Introduction to NSLS-II Beamlines and Infrastructure

Dr. Marcus D. Hanwell

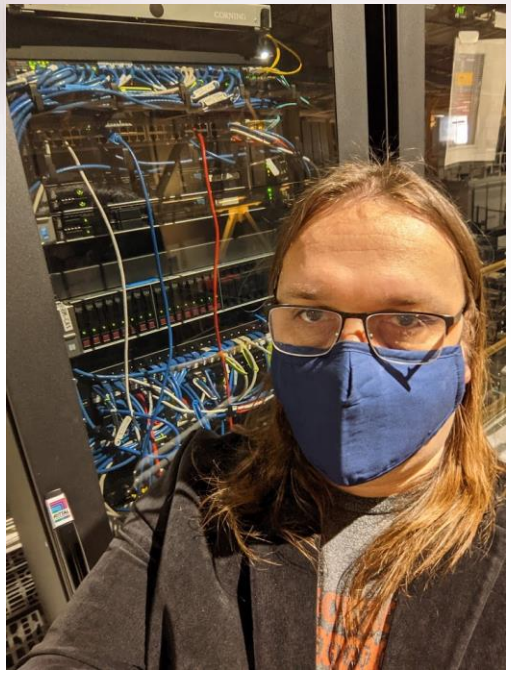
Data Science and Systems Integration Program, NSLS-II

23 July, 2021

U.S. DEPARTMENT OF ENERGY | Office of Science

BROOKHAVEN NATIONAL LABORATORY

Who Am I?

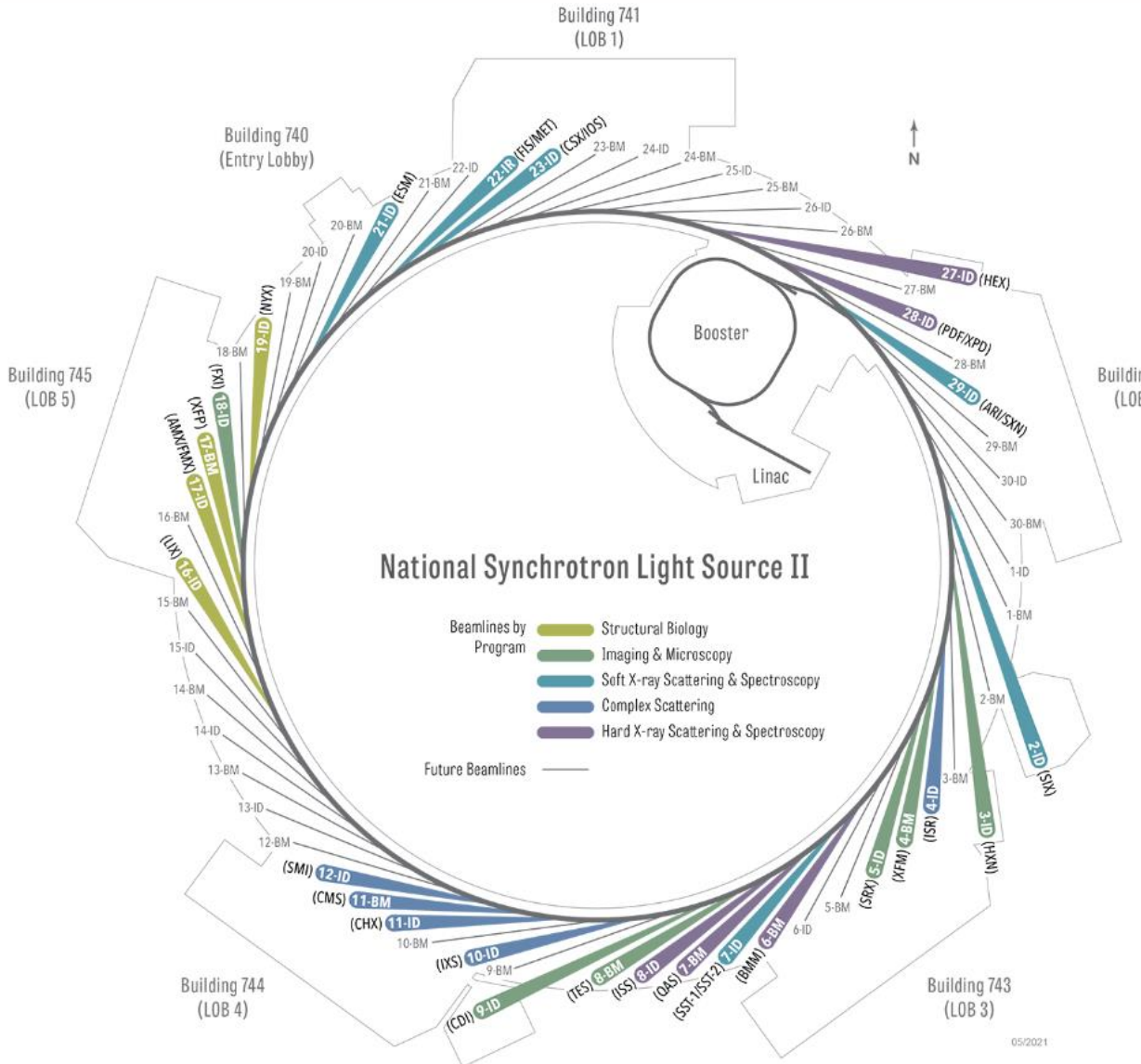


- A lad from Sheffield, South Yorkshire, UK
- B.Sc. and Ph.D. in Physics from Sheffield
  - Nanomaterial Engineering Group
  - Mainly thiol encapsulated gold nanoparticle thin films
  - Characterization using many techniques from AFM, X-ray, neutron, TEM, …
- Open source developer and programmer in my spare time
  - Gentoo porting of scientific applications to AMD64 back when it was new
  - KDE developed Kalzium components, Avogadro libraries
- Kitware after a postdoc, started as an engineer, left as a tech lead
  - Developed VTK, ParaView, CMake, ITK, Tomviz, Open Chemistry mainly C++, Git, …
- Joined DAMA last year at NSLS-II, now DSSI, just passed one year at the lab
  - You get my interpretation of NSLS-II with some help (I hope)


741

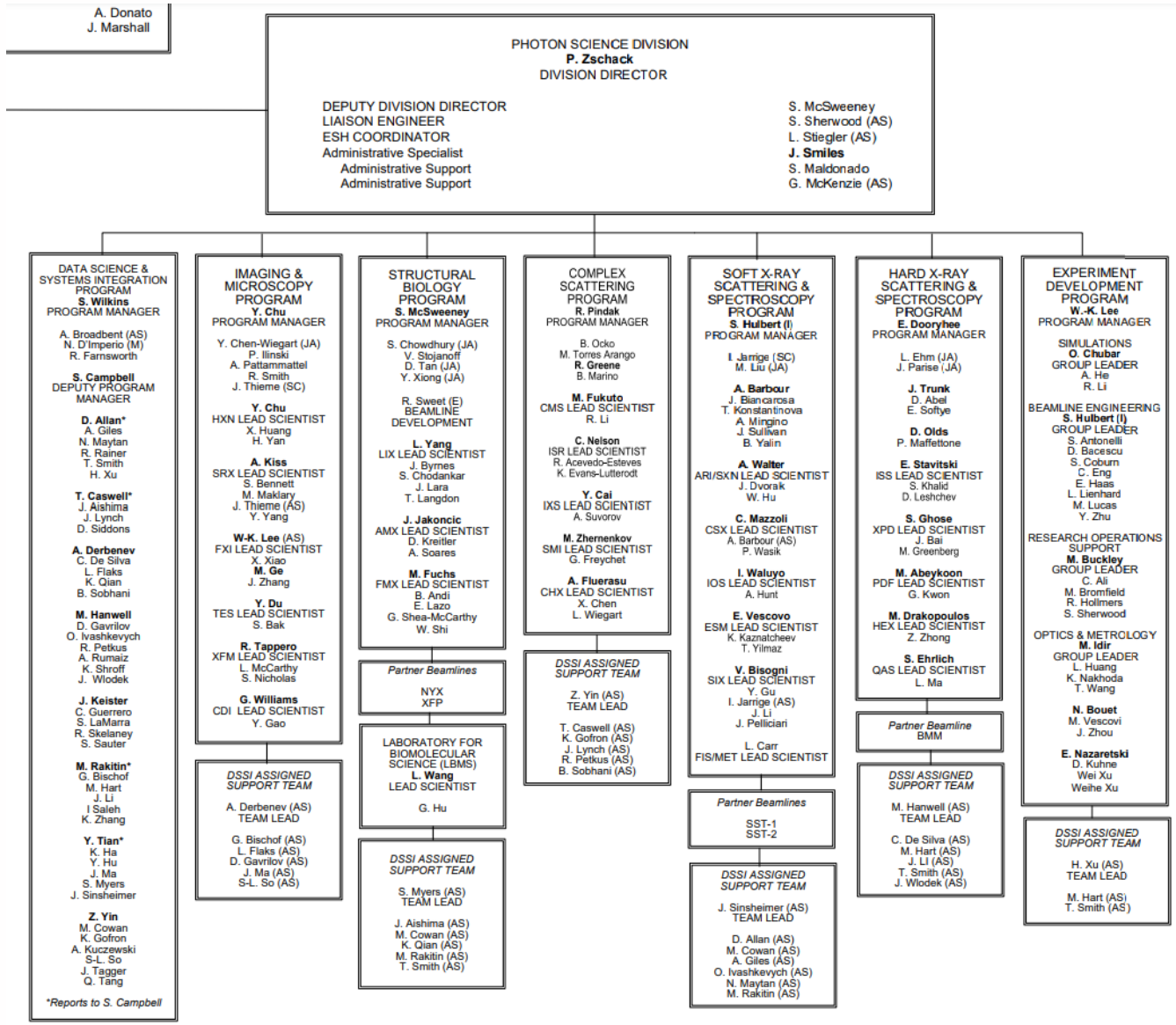
Organizational Structure

- Energy and Photon Sciences Directorate
  - National Synchrotron Light Source II
    - Accelerator Division
    - Photon Science Division
    - User Services, Communication & Outreach
    - Environment, Safety, Health & Quality (ESHQ)
- 4 LOBs housing offices along with a main entrance
- 28 experimental stations or beamlines
  - Probing electronic, chemical and atomic structure of materials
  - Largely independent infrastructure for each beamline right now


Building 741
(LOB 1)
Building 740
(Entry Lobby)
Building 745
(LOB 5)
Building 742
(LOB 2)
Building 744
(LOB 4)
Building 743
(LOB 3)
Booster
Linac
N
National Synchrotron Light Source II
Beamlines by Program
Structural Biology
Imaging & Microscopy
Soft X-ray Scattering & Spectroscopy
Complex Scattering
Hard X-ray Scattering & Spectroscopy
Future Beamlines
05/2021

What is a Synchrotron?

- Billion-dollar user facility
- Electron storage ring that produces very bright X-rays
- Consists of a ring surrounded by end stations that do specific science
- Divided into different programs (url):
  - Soft X-ray scattering and spectroscopy
  - Hard X-ray scattering and spectroscopy
  - Complex scattering
  - Imaging and microscopy
  - Structural biology
  - Data Science and Systems Integration (DSSI)
  - Experiment Development


A. Donato
J. Marshall
PHOTON SCIENCE DIVISION
P. Zschack
DIVISION DIRECTOR
DEPUTY DIVISION DIRECTOR
S. McSweeney
LIAISON ENGINEER
S. Sherwood (AS)
ESH COORDINATOR
L. Stiegler (AS)
Administrative Specialist
J. Smiles
Administrative Support
S. Maldonado
Administrative Support
G. McKenzie (AS)
DATA SCIENCE & SYSTEMS INTEGRATION PROGRAM
S. Wilkins
PROGRAM MANAGER
A. Broadbent (AS)
N. D'Imperio (M)
R. Farnsworth
S. Campbell
DEPUTY PROGRAM MANAGER
D. Allan*
A. Giles
N. Maytan
R. Rainer
T. Smith
H. Xu
T. Caswell*
J. Aishima
J. Lynch
D. Siddons
A. Derbenev
C. De Silva
L. Flaks
K. Qian
B. Sobhani
M. Hanwell
D. Gavrilov
O. Ivashkevych
R. Petkus
A. Rumaiz
K. Shroff
J. Wlodek
J. Keister
C. Guerrero
S. LaMarra
R. Skelaney
S. Sauter
M. Rakitin*
G. Bischof
M. Hart
J. Li
I Saleh
K. Zhang
Y. Tian*
K. Ha
Y. Hu
J. Ma
S. Myers
J. Sinsheimer
Z. Yin
M. Cowan
K. Gofron
A. Kuczewski
S-L. So
J. Tagger
Q. Tang
*Reports to S. Campbell
IMAGING & MICROSCOPY PROGRAM
Y. Chu
PROGRAM MANAGER
Y. Chen-Wiegart (JA)
P. Ilinski
A. Pattammattel
R. Smith
J. Thieme (SC)
Y. Chu
HXN LEAD SCIENTIST
X. Huang
H. Yan
A. Kiss
SRX LEAD SCIENTIST
S. Bennett
M. Maklary
J. Thieme (AS)
Y. Yang
W-K. Lee (AS)
FXI LEAD SCIENTIST
X. Xiao
M. Ge
J. Zhang
Y. Du
TES LEAD SCIENTIST
S. Bak
R. Tappero
XFM LEAD SCIENTIST
L. McCarthy
S. Nicholas
G. Williams
CDI LEAD SCIENTIST
Y. Gao
DSSI ASSIGNED SUPPORT TEAM
A. Derbenev (AS)
TEAM LEAD
G. Bischof (AS)
L. Flaks (AS)
D. Gavrilov (AS)
J. Ma (AS)
S-L. So (AS)
STRUCTURAL BIOLOGY PROGRAM
S. McSweeney
PROGRAM MANAGER
S. Chowdhury (JA)
V. Stojanoff
D. Tan (JA)
Y. Xiong (JA)
R. Sweet (E)
BEAMLINE DEVELOPMENT
L. Yang
LIX LEAD SCIENTIST
J. Byrnes
S. Chodankar
J. Lara
T. Langdon
J. Jakoncic
AMX LEAD SCIENTIST
D. Kreitler
A. Soares
M. Fuchs
FMX LEAD SCIENTIST
B. Andi
E. Lazo
G. Shea-McCarthy
W. Shi
Partner Beamlines
NYX
XFP
LABORATORY FOR BIOMOLECULAR SCIENCE (LBMS)
L. Wang
LEAD SCIENTIST
G. Hu
DSSI ASSIGNED SUPPORT TEAM
S. Myers (AS)
TEAM LEAD
J. Aishima (AS)
M. Cowan (AS)
K. Qian (AS)
M. Rakitin (AS)
T. Smith (AS)
COMPLEX SCATTERING PROGRAM
R. Pindak
PROGRAM MANAGER
B. Ocko
M. Torres Arango
R. Greene
B. Marino
M. Fukuto
CMS LEAD SCIENTIST
R. Li
C. Nelson
ISR LEAD SCIENTIST
R. Acevedo-Esteves
K. Evans-Lutterodt
Y. Cai
IXS LEAD SCIENTIST
A. Suvorov
M. Zhernenkov
SMI LEAD SCIENTIST
G. Freychet
A. Fluerasu
CHX LEAD SCIENTIST
X. Chen
L. Wiegart
DSSI ASSIGNED SUPPORT TEAM
Z. Yin (AS)
TEAM LEAD
T. Caswell (AS)
K. Gofron (AS)
J. Lynch (AS)
R. Petkus (AS)
B. Sobhani (AS)
SOFT X-RAY SCATTERING & SPECTROSCOPY PROGRAM
S. Hulbert (I)
PROGRAM MANAGER
I. Jarrige (SC)
M. Liu (JA)
A. Barbour
J. Biancarosa
T. Konstantinova
A. Mingino
J. Sullivan
B. Yalin
A. Walter
ARI/SXN LEAD SCIENTIST
J. Dvorak
W. Hu
C. Mazzoli
CSX LEAD SCIENTIST
A. Barbour (AS)
P. Wasik
I. Waluyo
IOS LEAD SCIENTIST
A. Hunt
E. Vescovo
ESM LEAD SCIENTIST
K. Kaznatcheev
T. Yilmaz
V. Bisogni
SIX LEAD SCIENTIST
Y. Gu
I. Jarrige (AS)
J. Li
J. Pelliciari
L. Carr
FIS/MET LEAD SCIENTIST
Partner Beamlines
SST-1
SST-2
DSSI ASSIGNED SUPPORT TEAM
J. Sinsheimer (AS)
TEAM LEAD
D. Allan (AS)
M. Cowan (AS)
A. Giles (AS)
O. Ivashkevych (AS)
N. Maytan (AS)
M. Rakitin (AS)
HARD X-RAY SCATTERING & SPECTROSCOPY PROGRAM
E. Dooryhee
PROGRAM MANAGER
L. Ehm (JA)
J. Parise (JA)
J. Trunk
D. Abel
E. Softye
D. Olds
P. Maffettone
E. Stavitski
ISS LEAD SCIENTIST
S. Khalid
D. Leshchev
S. Ghose
XPD LEAD SCIENTIST
J. Bai
M. Greenberg
M. Abeykoon
PDF LEAD SCIENTIST
G. Kwon
M. Drakopoulos
HEX LEAD SCIENTIST
Z. Zhong
S. Ehrlich
QAS LEAD SCIENTIST
L. Ma
Partner Beamline
BMM
DSSI ASSIGNED SUPPORT TEAM
M. Hanwell (AS)
TEAM LEAD
C. De Silva (AS)
M. Hart (AS)
J. LI (AS)
T. Smith (AS)
J. Wlodek (AS)
EXPERIMENT DEVELOPMENT PROGRAM
W.-K. Lee
PROGRAM MANAGER
SIMULATIONS
O. Chubar
GROUP LEADER
A. He
R. Li
BEAMLINE ENGINEERING
S. Hulbert (I)
GROUP LEADER
S. Antonelli
D. Bacescu
S. Coburn
C. Eng
E. Haas
L. Lienhard
M. Lucas
Y. Zhu
RESEARCH OPERATIONS SUPPORT
M. Buckley
GROUP LEADER
C. Ali
M. Bromfield
R. Hollmers
S. Sherwood
OPTICS & METROLOGY
M. Idir
GROUP LEADER
L. Huang
K. Nakhoda
T. Wang
N. Bouet
M. Vescovi
J. Zhou
E. Nazaretski
D. Kuhne
Wei Xu
Weihe Xu
DSSI ASSIGNED SUPPORT TEAM
H. Xu (AS)
TEAM LEAD
M. Hart (AS)
T. Smith (AS)

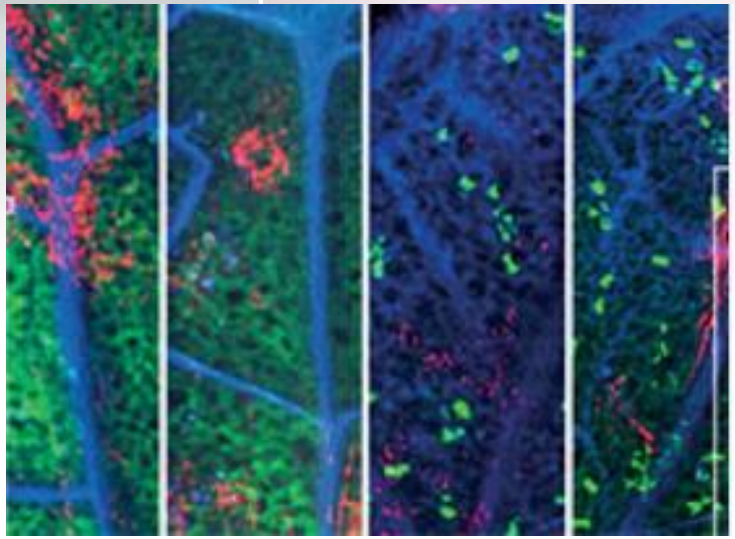
Data Science and Systems Integration Program

- Reinvention from the former Controls Program
  - Consolidated some related groups
- Goes from interfacing with hardware to the workstations
  - People working on new detectors
  - IOCs that speak EPICS for control/data acquisition
  - CS-Studio to display status and talk to EPICS IOCs
  - Bluesky to coordinate data acquisition, storage
  - Data Broker to retrieve/display historic data
  - GUIs, data visualization, analysis, processing and other steps
- Since inception we have largely been dealing with cyber security

Scientific View of a Beamline

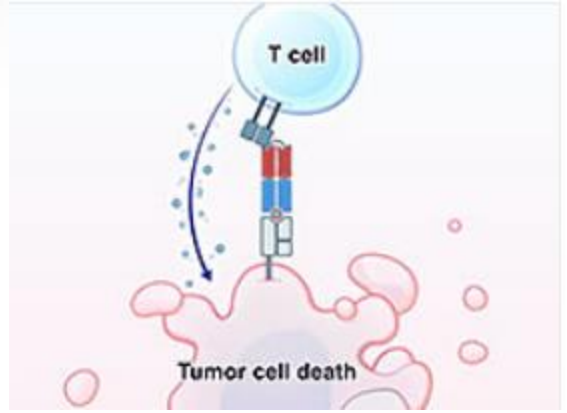
- X-rays, samples, detectors – SCIENCE!
- Lead beamline scientist responsible for scientific activity
- Proposals are made and time is granted at each beamline
  - Each beamline fills a scientific niche that others want access to
- The heart of science is publications, citations, impact
  - This is generally how the high-level success is measured
- Accelerator and beamline uptime is precious
  - Users often only have a short time window to collect data
  - They must collect data, analyze it, take that away, publish, rinse and repeat

SRX: Submicron X-ray Spectroscopy



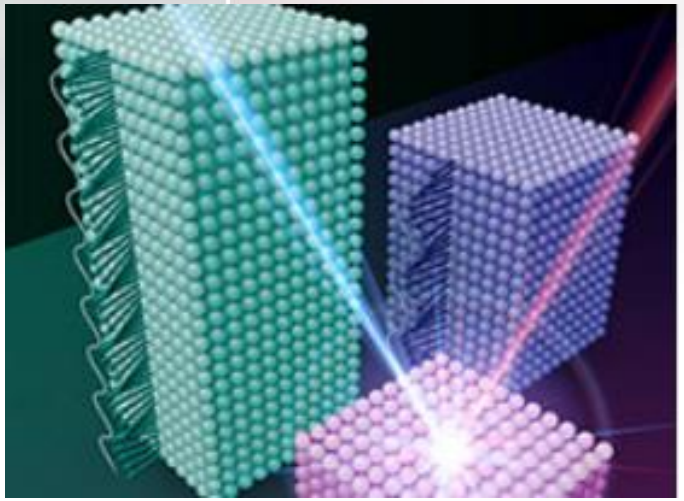
- Lead beamline scientist: Andrew Kiss
- Program: Imaging and Microscopy
- Scientific scope: "Submicron Resolution X-ray Spectroscopy (SRX) beamline is an undulator beamline at sector 5-ID providing world-leading, high-throughput spectroscopic imaging capability with submicron spatial resolution and millisecond dwell times/pixel. Scientific communities such as energy, materials, environmental, and life sciences take advantage of this beamline to understand complex natural and engineered systems that are heterogeneous on the submicron scale."

AMX: Automated Macromolecular Crystallography



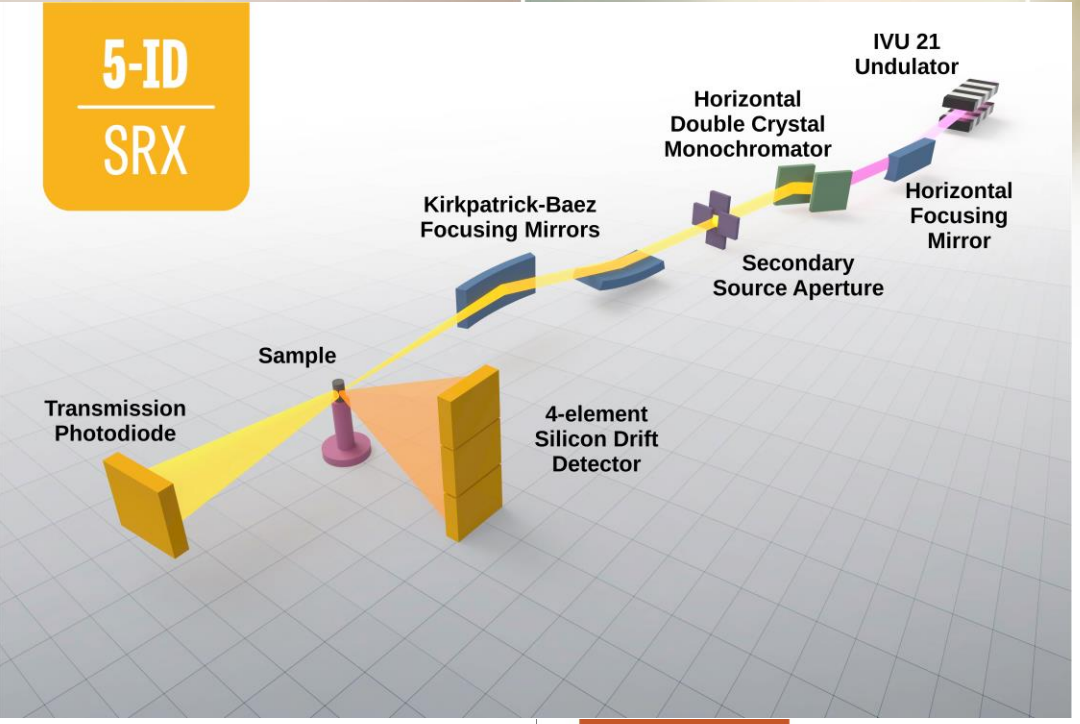
- Lead beamline scientist: Jean Jakoncic
- Program: Structural Biology
- Scientific scope: "The Highly Automated Macromolecular Crystallography (AMX) beamline is designed to meet the needs of the biomedical researcher to reveal structures and functions of proteins and other macromolecules. Researchers can use its ultrabright x-rays to investigate small crystals of proteins and macromolecules. The beamline offers a high-flux mini-beam that allows scientists to scan their crystals and collect best possible quality diffraction data for a large number of samples sizes."

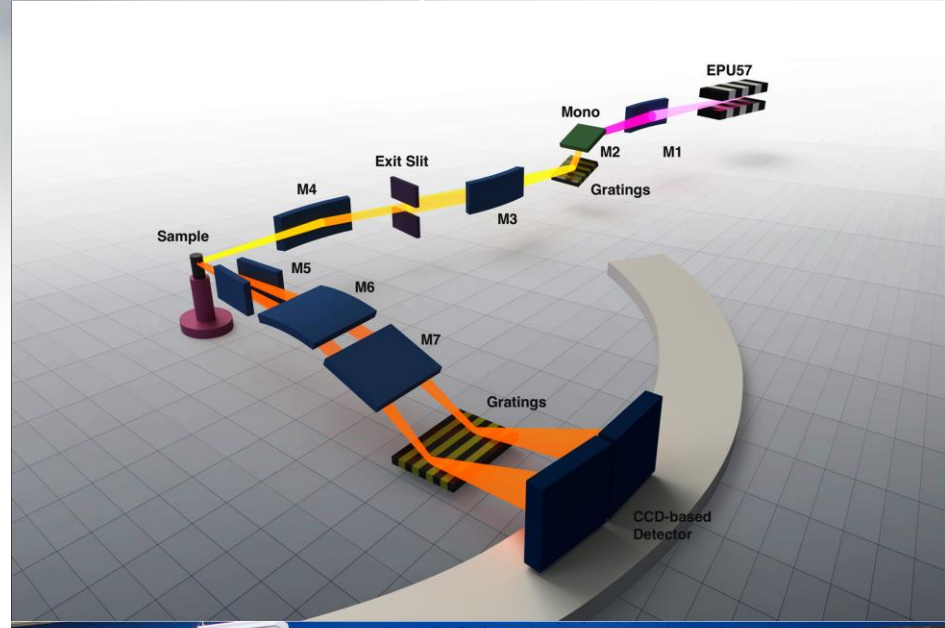
SIX: Soft Inelastic X-ray Scattering



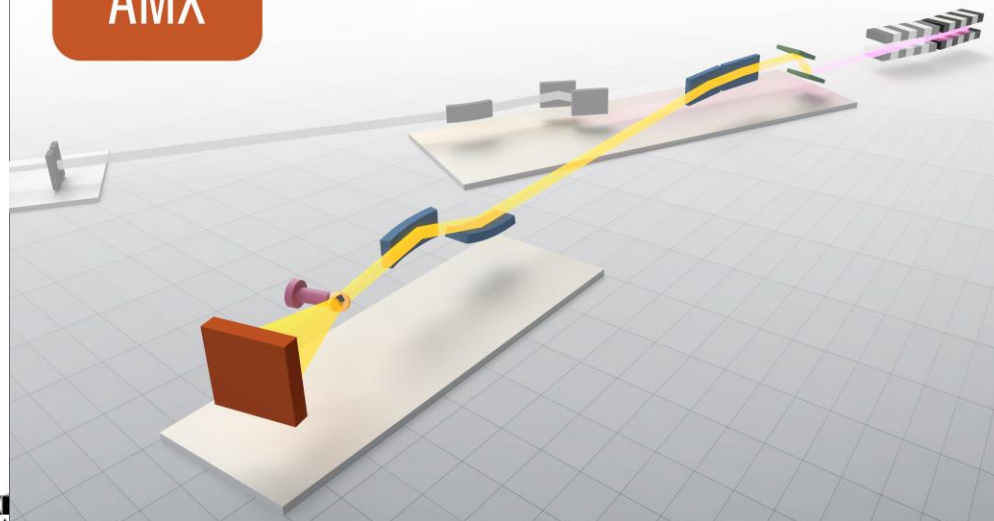
- Lead beamline scientist: Valentina Bisogni
- Program: Soft X-ray Scattering and Spectropscopy
- Scientific scope: "The Soft Inelastic X-ray Scattering (SIX) beamline utilizes resonant inelastic x-ray scattering (RIXS) to study the elementary excitations (spin, charge, orbital, and lattice) in materials with an ultrahigh energy resolution. This allows researchers to investigate a wider variety of materials in the areas of condensed matter physics and quantum materials, unveiling the interactions leading to their unconventional properties."

5-ID
SRX





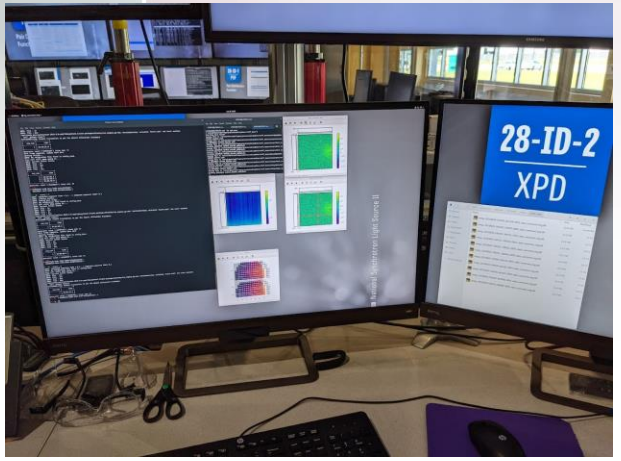
17-ID-1
AMX



U.S. DEPARTMENT OF ENERGY | Office of Science

BROOKH
NATIONAL LA

Computational View of a Beamline



- Detectors and motors either networked, serial or USB
- IOC servers on the "EPICS" VLAN talk to detectors, motors, etc
  - Cameras live on a "CAM" VLAN stream images mainly
  - Instruments on an "INST" VLAN for general instruments
- Some servers act in special roles
  - GPFS clusters, processing, etc
- Channel archiver servers used for various beamline services
  - Alarm servers, olog, channel archiving, beamline MongoDB
- Workstations on the "SCI" VLAN used to control beamline operations
  - Usually dual-homed with "EPICS" VLAN to talk to IOC services
  - These are often accessed remotely with NX or Guacamole


05-07-2021 01:35:49 PM
LOREX
28-ID-2
XPD
X-ray Powder
Diffraction

Assigned Support Teams

- The new DSSI program has assigned support teams
  - A lead for the program and specialists in different areas
- Hard X-ray scattering and spectroscopy (HXSS)
  - Led by Marcus Hanwell
  - Ji Li and Chanaka de Silva acted as points of contact for HXSS before
  - Jakub Wlodek on EPICS development, acquisition software
  - Michael Hart on Bluesky development
  - Thomas Smith from the former sysadmin group
- Day-to-day operations, troubleshooting, minor development tasks
- Six beamlines: ISS, QAS, PDF, XPD, BMM and HEX (being built)

Services DSSI Offers

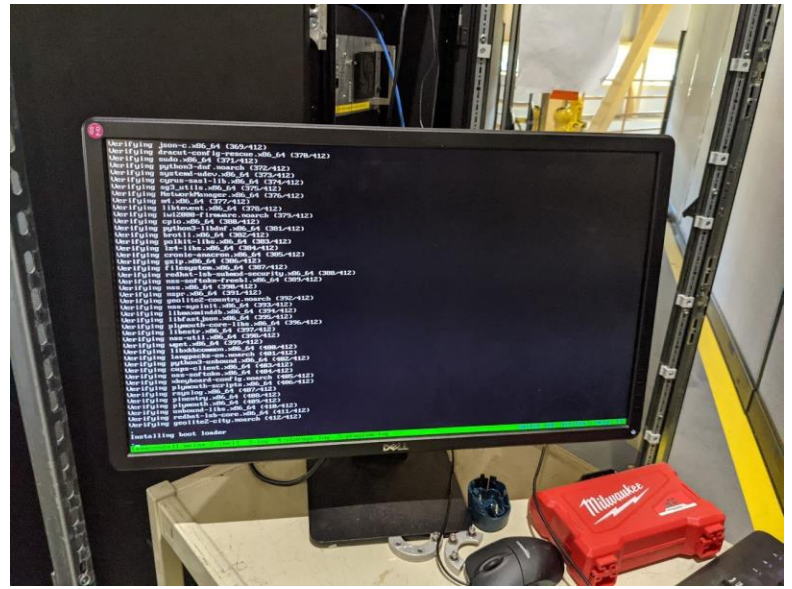
- Data Science and Systems Integration!
- Interface with the beamlines to achieve their scientific goals
- Ensure all equipment can talk to relevant services
  - Motion control, detectors, cameras, temperature monitors, encoders
- Racked servers at the beamlines providing services
  - IOC services to control equipment, acquire data, monitor
  - File systems, databases, archival services, etc
- Workstations, detector PCs, analysis machines
  - Usually RHEL 8, formerly Debian 7, 8, 9, 10

Challenges for DSSI and NSLS-II

- Getting and remaining cyber compliant
  - Operational schedule restricts when updates/reboots are possible
  - Various device drivers can be vendor specific without upgrade paths
  - Resistance to change without clear benefits
- Catering to the user facility with general users
  - Domain scientists interested in characterizing data
  - Familiarity with SSH, Linux, coding, version control are not guaranteed
- Need access to resources as experiments run
  - Batch schedulers not fit for purpose
  - Samples may degrade as data is acquired in beam

Challenges for Central Services

- Moving from hand-curated machines to mass deployments
  - Satellite for RHEL provisioning
  - Tower for configuration deployment
  - RPM packaging
  - Conda packaging
- Centralized services migrating from beamlines
  - MongoDB single node to central cluster
  - Filesystem GPFS clusters to central Lustre/others
  - EPICS services moving from channel archiver
- Developing analysis cluster, computational cluster, data processing
  - Tackling both post experiment and real-time processing/feedback/vis



Future Plans

- Assigned support teams integrate and participate in beamline work
- Centers form around core areas
  - Motion control
  - Area detector
  - Bluesky
  - EPICS services
  - GUIs, UX, data visualization
  - …
- DSSI moves to greater emphasis on research and development
  - Enable science through state-of-the-art data science and systems integration

Strategic Directions

- Vision is aligned with the five DOE light sources
- Forming partnerships with relevant lab facilities
- Leverage common use cases where we can work together
- Build capabilities where we need to do things differently
- Strong emphasis on open source at the facility
  - Contribute where reasonable
  - Default to open when developing code
- As with many units timelines are tight, resources are scarce
  - Leverage expertise from other groups where
- Partnering to develop code, GUIs, visualization, automation

Questions?

- DSSI is a young program with big challenges
  - The interface of computational with scientific
- Unique challenges with user facilities
  - Domain scientists with short-lived experiments visit frequently
  - Unique samples that may degrade as they are characterized
- Each beamline is a one-off
  - Commonalities such as technique, detectors, software
  - Likely wouldn't have been commissioned without unique elements
- Software is at the heart of the modern scientific enterprise
  - How can we better partner with scientists to enable their science?


RAM
MOUNTS
X-GRIP