

***Life Sciences Collaborative
Access Team (LS-CAT) @ APS:
UI LNode***

Joseph S Brunzelle
j-brunzelle@northwestern.edu

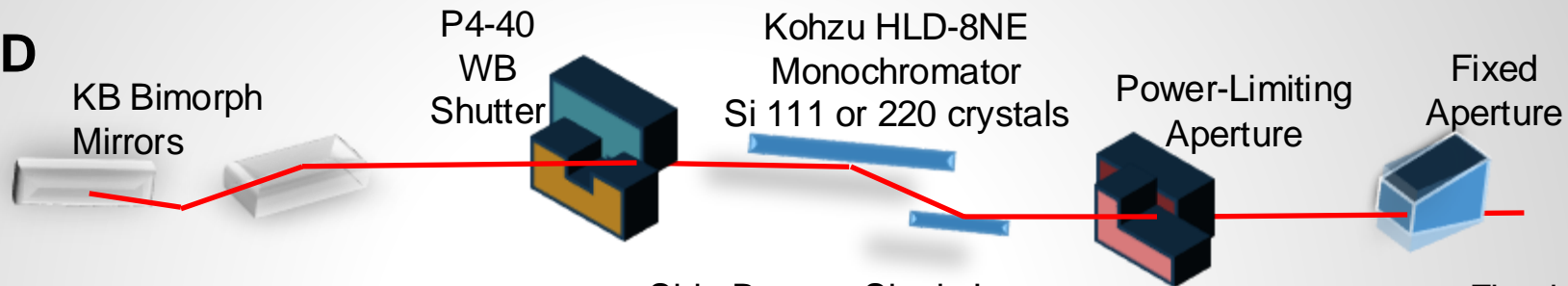


The Life Sciences Collaborative Access Team (LS-CAT)

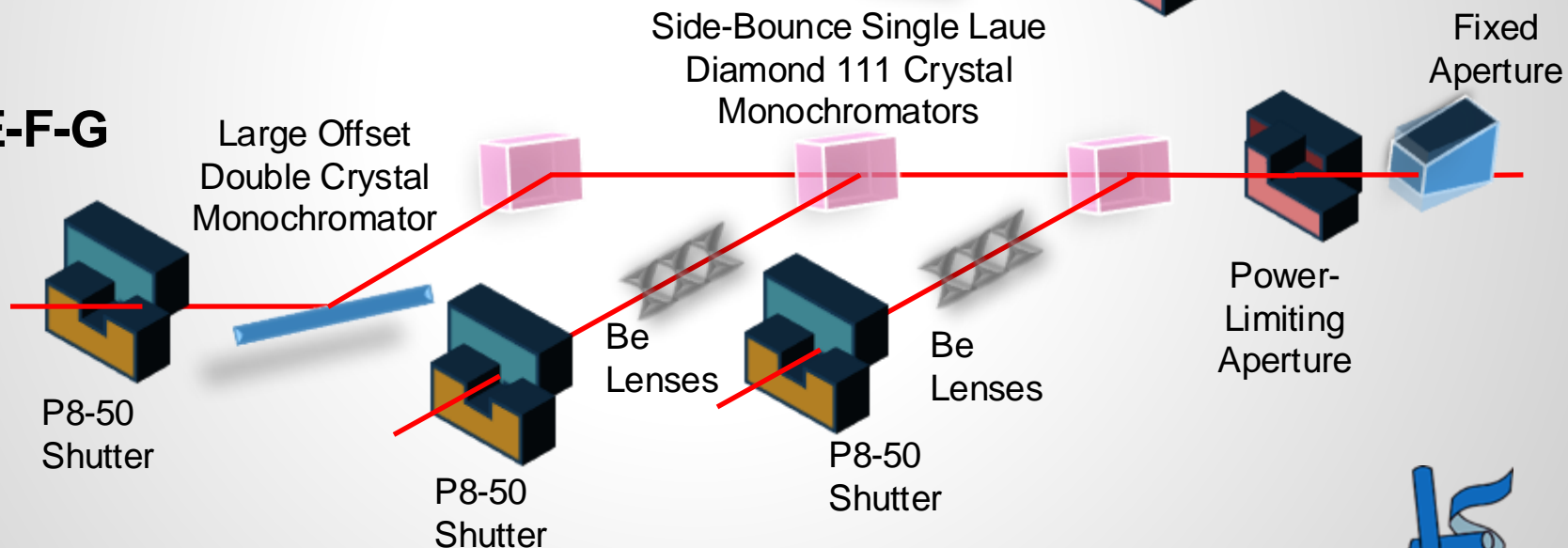
- A consortium of academic and research institutions comprised of:
 - Northwestern University
 - Michigan State University
 - University of Michigan
 - Wayne State University
 - University of Illinois
 - Vanderbilt University
 - University of Wisconsin at Madison
 - eBERLight a DOE/BER group @ ANL
- Areas of research
 - Multi-component systems in cellular signaling and protein transport
 - Protein/nucleic acid complexes involved in genome replication, regulation, and expression
 - Enzymes that are novel targets for mechanistic studies and for biotechnology or drug design
 - Biological and environmental research objectives of the DOE
- Beamlines incorporate a 1 milliradian canted undulator design
 - 2.1 cm inboard undulator device
 - 3.0 cm outboard undulator device



21ID-D

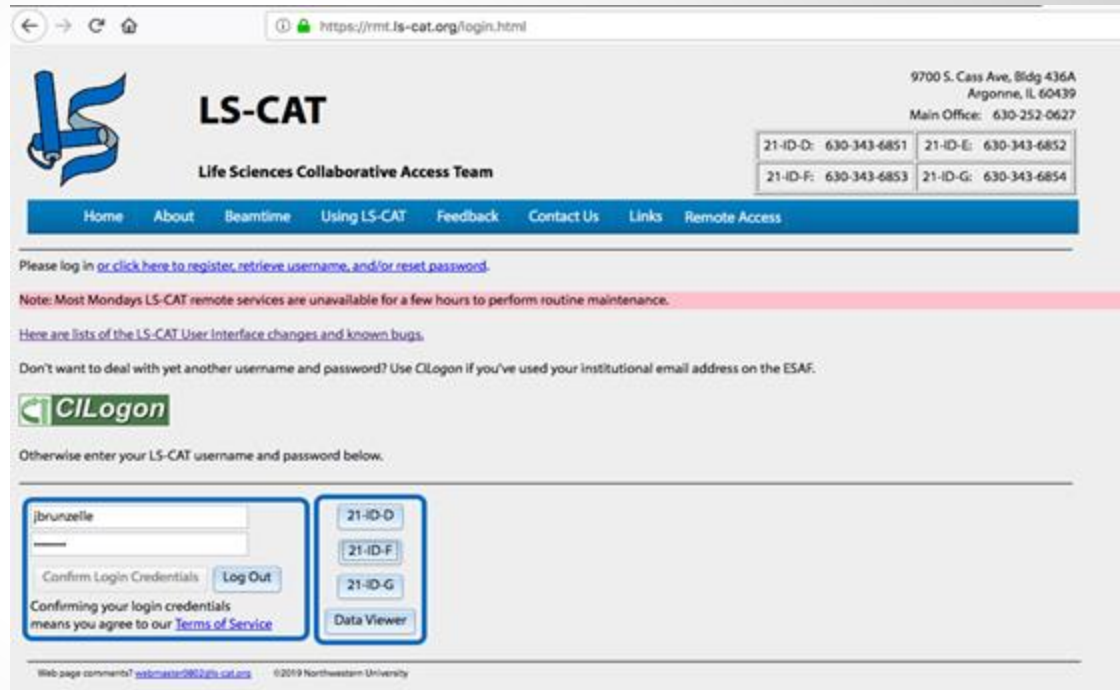


21ID E-F-G



Current User Interface: Login

- LSnode: Web based frontend w/ node.JS backend and various DBs
- Uses CILogon
 - Enables researchers to use their home organization identities to access
 - In conjunction with ORCID, an identity provider that is support by ANL/APS
- User accounts linked w/experimental session (ESAF submission)



The screenshot shows the LS-CAT login page in a web browser. The URL is <https://rmt.ls-cat.org/login.html>. The page features the LS-CAT logo (a blue ribbon forming the letters 'L' and 'S') and the text "LS-CAT Life Sciences Collaborative Access Team". In the top right corner, the address "9700 S. Cass Ave, Bldg 436A Argonne, IL 60439" and "Main Office: 630-252-0627" are displayed. Below this is a table of phone numbers:

21-ID-D: 630-343-6851	21-ID-E: 630-343-6852
21-ID-F: 630-343-6853	21-ID-G: 630-343-6854

A blue navigation bar contains links for Home, About, Beamtime, Using LS-CAT, Feedback, Contact Us, Links, and Remote Access. Below the navigation bar, there is a login prompt: "Please log in or [click here to register, retrieve username, and/or reset password.](#)" A pink banner states: "Note: Most Mondays LS-CAT remote services are unavailable for a few hours to perform routine maintenance." Below this, there is a link: "[Here are lists of the LS-CAT User Interface changes and known bugs.](#)" A message says: "Don't want to deal with yet another username and password? Use CILogon if you've used your institutional email address on the ESAF." The CILogon logo is shown. Below it, the text reads: "Otherwise enter your LS-CAT username and password below." There are two input fields for username and password. The username field contains "jbrunzelle". Below the input fields are buttons for "Confirm Login Credentials", "Log Out", and "Data Viewer". A note says: "Confirming your login credentials means you agree to our [Terms of Service](#)". At the bottom, there is a footer with the text: "Web page comments? webmaster@rmt2@ls-cat.org ©2019 Northwestern University".



Current User Interface: Sample Mounting

- Simple sample selection for robotic mounting
- Error handling/mitigation
- Can mount from EMBL or Rigaku pucks

LS-CAT
Life Sciences Collaborative Access Team

Schedule 21-ID-D

1E1045 Station
Log Out ESAF

You Control This Station
Code

Station A not enabled

Open FS.
Open Stn. Close Stn.

No Sample Present

Energy (KeV) 11.501

Attenuation Actual 0.00% Requested 0

Chat (2)

Sample Center Collect Expert

Sample Mounted: No Sample Present
Sample in Gripper: none
Robot Progress: 100%

Robot Status: **Power Of LN2 is OFF** Turn LN2 On: LN2 very low, remove samples

MCQ Status: MCQ Started
Detector Distance: 130.0 mm
File Base: A3
File Prefix: A3_1_1

Dewar 1: Open View
Dewar 2: Open View
Dewar 3: Open View

Auto Recovery

Reset and Run Back Sample Missing or Empty Vial Put Robot in Known State

Manual Recovery

Stop robot now: Abort
Move to the home position safety: Safe
Try to recover by backtracking: Back

Expert Recovery

Panic Home Open Tool Close Tool Turn Magnet On Turn Magnet Off
Dry the gripper Clear Robot Memory Reset Robot Parameters Reset Robot Motion

D Mount Area



Current User Interface: Sample Centering

- Standard 3-click centering
- Quickly change MD2 Mode
- Ease to adjust orientation
- Lighting
- Zoom

The screenshot shows the LS-CAT (Life Sciences Collaborative Access Team) web interface. At the top, it displays the LS-CAT logo and the user ID 'e161045'. Below this is a 'Schedule' section for '21-ID-D' with a 'Log Out ESAF' button. A row of status indicators includes 'You Control This Station' (with a 'Code' button), 'Station A not enabled', 'Open File' (with 'Open Site' and 'Close Site' buttons), 'No Sample Present', 'Energy (KeV)' (11.501 / 11.500), and 'Attenuation' (Actual 0.00%, Requested 0%). A 'Chat (2)' button is on the right.

The main control area has tabs for 'Sample', 'Center', 'Collect', and 'Expert'. Under 'Centering Mode', there are buttons for 'Live 3-Click', 'MD2 Mode', and 'Beam Marker' (set to '50 µm dia circle'). Below this is the 'Live 3 Click Crystal Alignment' section with 'Long Pin' and 'Short Pin' buttons, an 'Omega 540.00' slider, and buttons for '-180', '-90', '-10', '+10', '+90', '+180', and 'Reset'.

The 'Instructions' section provides a 5-step guide for crystal centering. The 'Hints' section offers additional tips, such as waiting for the sample to stop rotating and adjusting the angle with the omega slider.

On the right, there is a 'Zoom' control (1-10) and a 'Reciprocate Video' button. The main video window shows a live feed of the crystal with a red crosshair and a 'D Sample' dropdown menu.



Current User Interface: Data Collection

- Essential collection parameters
- Single and/or Ortho snap analysis

GridIn to transfer your data. Our Globus endpoint is: 'iscat@Data' with path: '~e161045'."/>

LS-CAT
Life Sciences Collaborative Access Team

Schedule 21-ID-D

161045 Brister
Log Out ESAF

You Control This Station
Code

Station A not enabled

Open FE
Open Sn
Close Sn

No Sample Present

Energy (KeV)
11.501
11.500

Attenuation
Actual
0.00%
Requested
0 %

Chat (2)

Sample Center Collect Expert

Directory: d:04192017\ina\screen
Prefix: 546-1
Distance (mm): 200 Spindle Rate (1/Sec): 20
Start (°): 360 Snap Delta (°): 0.2
Range (°): 180 Frame Rate (1/mg): 5
Collection Time (secs): 9 *Oscillation* Angle (°): 0.2
Number of Frames: 900 Frame Rate (Hz): 100

Ortho Snap Snap Pause Resume

Run

MD2 Status:
APS Status: Station A not enabled
Detector: Cover is closed
Free Space: 170.0GB Clear Now
Omega: 540.001°
Fast Shutter: Closed
Count Cutoff:
Saturated Count: 0
Spots: 212
Max: 23307
RMS: 135.41
Min: 0

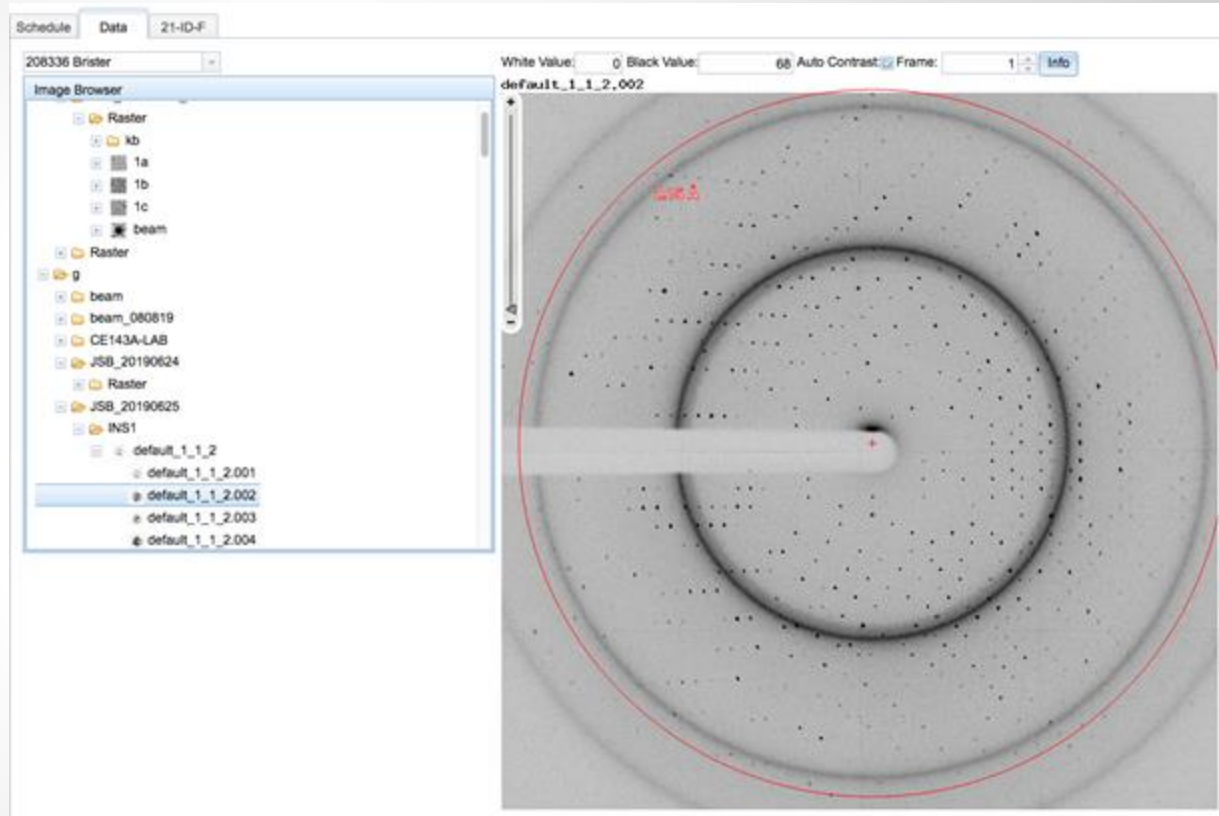
File Series	Start (°)	Range	Status
546-1_S.001	-80	360	Done
546-1.001	-80	360	Done
546-1.002	-80	360	Done
546-1.003	-80	360	Done

You can use [GridIn](#) to transfer your data. Our Globus endpoint is: 'iscat@Data' with path: '~e161045'

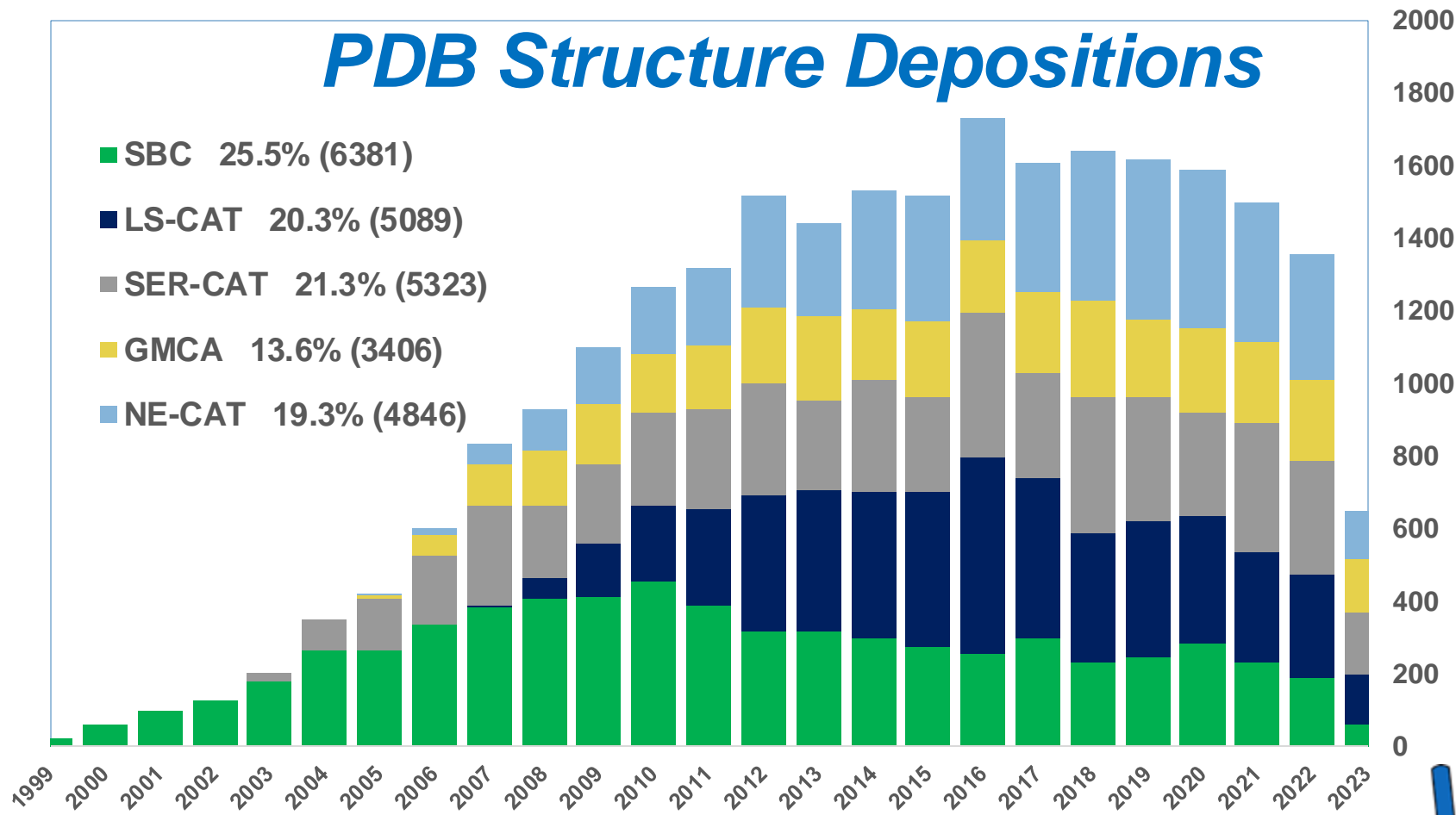


Current User Interface: Data Viewer

- Browse thru directory tree
- Simple indexing and data analysis



PDB Structure Depositions



Current User Interface: Pros and Cons

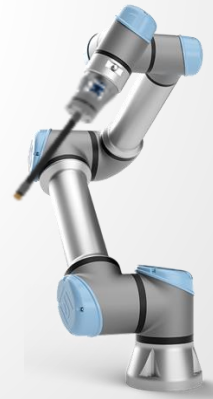
Pros

- Simple
- Clean
- Intuitive
- Secure

Cons

- Demanding development time for single group
- Lacked automation
- Lacked reporting system/LIMS
- Needed hardware updates

-
- LSnode needs to be replaced
 - Need a UI to complement new devices
 - MD3-up
 - UR5 sample changer/37 puck dewar
 - SSX
 - Support new automation ideas



Future User Interface: MXCuBE-Web

- APS-U Dark period experiences
 - Extensive exposure to various facilities
 - SSRL, NSLS-II, DLS, ESRF, Soleil, and MAX-IV
- Philosophy is similar
- Overall concept is like LSnode
- Intuitive
- Secure
- Wide community implementation and support
- Continued development
- Compatibility with a reporting system/LIMS

