Protein Crystallography at NSLS2

System Administrator view

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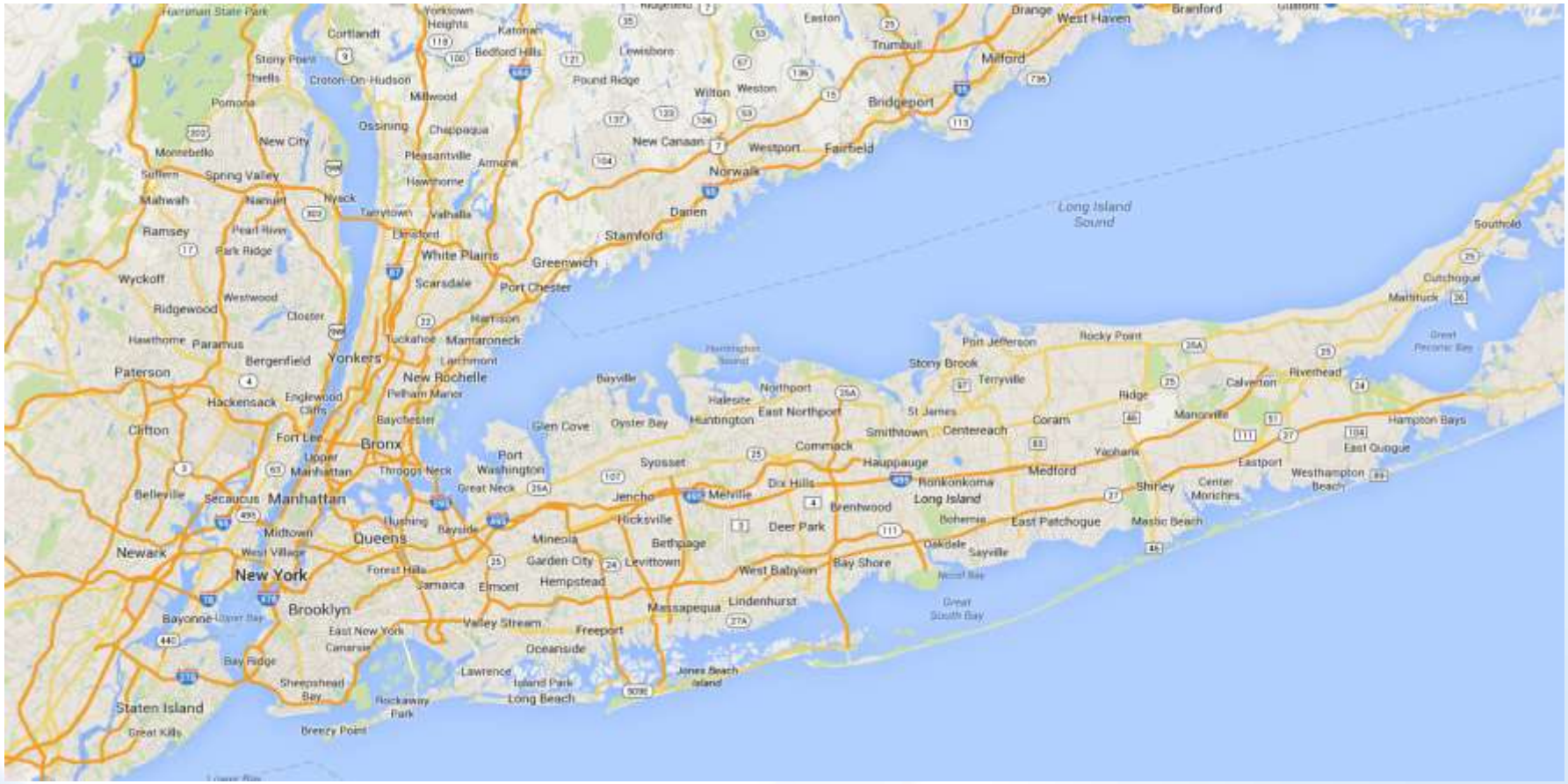
Photon Sciences Directorate

BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

What is NSLS2? Where is it?



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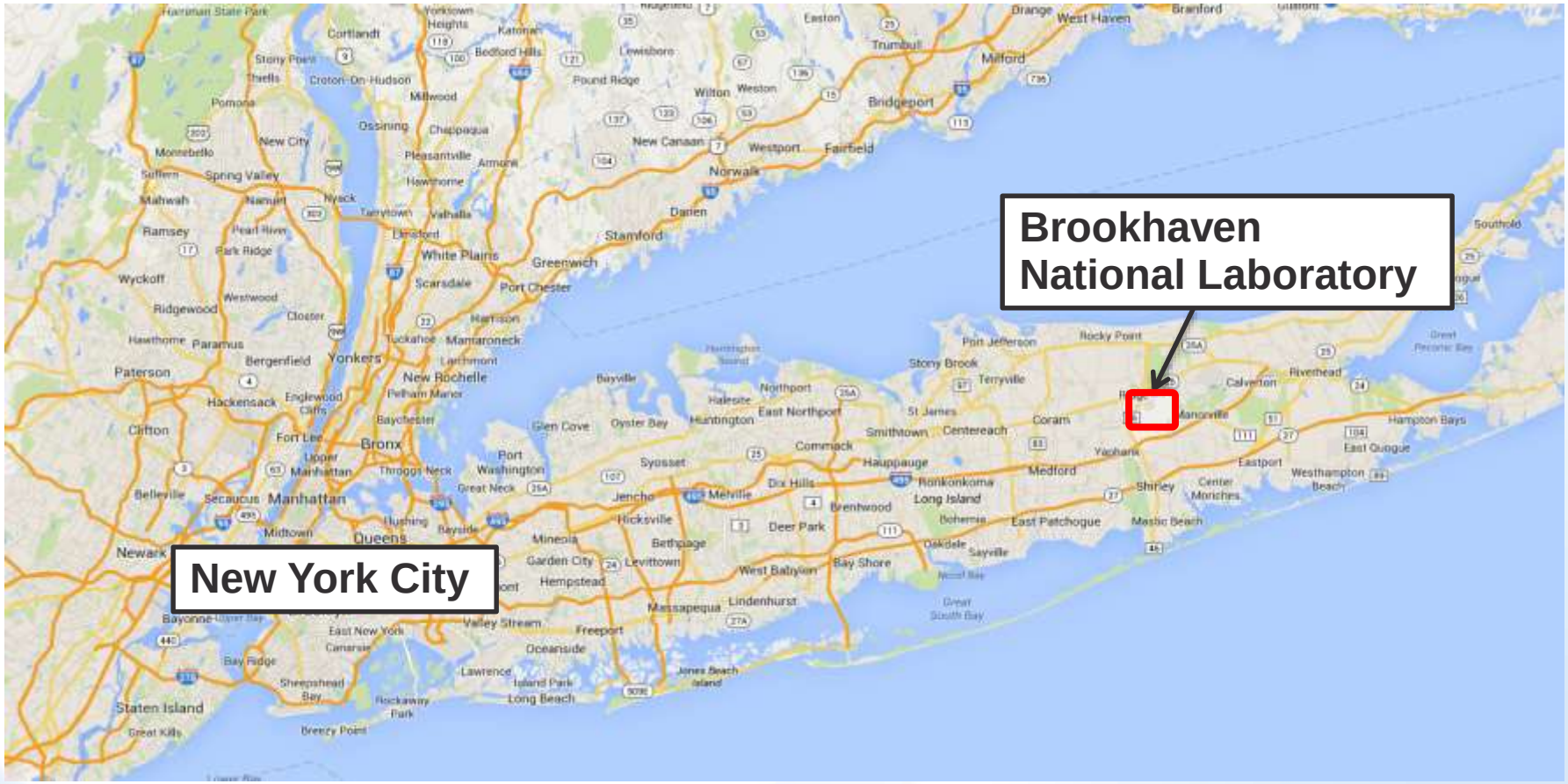

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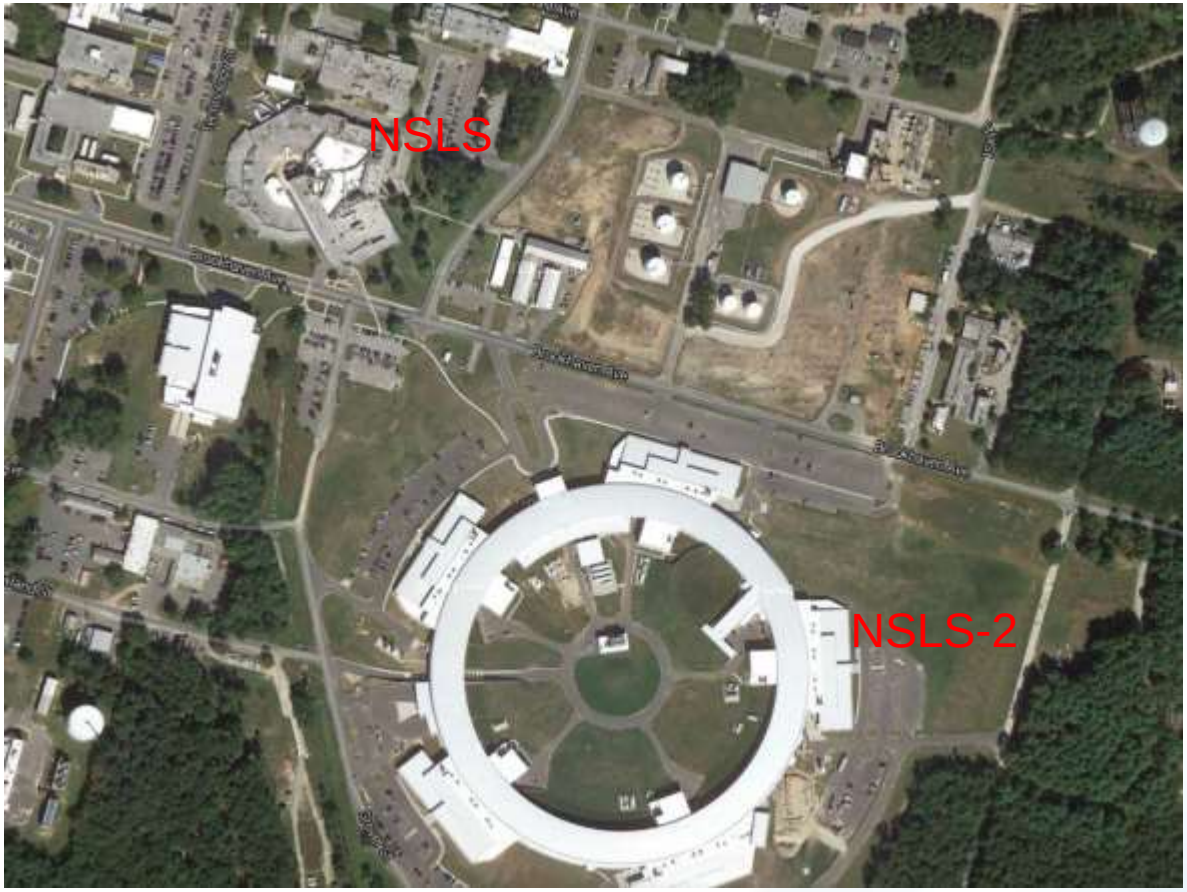
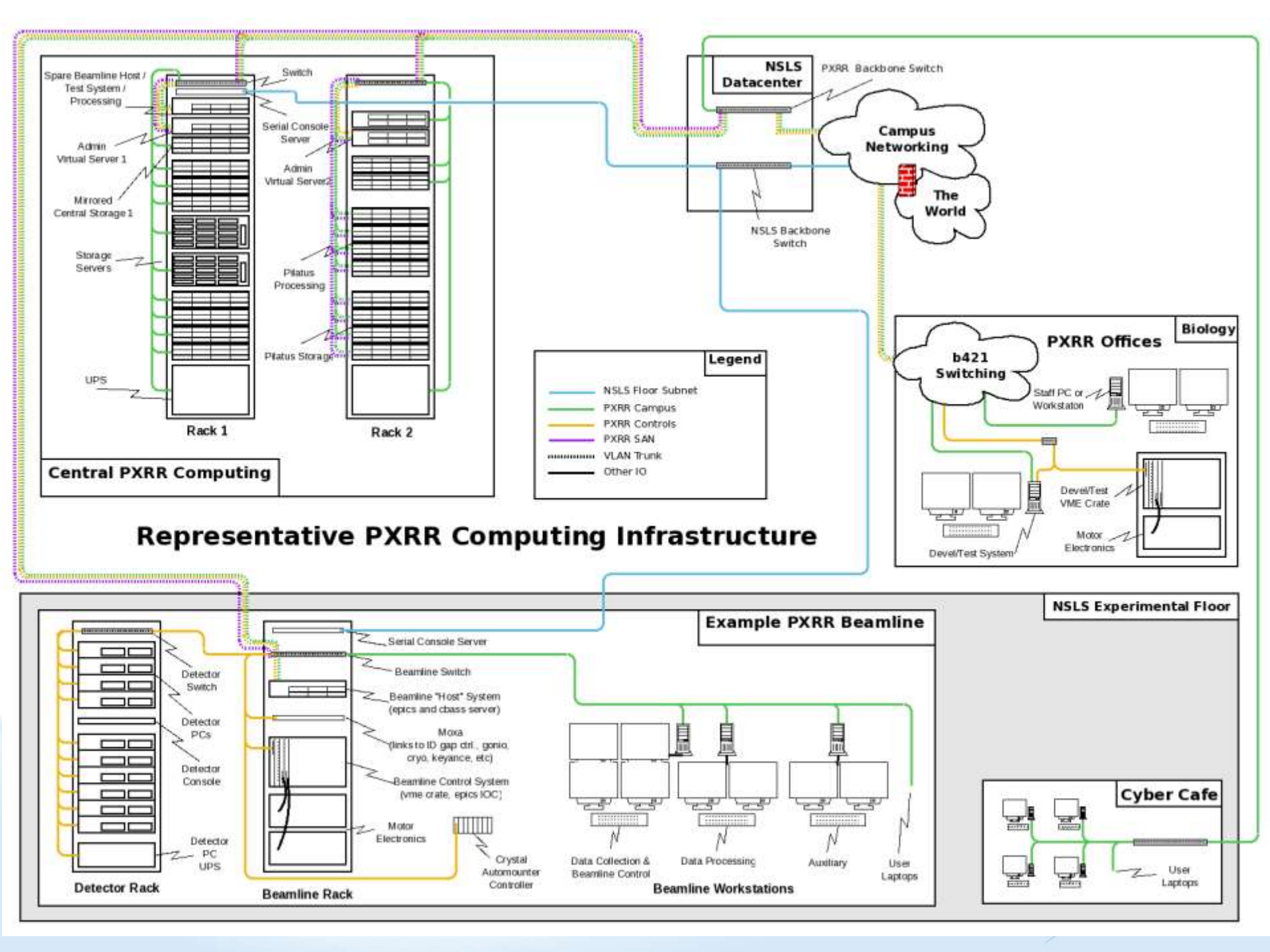


NSLS MX highlights

- 5 Beamlines
- Dectris Pilatus 6M detector: 12 frames/second, 6MB image size
- Storage: 20TB gluster array
- Network: 2Gb aggregate links
- Other detectors – ADSC Q315r, Q210; Storage – 4x 3TB RAID5 systems


Spare Beamline Host / Test System / Processing
Switch
Serial Console Server
Admin Virtual Server 1
Admin Virtual Server2
Mirrored Central Storage 1
Storage Servers
Pilatus Processing
Pilatus Storage
UPS
Rack 1
Rack 2
Central PXRR Computing
NSLS Datacenter
PXRR Backbone Switch
Campus Networking
The World
NSLS Backbone Switch
Legend
NSLS Floor Subnet
PXRR Campus
PXRR Controls
PXRR SAN
VLAN Trunk
Other IO
Biology
PXRR Offices
b421 Switching
Staff PC or Workstation
Devel/Test VME Crate
Devel/Test System
Motor Electronics
Representative PXRR Computing Infrastructure
NSLS Experimental Floor
Example PXRR Beamline
Detector Switch
Detector PCs
Detector Console
Detector PC UPS
Detector Rack
Serial Console Server
Beamline Switch
Beamline "Host" System (epics and cbass server)
Moxa (links to ID gap ctrl., gonio, cryo, keyance, etc)
Beamline Control System (vme crate, epics IOC)
Motor Electronics
Crystal Automounter Controller
Beamline Rack
Data Collection & Beamline Control
Data Processing
Auxiliary
User Laptops
Beamline Workstations
Cyber Cafe
User Laptops

PXRR Systems at NSLS

- 140 computers 81 linux, 58 windows (31 for detectors)
- 12 managed switches (1 managed by ITD)
- 9 ups's
- 8 camera servers
- 7 vme crates
- 6 printers
- 6 compumotors (gonios)
- 5 wago controllers (robots)
- 3 dvd robots
- 3 cyclades terminal servers
- 2 moxa serial device servers
- 1 automatic transfer switch
- 1 firewall (managed by ITD)
- Over 200 hard drives in 2 Racks

= just over 200 networked devices

System Administration Tools

- Scientific Linux 6 servers and workstations
- Cobbler provisioning for new system builds
- System management with Puppet with ENC using Cobbler and ssh power tools – pdsh, pdcp, dshbak
- Monitoring with Nagios and centralized logging

NSLS PX Control System

- EPICS based home built system running on Scientific Linux and Fedora.
- Data collection: CBASS – python based
- Database system PXDB: postgresql used to manage samples, datasets, users, scheduling etc.

Timeline

- NSLS will stop operations in 5 days.
- NSLS-2 general construction is finished
- First new detector Dectris Eiger 16M is scheduled to arrive in March of 2015 – in 6 months
- Beamline components arrive fall of 2015
- MX beamlines will start operations in January 2016.

NSLS2 MX operations

- Defining factors:
  - Beam brightness
  - Detector speed
  - Storage capacity
  - Data retention policy
  - Funding

NSLS2 MX operations

- Defining factors:
  - Beam brightness
    - $2x10^{13}$ photon/sec (AMX) 5μm^2
    - $1x10^{13}$ photon/sec (FMX) 1μm^2
    - Sample will be dead with exposure time of 1 second. Full data set should be measured within this time
    - Merging data sets from multiple samples

Detector Speed

EIGER X DETECTOR SERIES TECHNICAL SPECIFICATIONS

	1M	4M	9M	16M
				
Number of detector modules	1 x 2	2 x 4	3 x 6	4 x 8
Sensitive area (width x height) [mm²]	77.2 x 79.9	155.2 x 162.5	233.2 x 245.2	311.2 x 327.8
Pixel size [µm²]	75 x 75			
Total number of pixels	1030 x 1065 = 1,096,950	2070 x 2167 = 4,485,690	3110 x 3269 = 10,166,590	4150 x 4371 = 18,139,650
Gap width, hor. / ver. [pixel]	- / 37	10 / 37	10 / 37	10 / 37
Inactive area [%]	3.5	5.6	6.3	6.6
Defective Pixels [%]	< 0.03			
Maximum frame rate* [Hz]	3000	750	238	133
Readout time	continuous readout, 3 µs dead time, duty cycle > 99 %			
Point-spread function	1 pixel			
Sensor thickness [µm]	450			
Threshold energy [keV]	2.7 - 18			
Maximum count rate [phts/s/mm²]	$5 \cdot 10^8$			
Counter bit depth [bit]	12			
Image bit depth [bit]	16 or 32			
Data format	HDF5 / NeXus			
Dimensions (WHD) [mm³]	114 x 133 x 240	235 x 235 x 372	330 x 350 x 500	400 x 430 x 500
Weight [kg]	3.9	18	46	75
Power consumption [W]	75	300	675	1200

* Theoretical limit at maximum bandwidth | All specifications are subject to change without notice.

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133Hz

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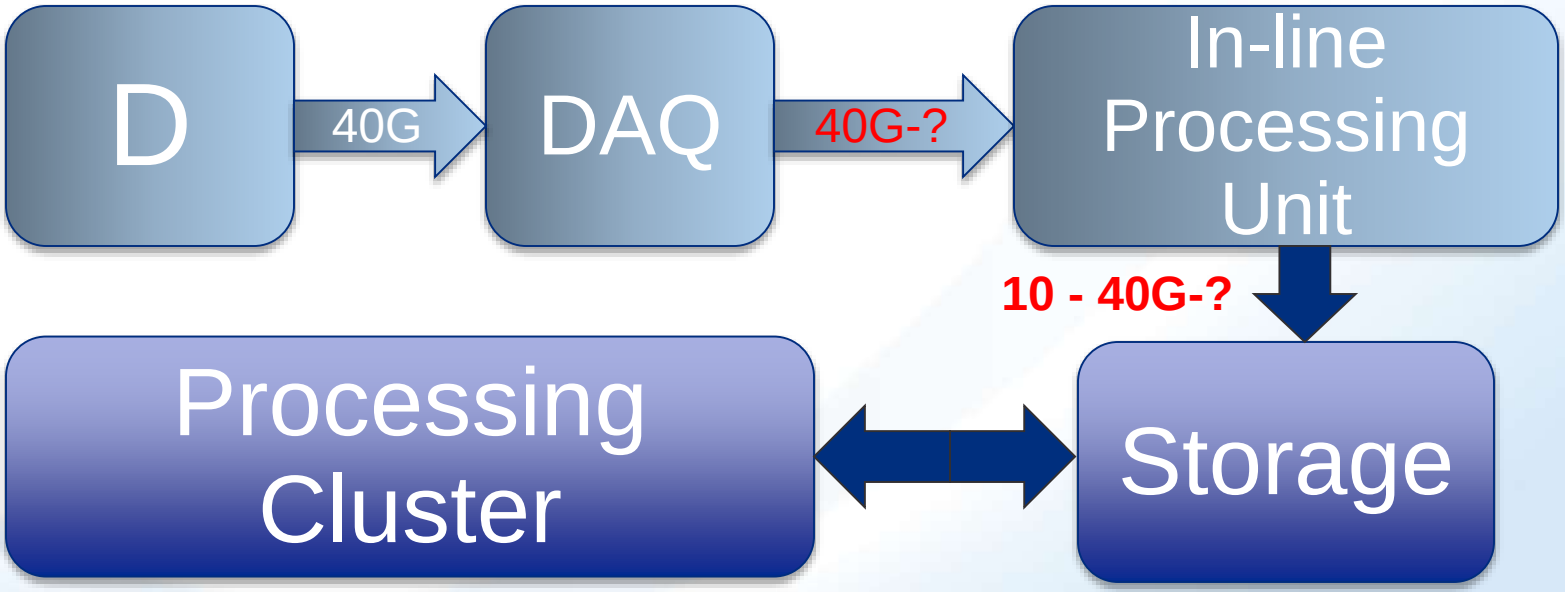
Detector Data Flow

- 18,139,650 pixels
- 12 or 16 bits/pixel
- 133 frames/second
- Total: 38,601,175,200 bits/sec ~40Gb/sec



Proposed Computing Facility

SRX
100 MB/s (peak)
15 TB/Month

SM3
ADSC Q270
34 MB/s (ub)
2 TB/Month ?

XFP ?

PILATUS 6M 25 Hz | *2 Gb*

"Pilatus Processing Unit"
24 cores (RAMDISK Buffering: 90 GB)
On the Fly data Processing
(integration/fast scoring)

Medium Storage
Processing Units
Control Stations

AMX

EIGER 16M 133 Hz (750 Hz 4M ROI) | *20 Gb*

"Eiger Processing Unit"
48 cores (RAMDISK Buffering: 1.5 TB)
On the Fly data Processing
(integration/fast scoring)

Large Storage
Processing Units
Control Stations

FMX

2x 20 Gb

3 x 10 Gb

20 Gb

100 TB + 200 Cores >>> 400 TB + 600 cores

+++

Scalable Storage and Processing Nodes
NSLS-II "standards" : IBM Server

2 Pilatus 300K + 1 Pilatus 1M

Mini PPU (8 Cores + 384 Gb RamDisk)

Modest Storage / Processing Units

LIX

10 Gb

Dedicated 40 TB + 40 cores in the HPC center

NSLS2 Beamline Controls

- Debian 7, EPICS prebuilt binary packages.
- Using NSLS2 infrastructure and support
- Storage:
  - IBM storage GPFS
  - alternatives (Winchester etc.)
  - GlusterFS, Ceph
- Data processing OS:
  - Debian ?
  - Scientific Linux ?

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