution may make use of a 400 element fluorescence detector array that covers 30% of 4π solid-angle;
- Each detector element gives rise an energy spectrum which is digitalized to 1024 channels at 12 bit dynamic range, with 0.1 ms dwell time;
- This leads to a peak data rate of 400x1024x 12x10000 = 50 Gb/sec;
- Complete 3D dataset on the 5 μm biological cell at 5 nm resolution will consist of 1000x1000 x1000 pixels, leading to ~1 TB per 3D dataset;
- Such 3D dataset may be collected at NSLS-II in about 1 day.




Courtesy of S. Vogt (APS)



# Scientific Computing Group at NSLS-II

- NSLS-II is designed to provide leading experimental capabilities based on high brightness, high flux, and exceptional beam stability over a broad range of photon energies from far infrared to hard x-rays
- Such capabilities, coupled with modern photon detectors, are expected to lead to unprecedented data rates and data-set quantities for many state-of-the-art experiments in a broad range of diverse scientific fields
- NSLS-II is in a unique position to seize this opportunity, with advanced planning, to engage early in the development of appropriate facilities to adequately support user science experiments and enhance scientific productivity and impact.
- NSLS-II is creating a new Scientific Data Acquisition & Computing Group in Experimental Facilities Division. The group will consist of 20-30 staff and be responsible for
  - Beamline experimental control and integration;
  - Planning and operation of computing and data storage infrastructure;
  - Data analysis and information feedback during experiments;
  - Post-experiment scientific computing and support.

# This Workshop

- We are searching for a Scientific Computing Group Leader to lead the effort in this important area of experimental facilities at NSLS-II; Advert will soon be posted at http://www.bnl.gov/nsls2/jobs.asp.
- The purpose of this workshop is (a) to identify the anticipated needs for scientific computing at synchrotron user facilities, and (b) to recommend a set of strategies and approaches to meet such needs at NSLS-II facility.
  - Data handling requirements in typical high-data-rate synchrotron experiments;
  - Experimental data storage policies for short-term and long-term;
  - Data reduction and analysis capabilities during user experiments;
  - Post-experiment data analysis support and accessibility;
  - Organization structure optimized to achieve the goals.
- The information discussed at this workshop will serve as guide to the development of scientific computing infrastructure at NSLS-II.