recent implementations

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Scientific Advisory Committee

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Outline

- Recent technical improvements
- Future short time improvements
- Protein express
- Remote access
- Summary

Constant interactions with experimenters …

… to make the beamline more user friendly, reliable, robust and efficient.

1. Better sample illumination (see K.Q. slides)

2. Better user interface (see K.Q. slides)
   Image size, faster (automated) fluorescence scan, new buttons, new tabs

Routine data collection at low energy (7 keV)

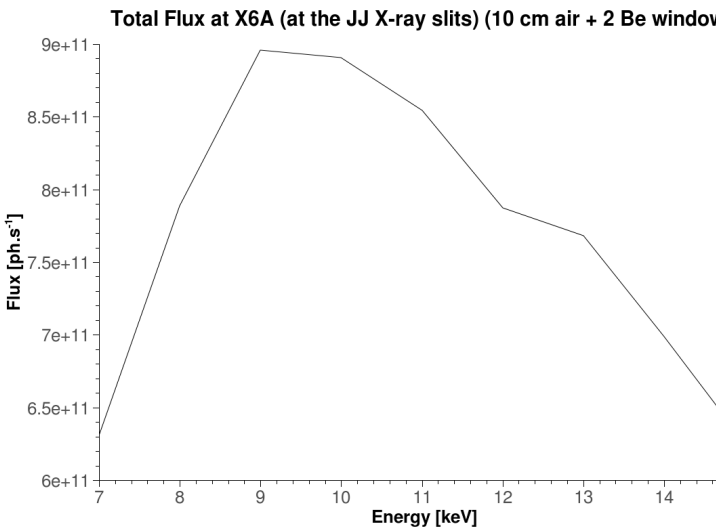
Currently on the to do list

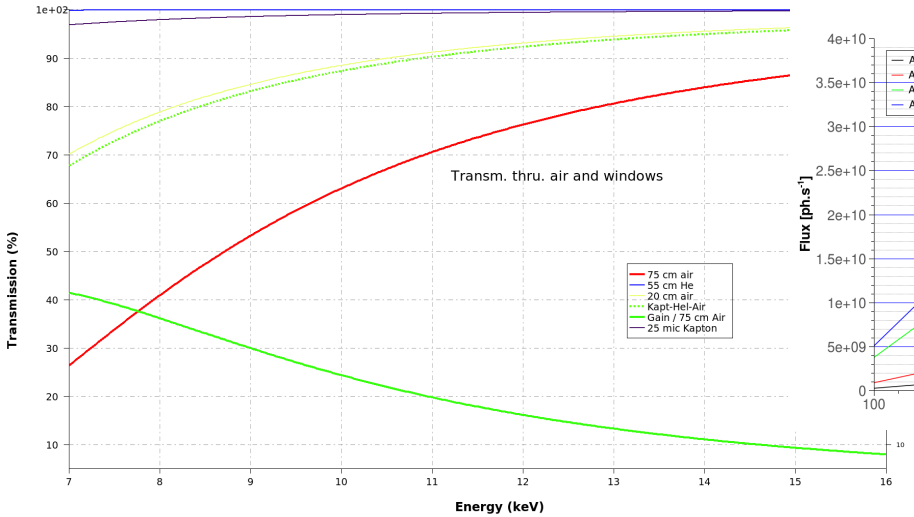
Automated beam stop

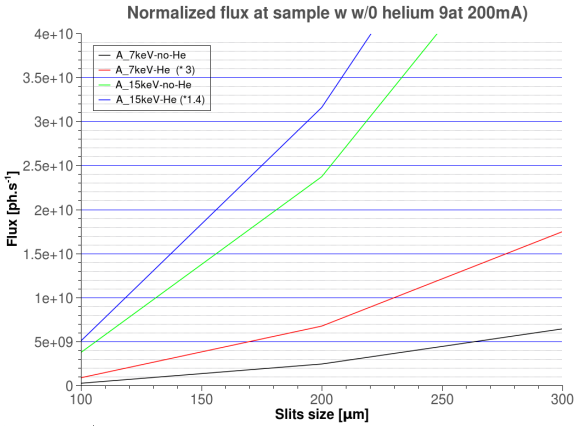
Data storage capacity

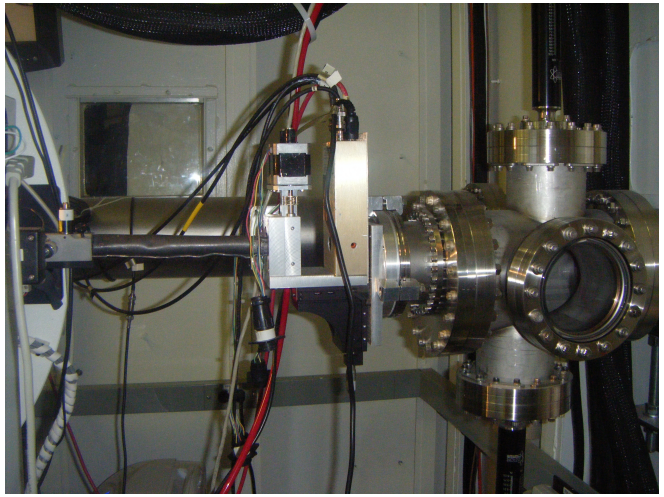
Routine data collection at 7 keV

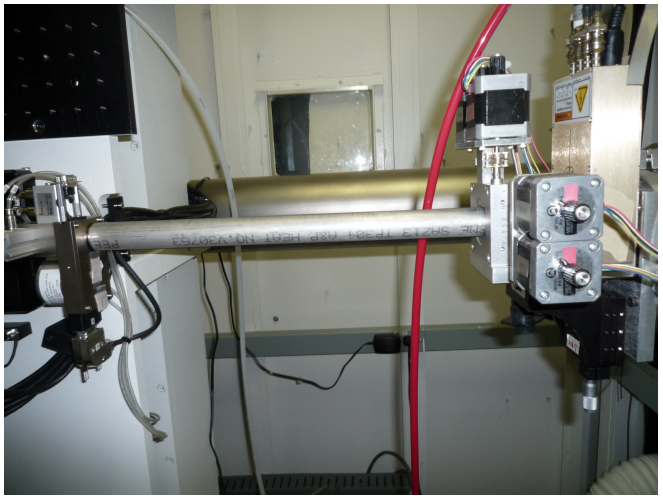
Data collection at the lowest (currently) energy accessible at X6A (7000 eV)
He path required to increase the flux

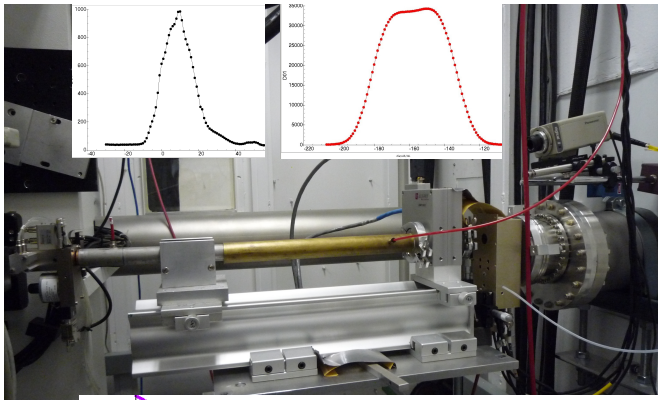


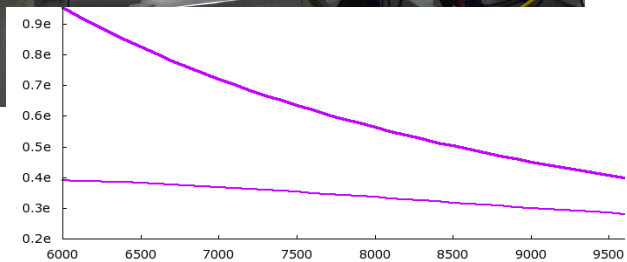








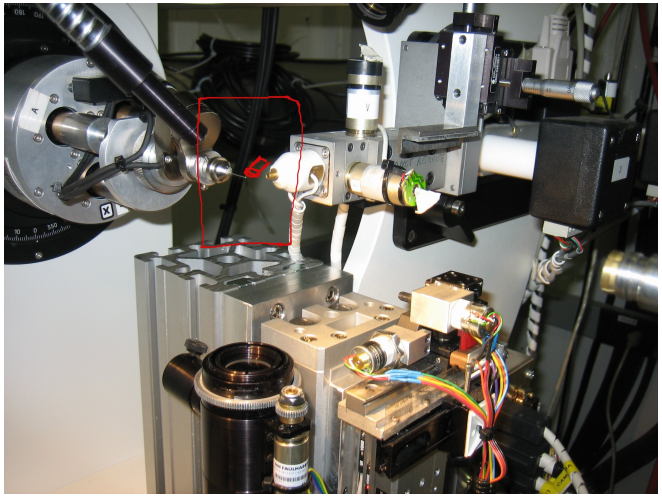


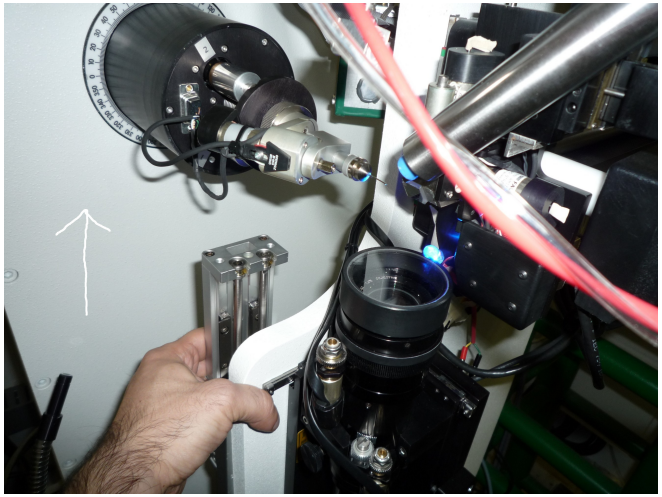


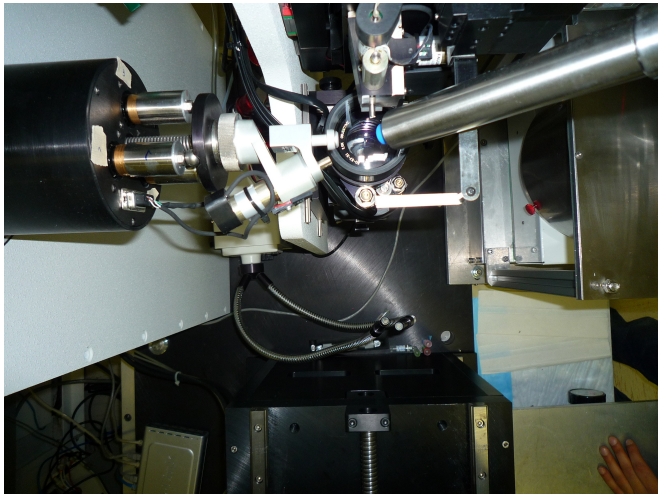
-> **Would like to achieve 6 keV**

Automated beamstop

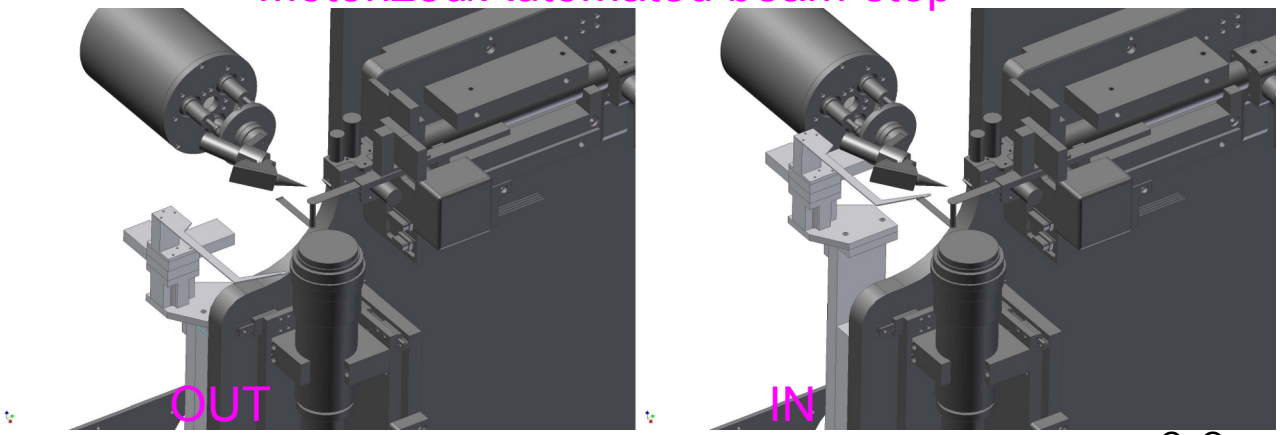
- Issues with the current beamstop design (rather delicate operation)
- Lack of real estate in the vicinity of the sample …
  due to Kappa/automounter considerations







Motorized/Automated beam-stop



C. Owen

-> Would like to implement it by summer 10

Protein eXpress
(http://protein.nsls.bnl.gov/mediawiki/index.php/Protein_Express)

Fedex / Mail In like

Users can send us protein crystal samples for diffraction measurements.
Users are responsible of submitting project and scheduling time (in cooperation with staff).
They provide spreadsheet containing priorities, requirements, size, loop, method, energy ...

We collect data for them and provide at least: sample images, diffraction data + sometimes processed files (x files + log + sca ...).

All samples are saved and stored until feedback (additional data required, E …).

For some users/collaborators, density map as well as partial structure can be provided.

More and more scientists are taking advantage of it (samples left behind …).

In the future : samples in pucks only will be "accepted" (automation needed …)

Last year
Groups : > 14
Crystals : > 200
Data sets : > 100
Structure : need to implement tracking method
Article : need to implement a tracking method

Remote Access

(http://protein.nsls.bnl.gov/mediawiki/index.php/Remote_Access)

User's requirements:

- BNL domain account as well as a cryptocard account.
MAC, WINDOWS, LINUX: OK
- VPN client
- Hardware : robust network connection AND high resolution display (Y > 1000)
2 connections preferred (one for data collection and one for data analysis)

NX no machine is robust (if connection lost, the session restart from the crash point)

Users send dry shipper containing pucks.

Use of live chat for support ...

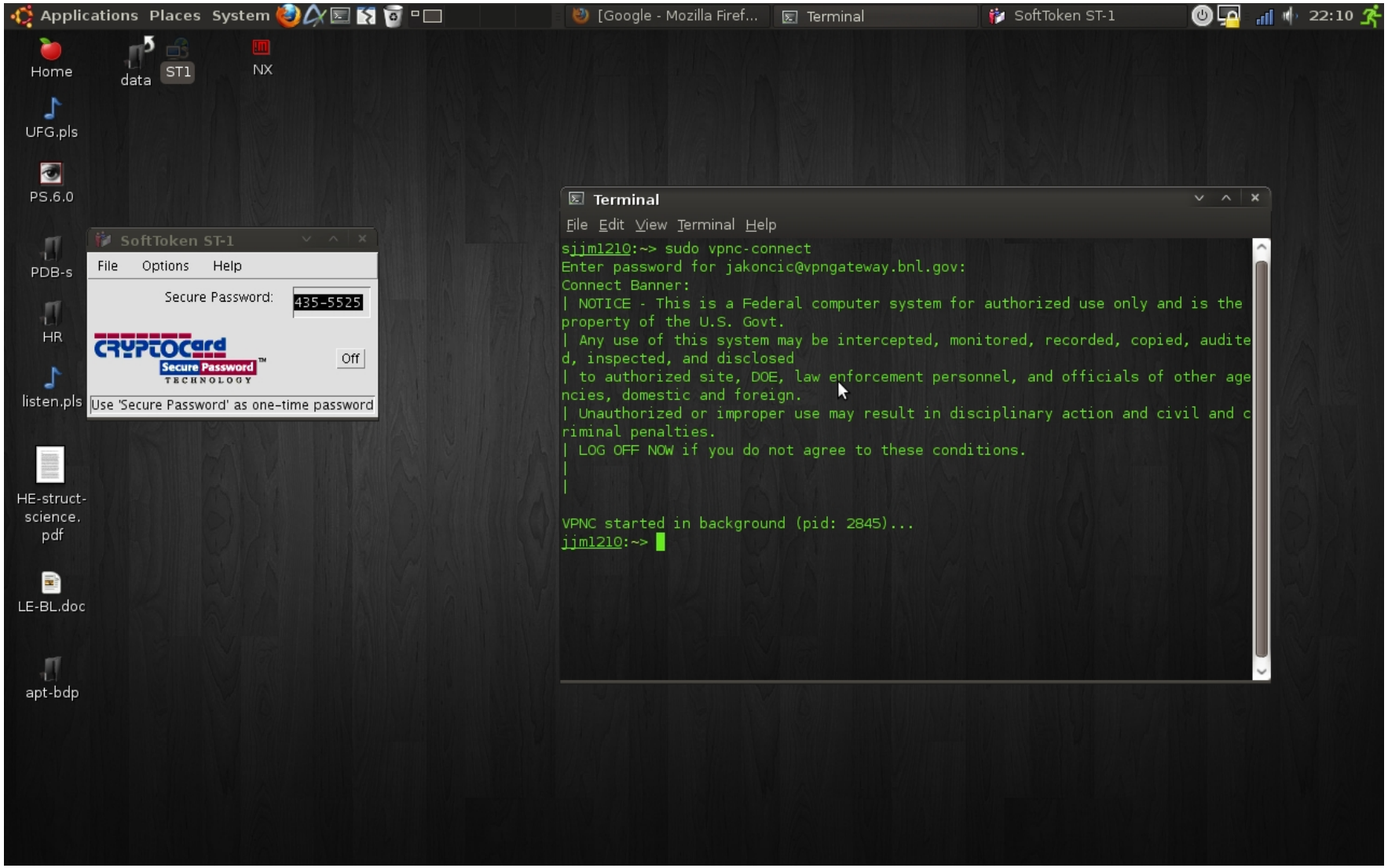
We load the pucks (4 * 16 at a time; ~ 150 mins total)

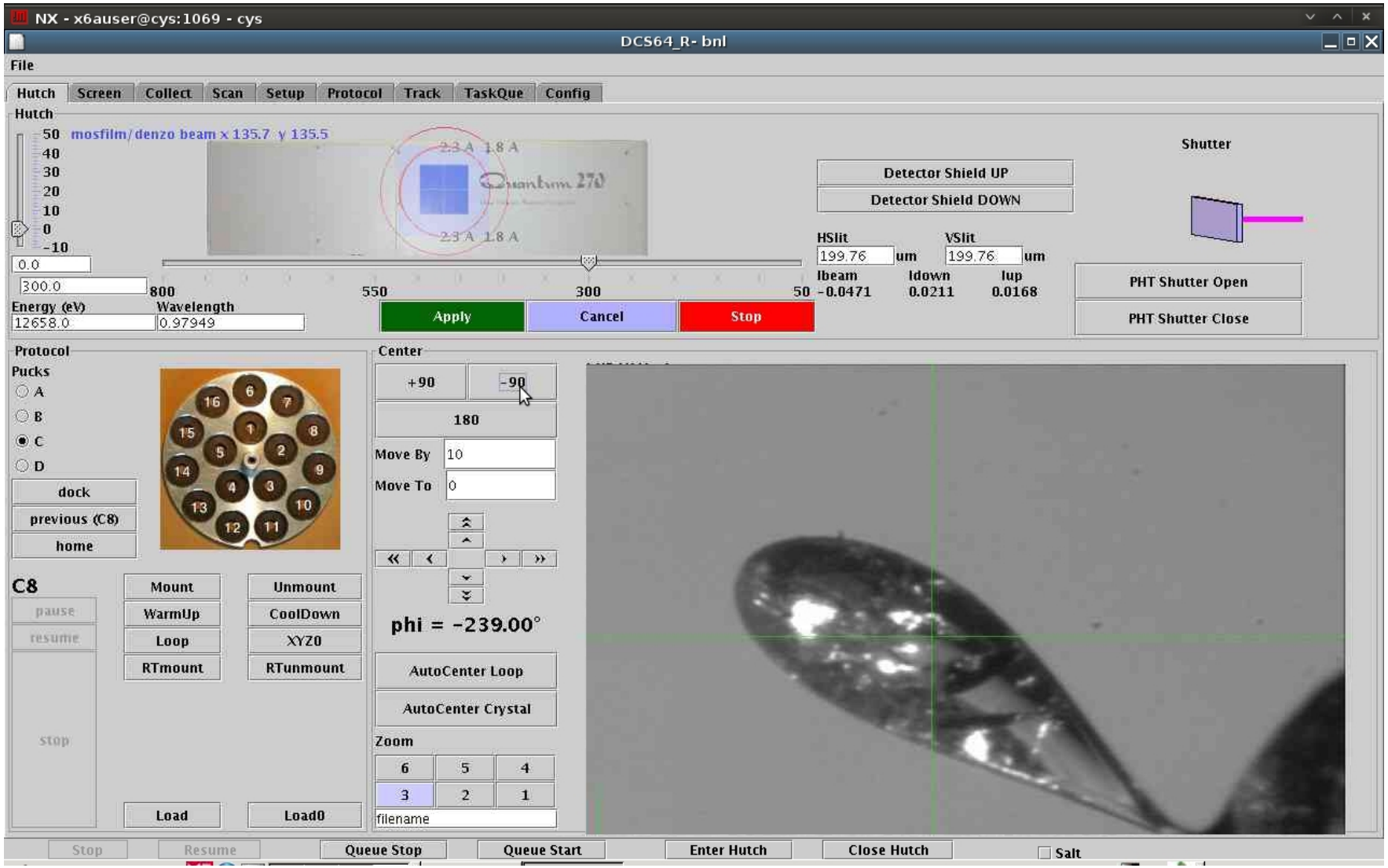
Users center samples and collect data …

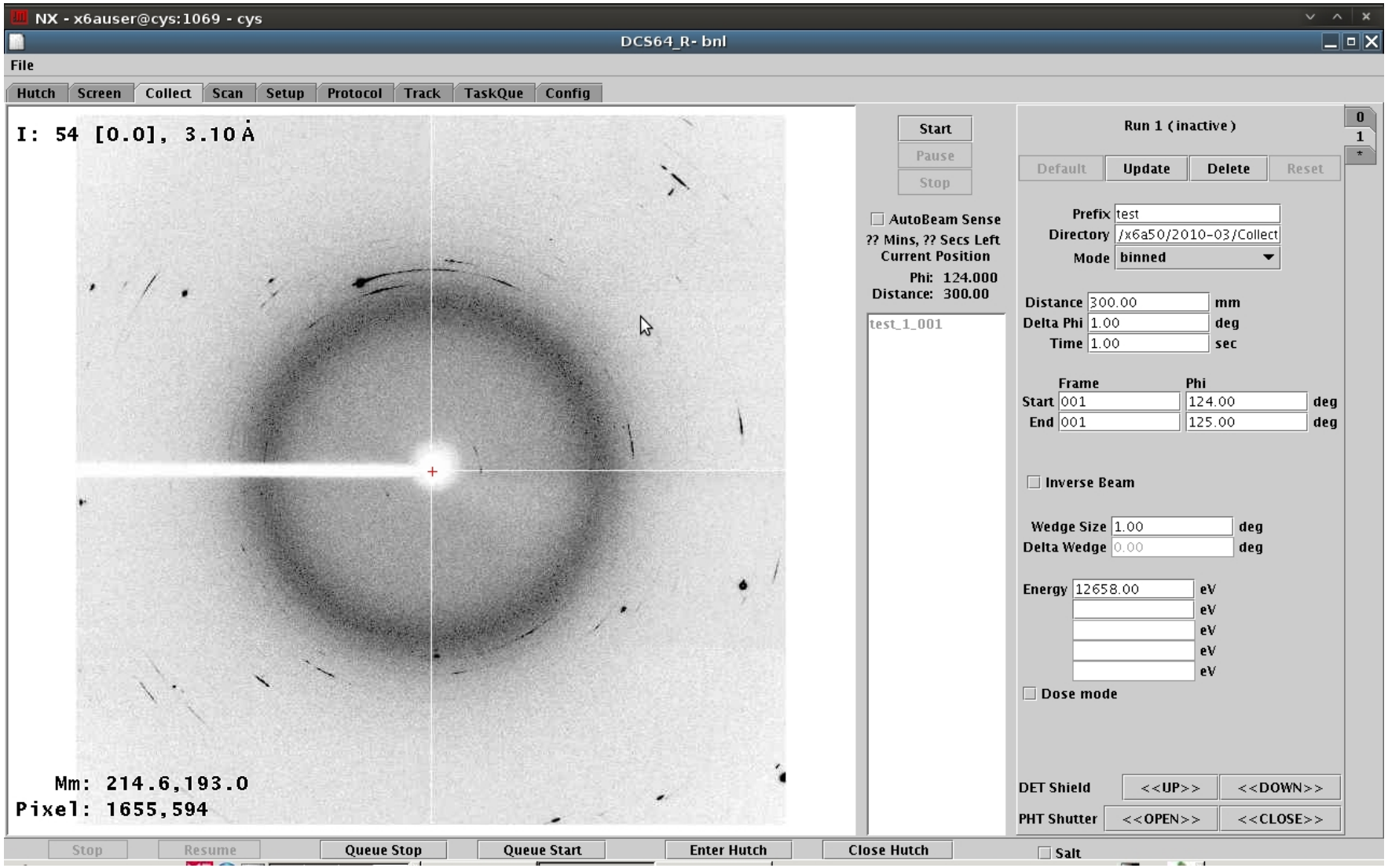
Future :
Full automation in preparation (see K.Q. slides, automated screening of all 64 samples …)
+ preferred method for protein eXpress

Remote Access

Step by step description


Applications Places System
[Google - Mozilla Firef...
Terminal
SoftToken ST-1
22:10
Home
data
ST1
NX
UFG.pls
PS.6.0
PDB-s
HR
listen.pls
HE-struct-science.pdf
LE-BL.doc
apt-bdp
SoftToken ST-1
File Options Help
Secure Password: 435-5525
CRYPTOCard Secure Password TECHNOLOGY
Off
Use 'Secure Password' as one-time password
Terminal
File Edit View Terminal Help
sjjm1210:~> sudo vpnc-connect
Enter password for jakoncic@vpngateway.bnl.gov:
Connect Banner:
| NOTICE - This is a Federal computer system for authorized use only and is the property of the U.S. Govt.
| Any use of this system may be intercepted, monitored, recorded, copied, audited, inspected, and disclosed
| to authorized site, DOE, law enforcement personnel, and officials of other agencies, domestic and foreign.
| Unauthorized or improper use may result in disciplinary action and civil and criminal penalties.
| LOG OFF NOW if you do not agree to these conditions.
VPNC started in background (pid: 2845)...
jjm1210:~>


NX - x6auser@cys:1069 - cys
DCS64_R- bnl
File
Hutch
Screen
Collect
Scan
Setup
Protocol
Track
TaskQue
Config
Hutch
mosfilm/denzo beam x 135.7 y 135.5
Detector Shield UP
Detector Shield DOWN
Shutter
HSlit
VSlit
199.76 um
199.76 um
Ibeam
Idown
Iup
-0.0471
0.0211
0.0168
PHT Shutter Open
PHT Shutter Close
Energy (eV)
Wavelength
12658.0
0.97949
Apply
Cancel
Stop
Protocol
Pucks
A
B
C
D
dock
previous (C8)
home
C8
pause
resume
stop
Mount
Unmount
WarmUp
CoolDown
Loop
XYZ0
RTmount
RTunmount
Load
Load0
Center
+90
-90
180
Move By
10
Move To
0
phi = -239.00°
AutoCenter Loop
AutoCenter Crystal
Zoom
6
5
4
3
2
1
filename
Stop
Resume
Queue Stop
Queue Start
Enter Hutch
Close Hutch
Salt


NX - x6auser@cys:1069 - cys
DCS64_R- bnl
File
Hutch
Screen
Collect
Scan
Setup
Protocol
Track
TaskQue
Config
I: 54 [0.0], 3.10 Å
Mm: 214.6,193.0
Pixel: 1655,594
Start
Pause
Stop
AutoBeam Sense
?? Mins, ?? Secs Left
Current Position
Phi: 124.000
Distance: 300.00
test_1_001
Run 1 (inactive)
Default
Update
Delete
Reset
Prefix test
Directory /x6a50/2010-03/Collect
Mode binned
Distance 300.00 mm
Delta Phi 1.00 deg
Time 1.00 sec
Frame
Phi
Start 001 124.00 deg
End 001 125.00 deg
Inverse Beam
Wedge Size 1.00 deg
Delta Wedge 0.00 deg
Energy 12658.00 eV
Dose mode
DET Shield
<<UP>>
<<DOWN>>
PHT Shutter
<<OPEN>>
<<CLOSE>>
Stop
Resume
Queue Stop
Queue Start
Enter Hutch
Close Hutch
Salt

Summary

Constant amelioration of the beamline …

Protein express usage increased …

Remote access is taking off …