

Optimising the Diamond experience from a user's perspective

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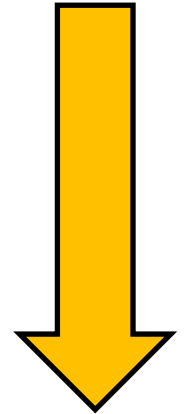
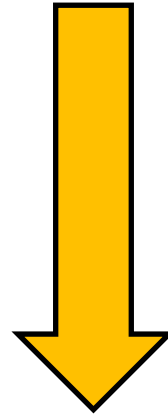
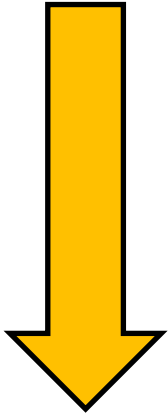
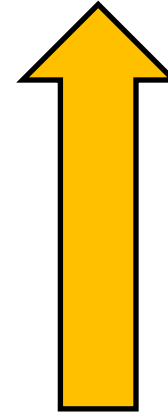
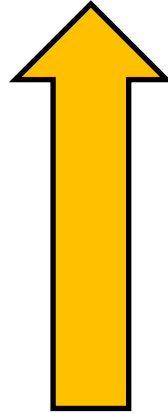


“Routine” data collection:

- on non-hazardous samples
- at cryogenic temperatures
- on pre-cooled crystals in pucks
- at conventional wavelengths

Disclaimer: the thoughts, views, and opinions expressed here are entirely my own and do not reflect the opinions of my employer, my wife, my kids, my...

Data collection philosophy...



Remote collection

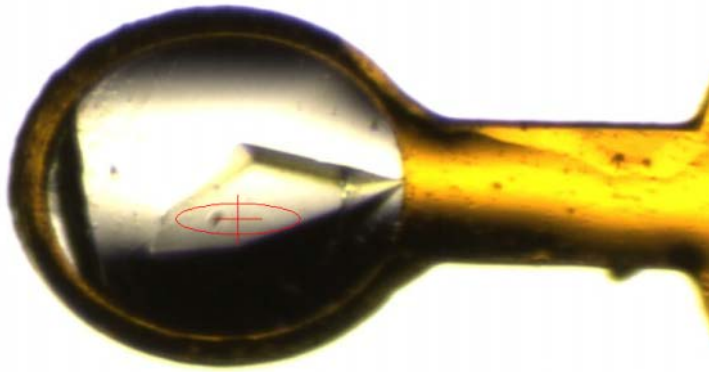




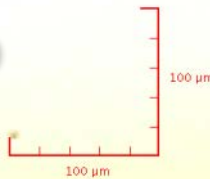
~160 miles

A 3-shift visit
requires two
full days

Some real data...

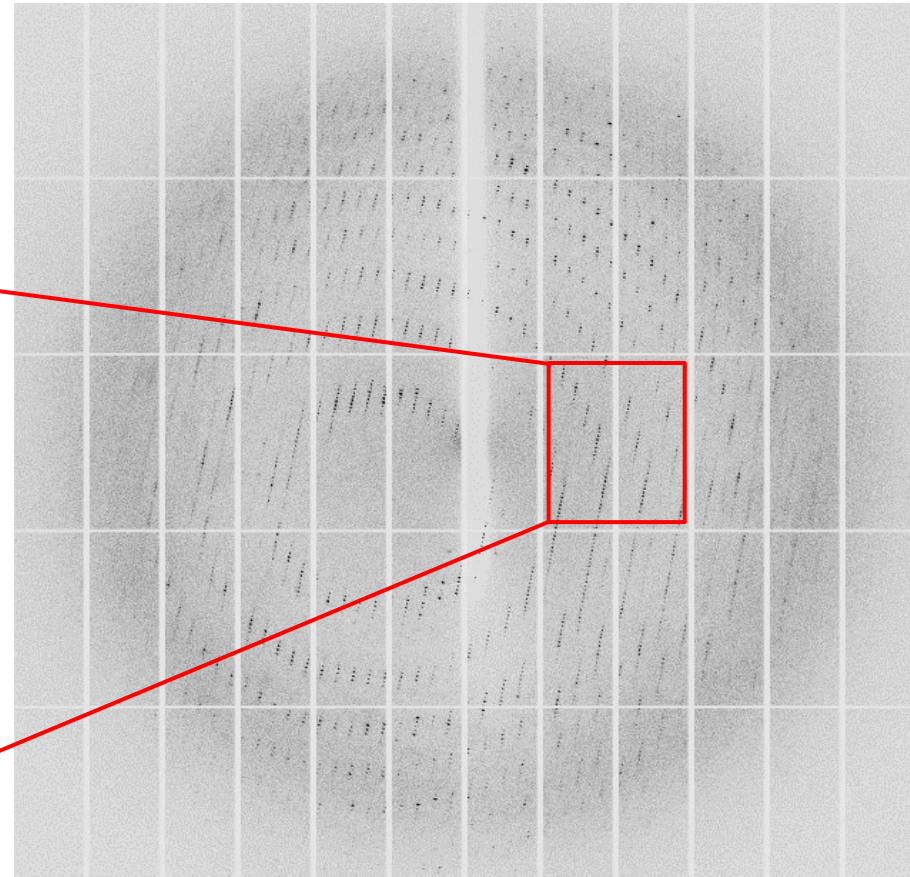
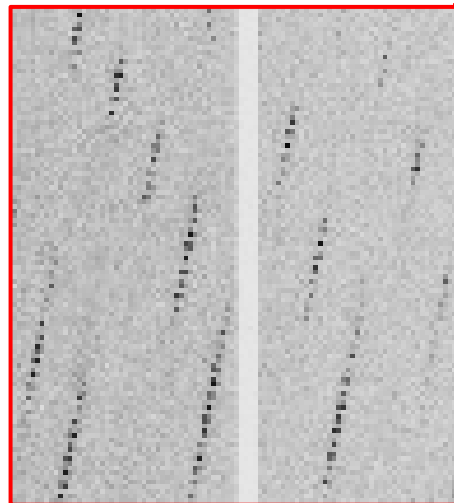


Crystal cooled in loop



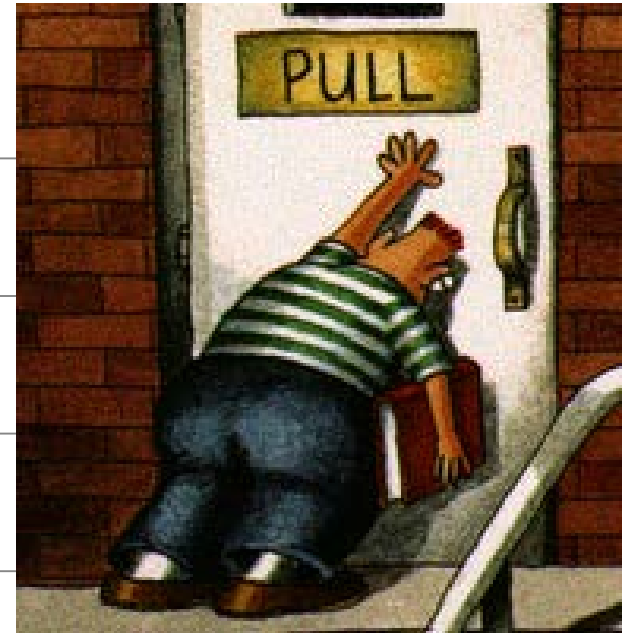
Beam size: $82.0 \times 21.0 \mu\text{m}$

Diffraction pattern recorded
from crystal at Diamond

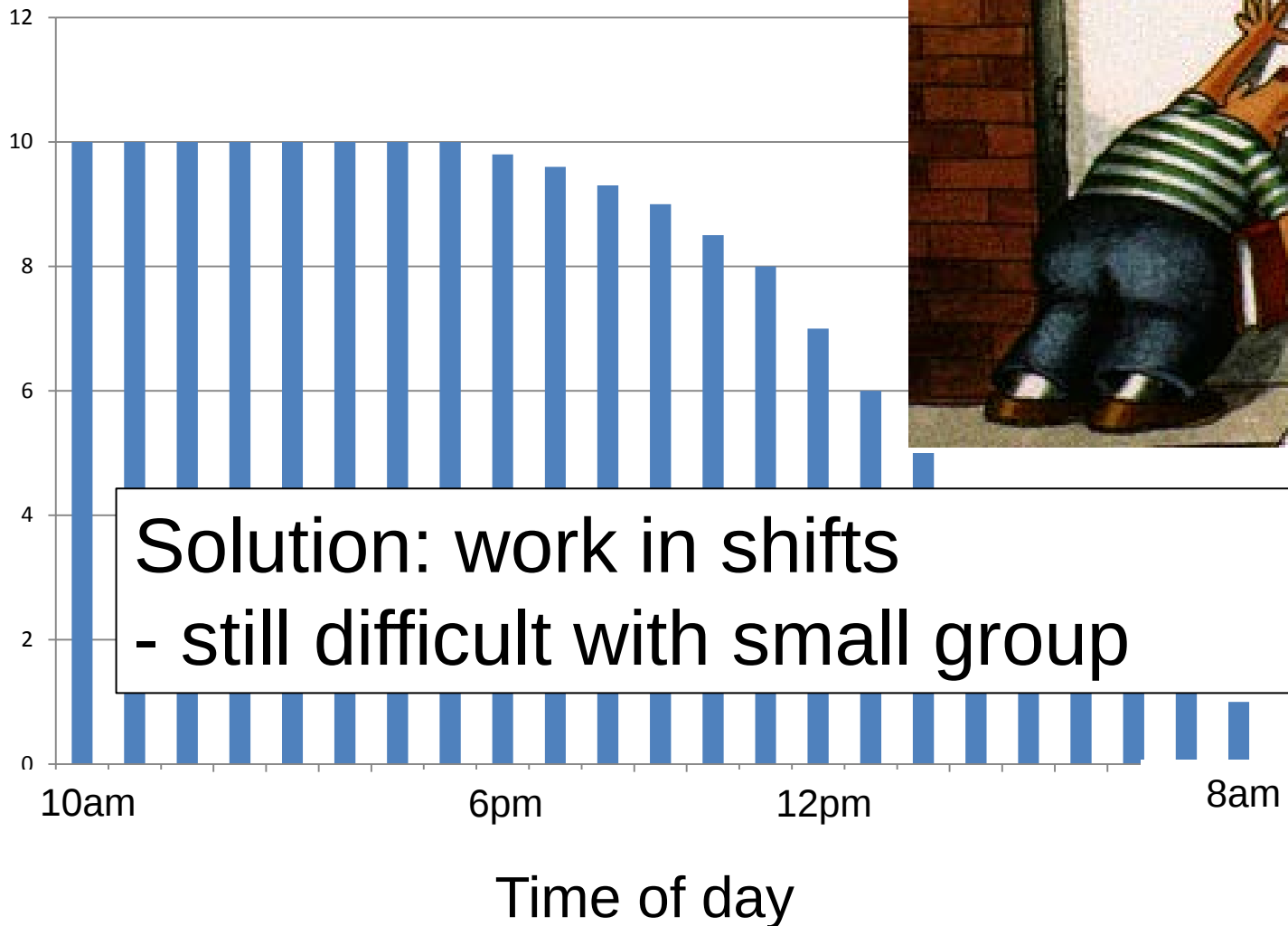


Some fictitious data...

A day at the beamline...



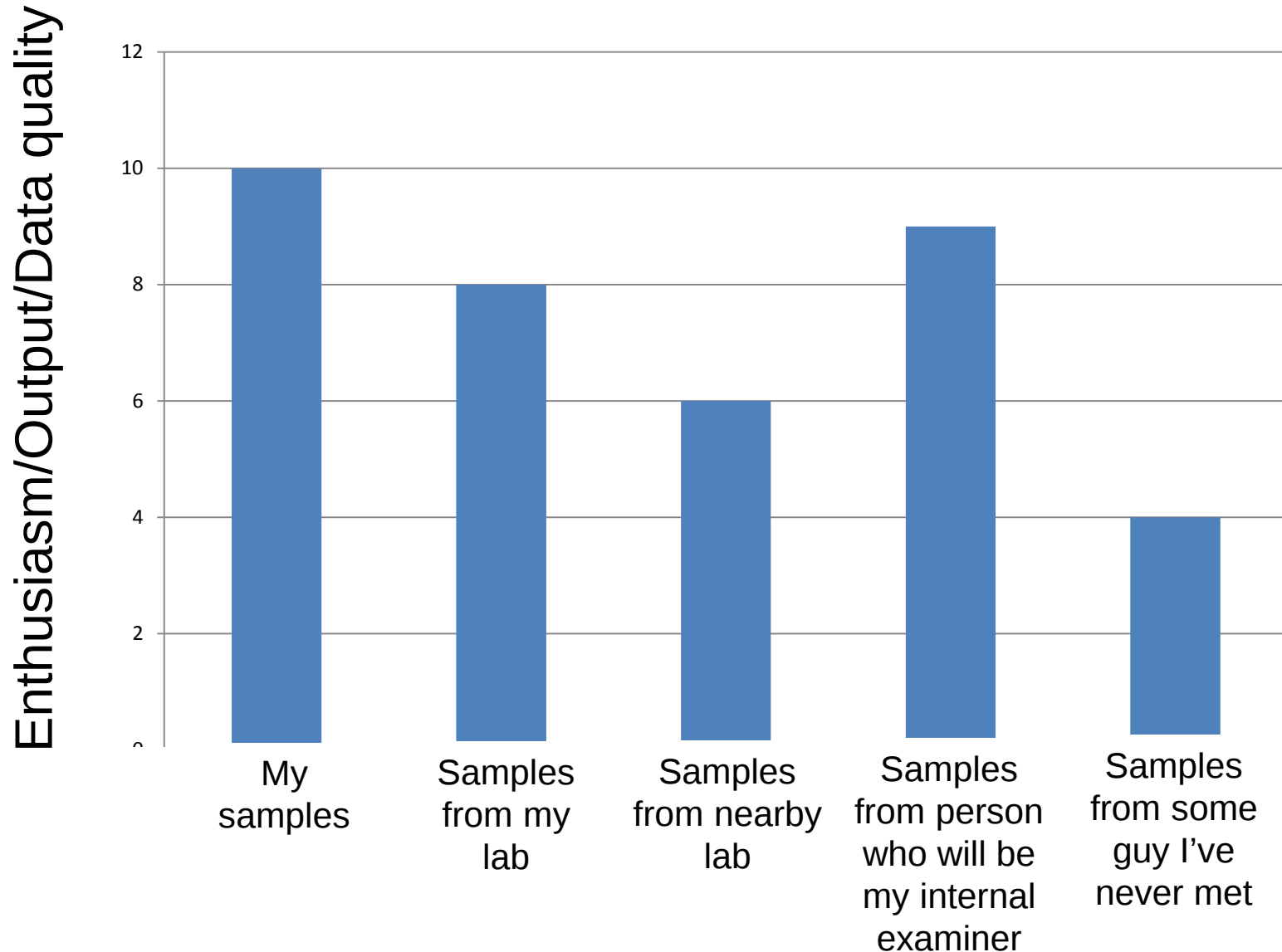
Data quality



Who should collect the data?

- Someone who knows the project
 - what data are required?
 - what space group/cell parameters/resolution to expect
- Someone who has a stake in the project
- Person who grew and mounted the crystals
- Someone who is not tired!

Some more fictitious data...



Ideal scenario:

- everyone collects data from their own crystals
- work in short shifts



Solutions:

1. everyone travels to Diamond (not practical ... and expensive)
2. small team travels to Diamond – everyone else collects data remotely (mixed access)
3. everyone collects data remotely (fully remote access)

Who travels to Diamond?

Without remote:

- 3 people minimum – at least 2 are experienced users

With remote (mixed access):

- 2-3 people – only 1 needs to be an experienced user
 - good way to introduce new users to DLS



Who collects data remotely?

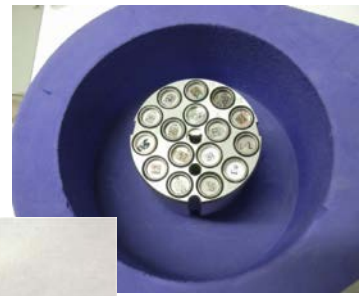
- 1 experienced user can cope, but better with 2
- any number of new users (at multiple sites)



Setting the scene for MX experiments

For routine data collection at 100 K:

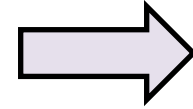
- Samples prepared and cryo-cooled in home lab
- Transported to DLS in dry shipping dewars
- Samples mounted robotically
- Data collection controlled through GDA GUI
- Only manual operation at DLS: loading/unloading pucks
 - between 144 or 592 samples can be loaded at once (depending on beamline)
 - may only need to enter hutch at beginning and end of visit
- Everything else computer driven...



Therefore you don't need to be there!

ISPyB database & shipping

- Create shipment in ISPyB
- Fill puck with samples (at home lab)
- Enter sample info. directly into ISPyB database

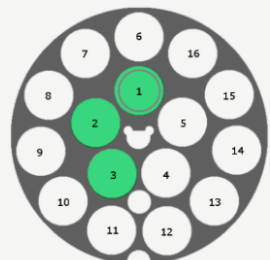


This page allows you to add containers to the selected dewar and shipment. If the protein you want to use isn't listed type in a new name and press tab. This will create a new protein

Shipment

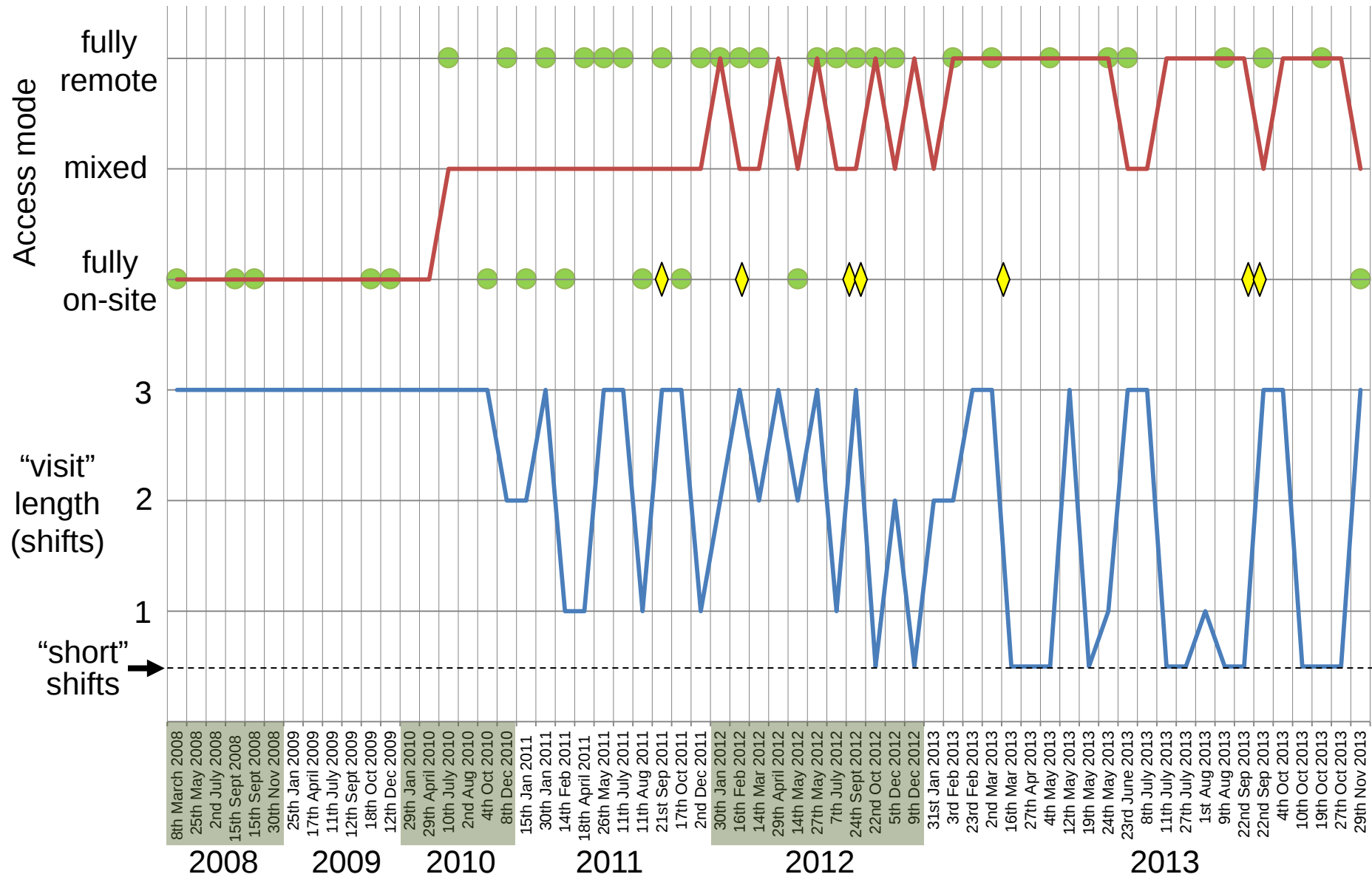
Dewar

Puck Name

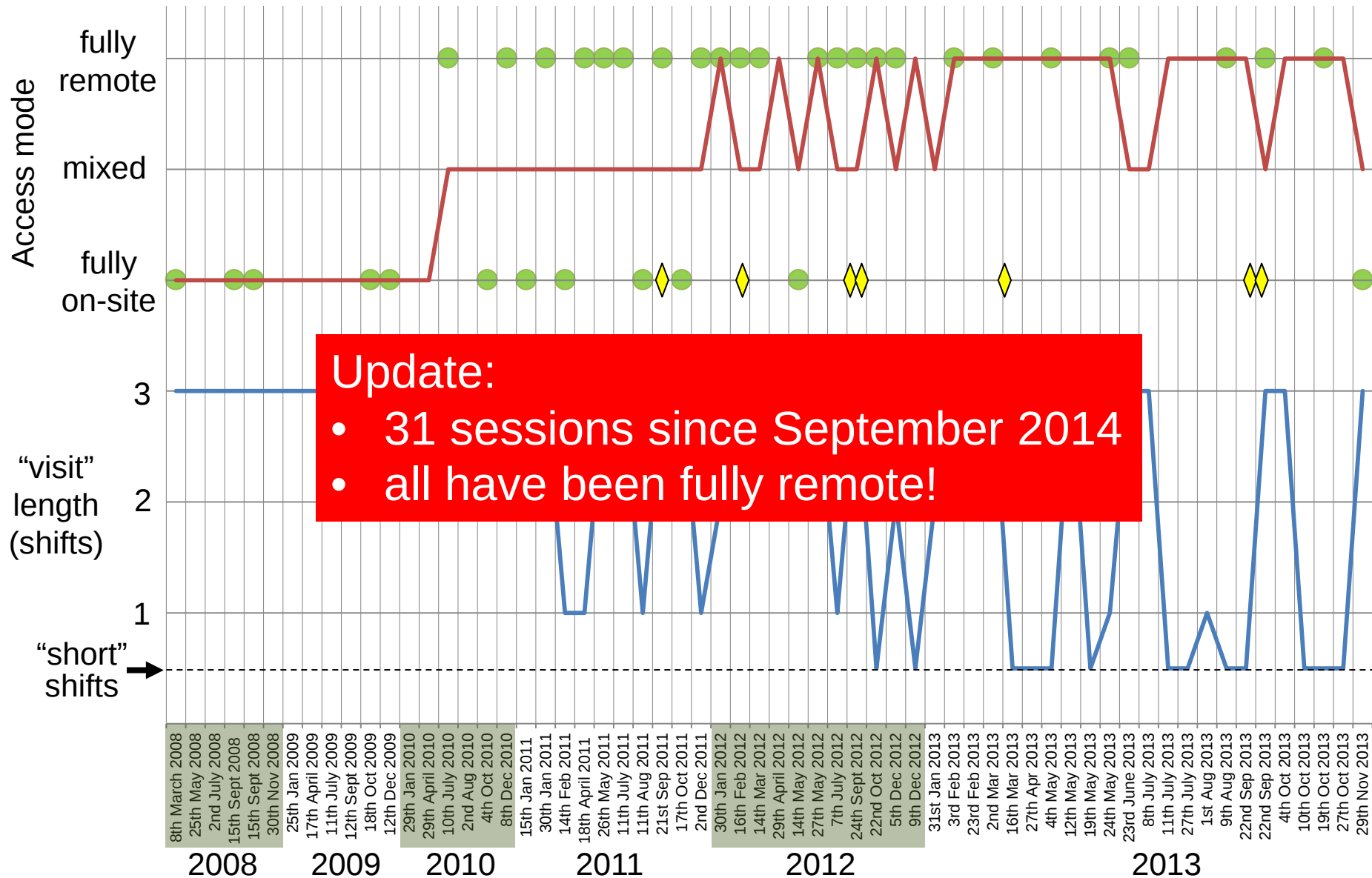


Location	Protein Acronym	Sample Name	Spacegroup	Barcode	Comment	
1	lys	lys1	P4			X
2	lys	lys2	P4			X
3	lys	lys3	P4			X

Shift usage by EEMaX BAG



Shift usage by EEMaX BAG





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Connection to Diamond

Remote Access

New remote access is available at Diamond to login on MX beamlines or NX cluster. Remote access is available from Linux, Mac OSX and Windows computers.

Please see the video below:



If you are experiencing issues you can try alternative ways to connect to Diamond:

- [From Linux or Mac OS X](#)

What you need:

- Linux/Mac/Windows Workstation
 - with at least one big monitor (24": 1920x1200 pixel) - preferably two
- Fast internet connection
 - >10 Mbit download speed (may be a bit optimistic if using at peak times...)
- Speaker phone or headset
- (Skype)

iMac with extra monitor:
(i) data collection
(ii) data evaluation

View
today's
jpgs

2nd iMac:
(i) data evaluation
(ii) data (re)processing
(iii) Skype

Useful
phone
numbers

GDA
interface

webcams

ISPyB
interface

Coffee!

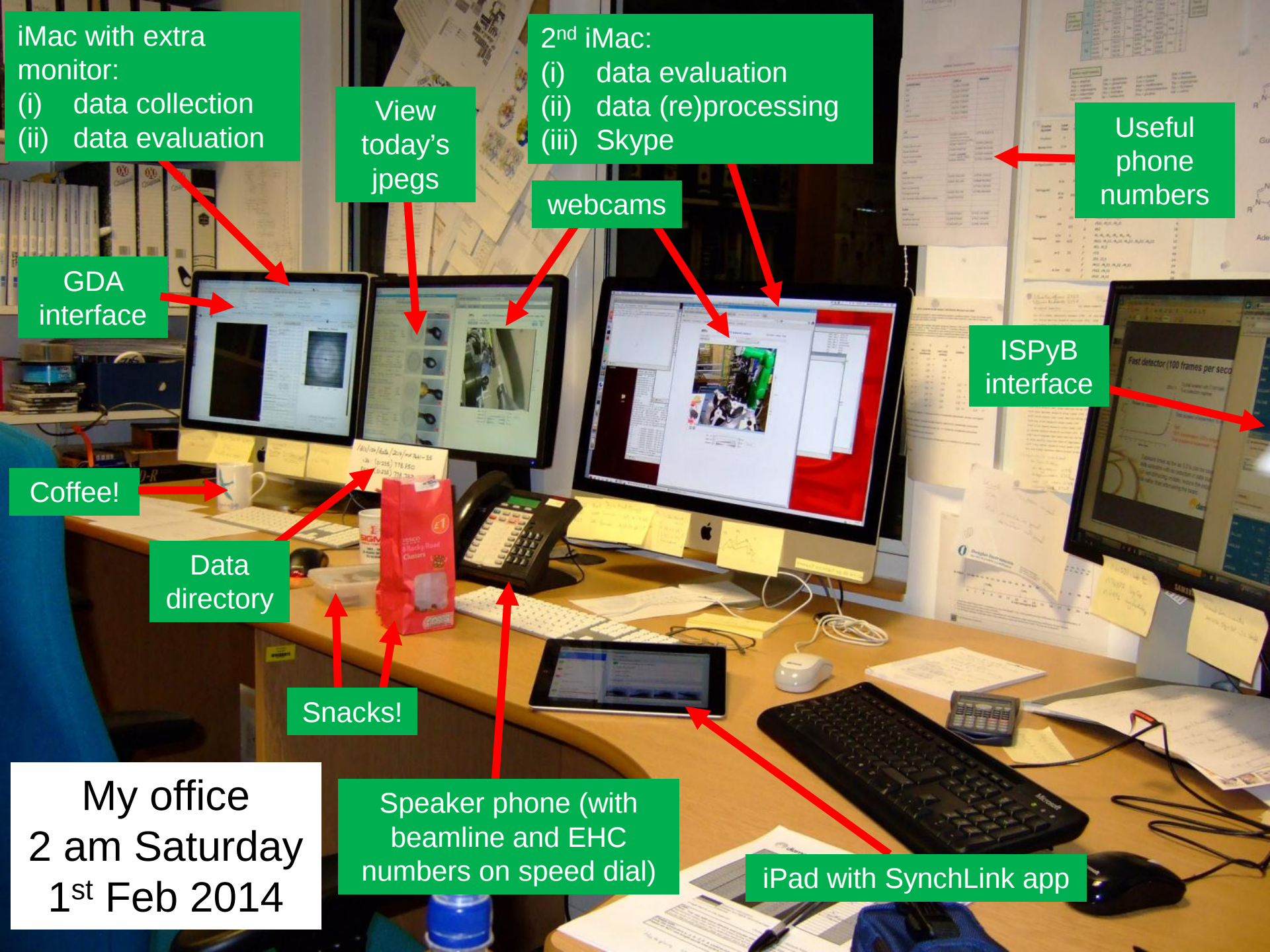
Data
directory

Snacks!

My office
2 am Saturday
1st Feb 2014

Speaker phone (with
beamline and EHC
numbers on speed dial)

iPad with SynchLink app



How do we manage the beamtime?

Several groups may participate in one visit, so we need to be organised..

Beamtime requirements are entered into a BAG wiki

Scheduled beamtime and associated deadlines (with reminders) sent as meeting requests to Outlook diaries

The image shows two overlapping windows. The top window is a web browser displaying a 'SCHEDULED BEAMTIME (AP18)' announcement. The bottom window is an Outlook 'Meeting' request for the same event.

SCHEDULED BEAMTIME (AP18)
[MX9475-53: 5 hrs I04 from 04:00 Sat 28 Nov 2015 until 09:00 Sat 28 Nov 2015 - DEADLINE: 9 Nov](#)

CJD
local users (include team leader & dietary info):
arrival/departure dates & times:
remote users: Changjiang Dong, Yinghong Gu, Huanyu Li, Zhengyu Zhang, Hao hao Dong
contact numbers (contact name/landline/mobile): Changjiang Dong 01603 123456
pucks/time: 4 pucks 2.5 hrs
comments:
Priority (H/M/L): M

DML
local users (include team leader & dietary info):
arrival/departure dates & times:
remote users: Lawson, Stevenson, Caputi, Schafer

Outlook Meeting Request:
Subject: PBEAMTIME* MX9475-53: 5 hrs I04 from 04:00 Sat 28 Nov 2015 until 09:00 Sat 28 Nov 2015 - DEADLINE: 9 Nov
Location: N/A
Start time: Sat 28/11/2015 04:00
Eng time: Sat 28/11/2015 09:00
All day event: ☐

This "meeting request" is for information only - PLEASE DO NOT REPLY TO IT

The time of this "meeting" corresponds to scheduled beamtime.

To add this to your diary, simply accept the invitation (N.B. if it is a "short visit" in the middle of the night, you may not see it in your diary until you scroll up or down!)

This "meeting request" has been set with a 3 week reminder, which will pop-up a few days before the deadline shown in the subject line. There will be no separate reminder sent by me (although group leaders will continue to get email reminders from the User Office).

Group leaders: if you want to make use of this time, by the deadline (in the subject line), make sure you have:

- (1) Declared all samples via the Diamond User Administration System
- (2) Shared information on your beamtime requirements via the EEMaX wiki
- (3) Registered any new users (instructions on the wiki)

In Shared Folder: Calendar

See more about: David Lawson.

How do we manage the beamtime?

- Decide on running order and approximate changeover times beforehand
 - need to be flexible e.g. if there is downtime
- For mixed access:
 - remote users generally get the night shift
 - on-site team remain on-call e.g. to change pucks
 - remote users occasionally get daytime access (e.g. while on-site team analyse data or go for meals!)

How do we manage the beamtime?

During beamtime - keep in contact:

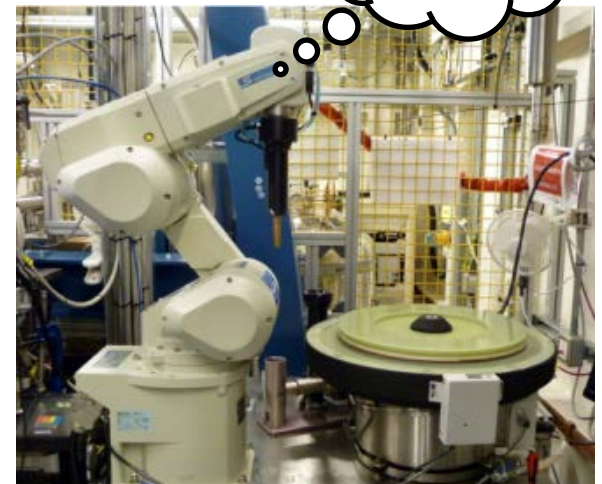
- let other users know what's going on – especially if schedule changes
- all parties need to be reasonable

“I need preliminary data for my grant application!”



“It’s taken me three years to get these crystals!”

?



- make sure all remote users know where their pucks are in the dewar!

Timeline for fully remote data collection

2 - 3 weeks before:

- decide who is going/sending samples (wiki)
- complete ERA and experiment notification form

Week before:

- decide on running order and rough division of beamtime (via email)
- prepare samples and enter sample information into ISPyB database

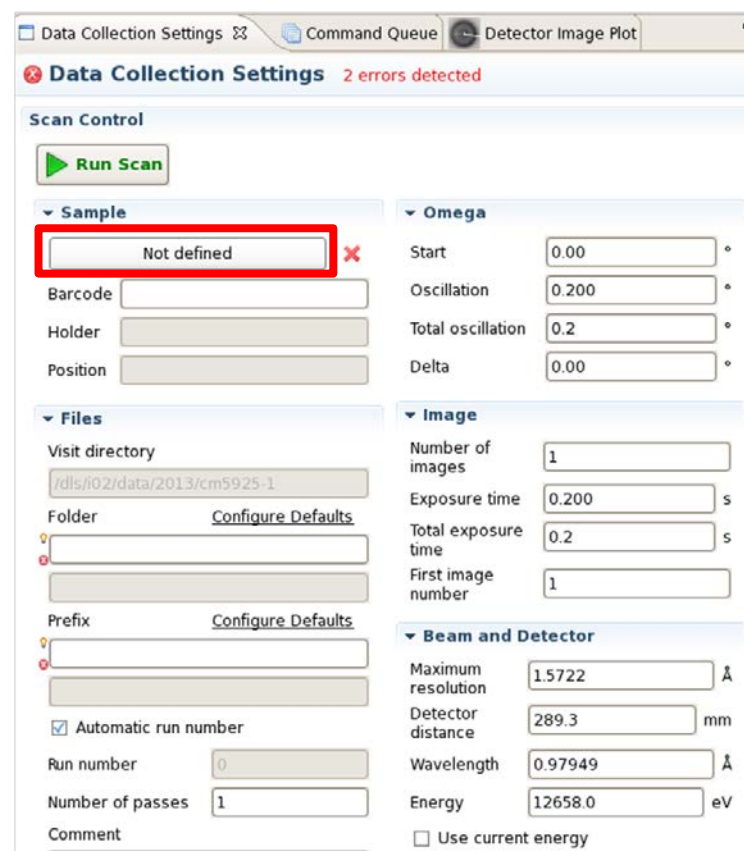
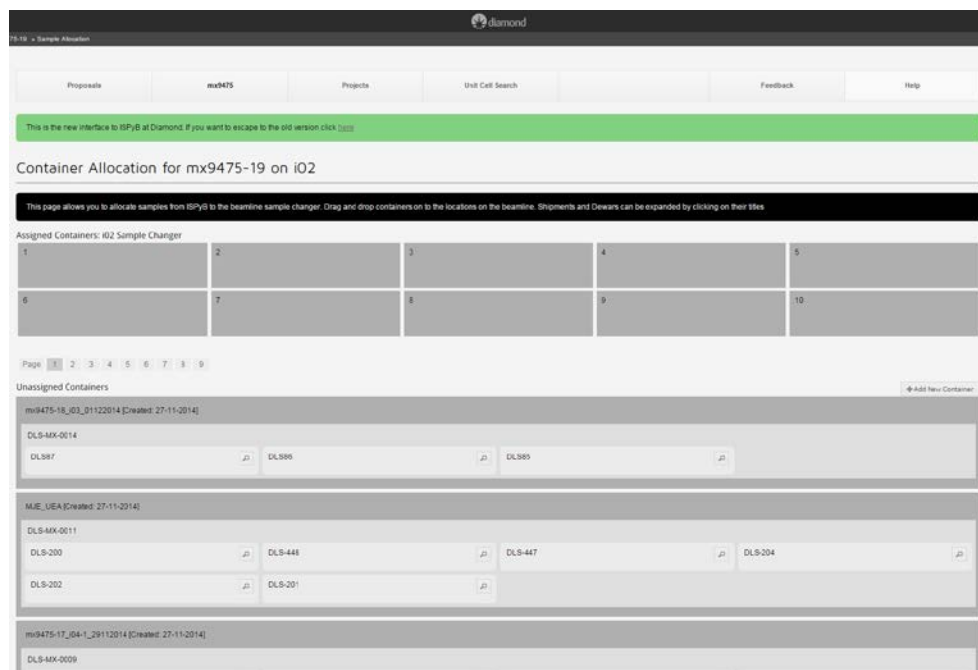
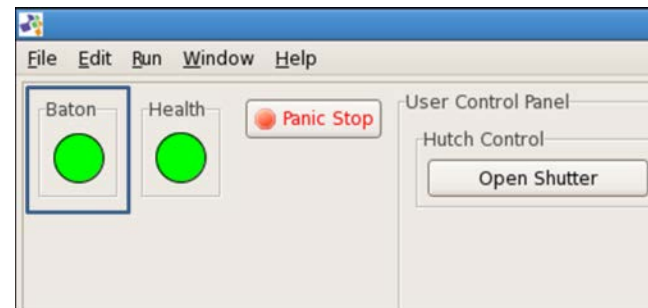
2 - 4 days before:

- ship samples (N.B. must arrive during normal working hours)
- upload files for autoprocessing into ISPyB database (PDBs, sequences)

Timeline for fully remote data collection

~1 hr before start of shift (or slot in running order):

- connect to beamline computer, start GDA
- LC/EHC loads pucks into beamline dewar
- enter puck positions into ISPyB database (LC/EHC)
- Zero hour – take the baton, select sample from menu, collect data!



This is the new interface to ISPyB at Diamond. If you want to escape to the old version click [here](#)

This page shows all data collections for the selected visit. If the visit is ongoing the page will automatically update as new data is collected. Auto processing results will be displayed

i03 Webcams & Beamline Status

Ring Current
232.281

Refill
130.903

Hutch
Locked

Port Shutter
Open

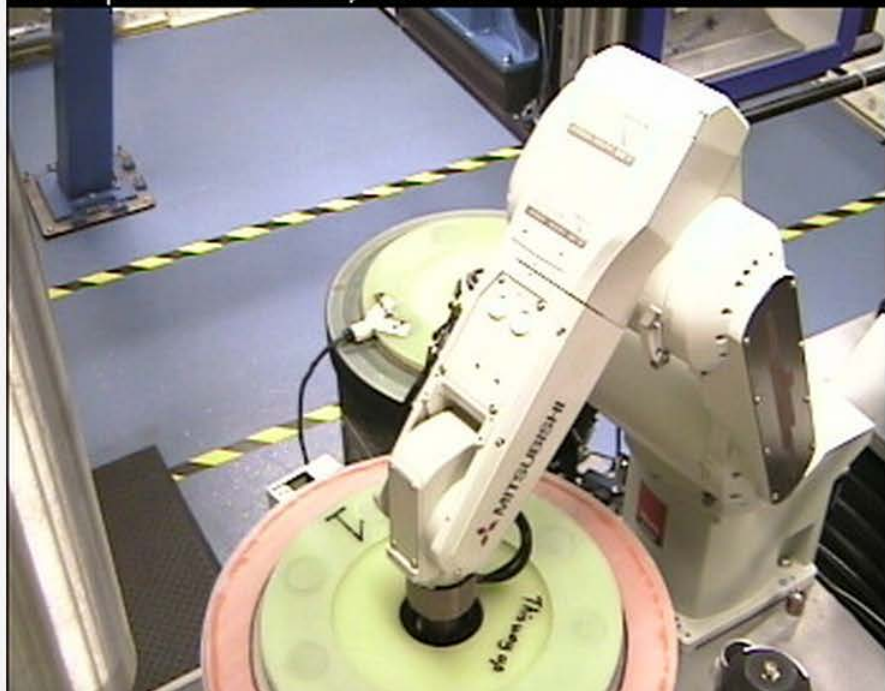
Expt Shutter
Open

Fast Shutter
Closed

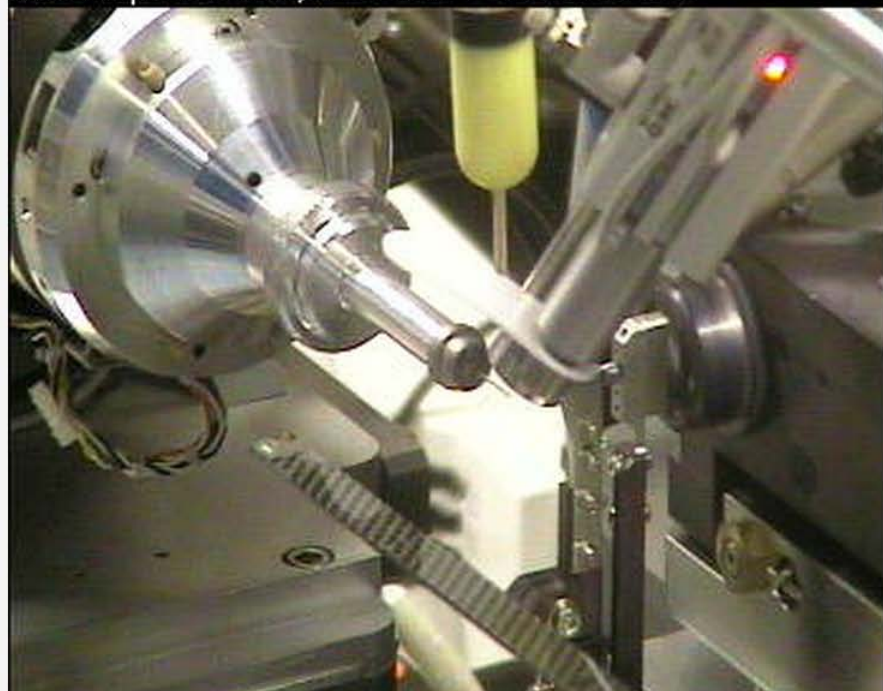
Wavelength
0.976254

Transmission
100

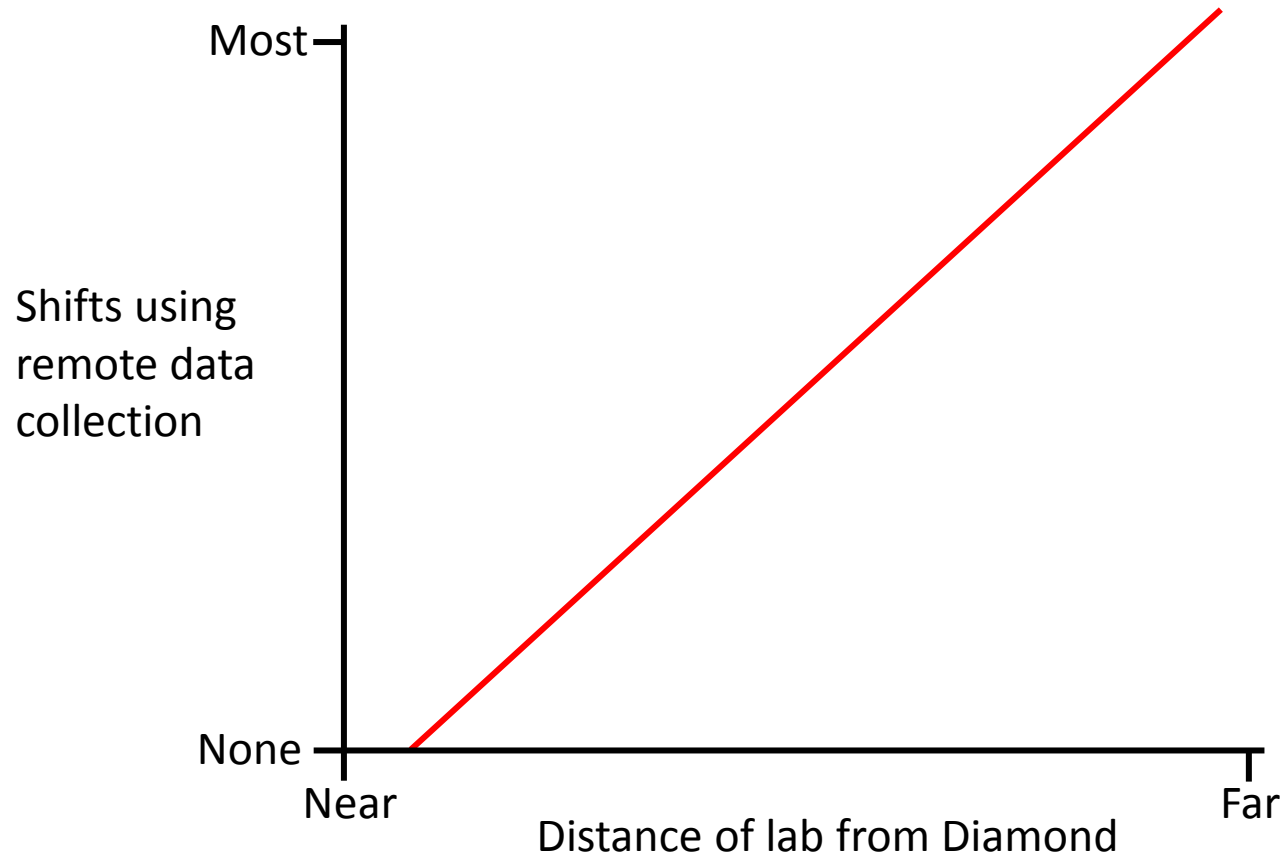
i03 Experimental Hutch, Mon Dec 1 2014 10:07:50



i03 Sample Position, Mon Dec 1 2014 10:07:50



How remote is “remote”?



People can be set in their ways...



Let go Luke...

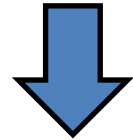


...use remote!

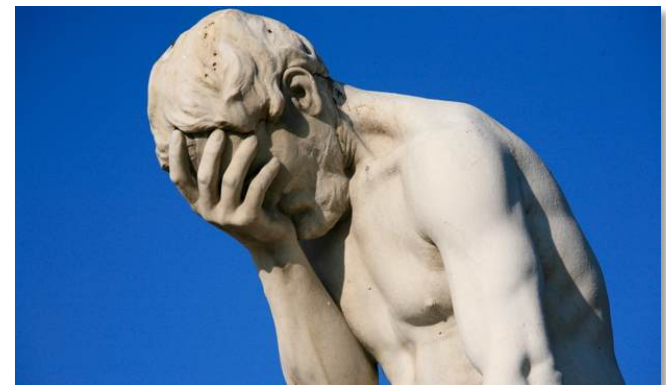
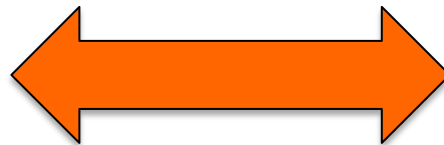
I know what
you're getting
for Christmas.

How?

Because I felt
your
presents!

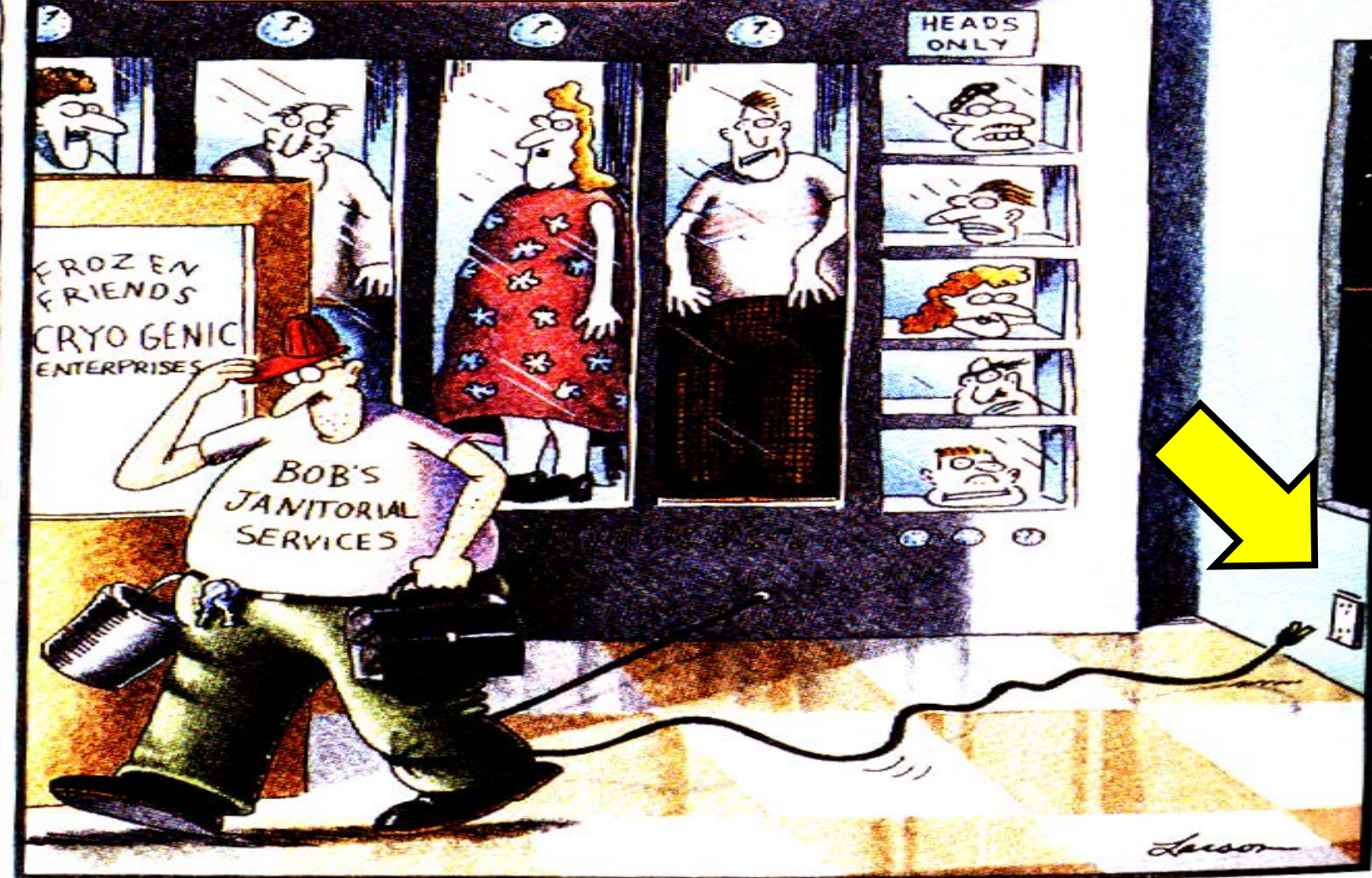


=



When things go wrong...

Warning: maintain at 100K



When things go wrong...

Can you fix things?

- probably not!

On-site user:

- During normal working hours – call local contact
- Out of hours – call EHC

Remote user:

- During normal working hours – call local contact
- Out of hours – call EHC

Therefore you don't need to be there!

Getting your data home...

- send hard drive with dewar
or...
- FTP data home



+



Both methods
are slow!

Alternative:

- (re)process data remotely on DLS computers and FTP output only
- archive raw data when hard drive gets home

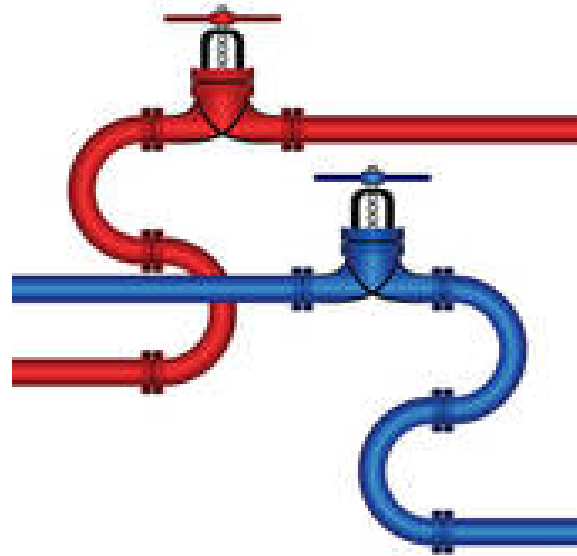
Advantages of remote data collection:

- Beamtime is fully used
- Users collect data on their own crystals
- Most/all of the users stay at home labs
 - time commitment is low for remote users
 - stakeholders can observe data collection
 - useful for training non-experts
- Time can be used flexibly
- Less stressful
- Everyone gets some sleep!
- Difficult to “break” the beamline

Disadvantages of remote data collection:

- Remote users get the night shift (mixed access)!
- Risk of losing touch with beamline staff and latest developments (do BAG training, go to User meeting)
- Dewars occasionally get misplaced...
- Don't get a cooked breakfast!
- Can't think of any more...

software tools and pipelines



Rules of thumb...

- Think!
- Be pessimistic about symmetry
 - if unsure - assume P1
- Be optimistic about resolution



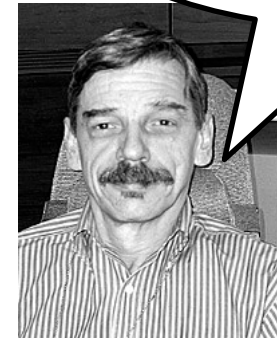
Goals for my beamtime...



Primary goals (data quantity **AND** quality...)

- To collect as much data as possible...
- To collect the best possible data...
- To collect the data that will enable me to:
 - Solve my structure
 - Extend the resolution of my structure
 - Show that my ligand is bound

Secondary goal (get a life!)



Zbyszek
Dauter

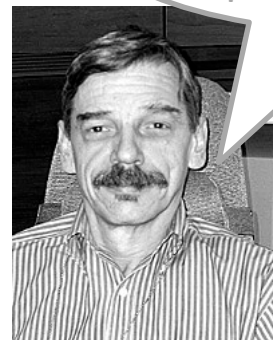
“Data collection is
the last
experimental step!”

Ask yourself:

- Do I spend a long time re-processing and analysing data at home?
- Does the next visit come along before I have analyzed all the data from the previous trip?

Primary goals (data quantity AND quality...)

- To collect as much data as possible...
- To collect the best possible data...
- To collect the data that will enable me to:
 - Solve my structure
 - Extend the resolution of my structure
 - Show that my ligand is bound



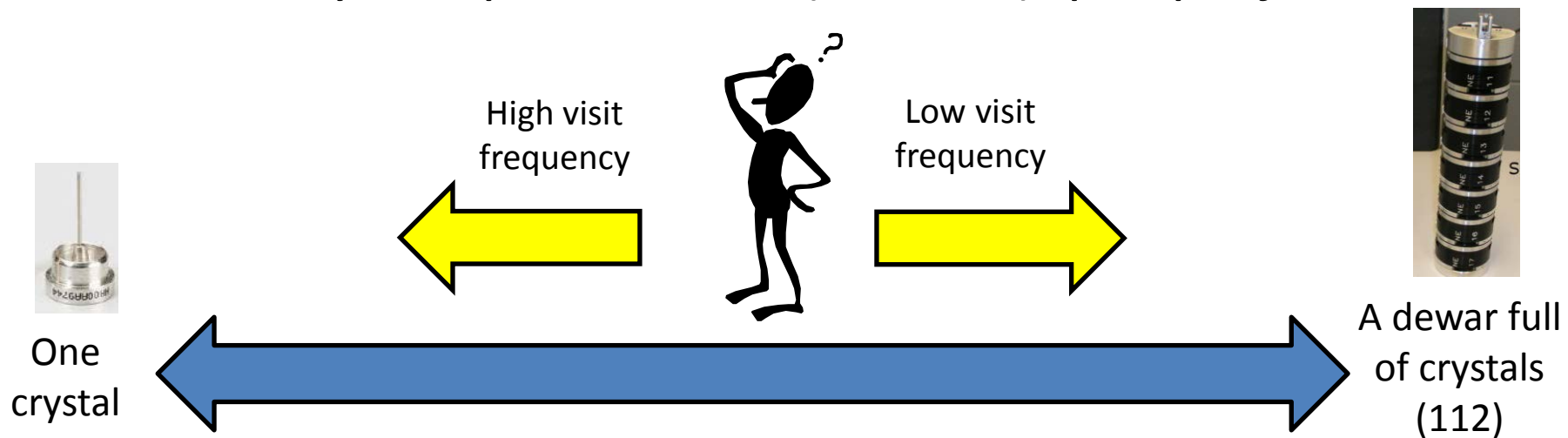
“Data collection is
the last
experimental step!”

Zbyszek
Dauter

Secondary goal (get a life!)

- Try to answer these questions before end of visit:
 - Can I solve my structure?
 - Can I extend the resolution of my structure?
 - Is my ligand bound?
- Minimise the amount of follow-up work...

How many samples to take (or send) per project...



Effort before, during and after beamtime

Time available for other projects/users

Number of crystals

Likelihood of 'success' within a single visit

Number of crystals

Data collection is always a compromise...

*How much
data do I
need?*

*What
resolution
do I need?*

*What are
the data
for?*

*How much
time do I
have?*

*How many
crystals do
I have?*



MX data collection has become faster...

20th century data collection



21st century data collection



MX data collection has become faster...

The Pilatus detector – a real game changer!

- Typical dataset takes <<5 min to collect
 - 10 - 20 GB raw data per data set!
 - >1.0 TB data possible in 24 hrs!
- In practice, 4 “useful” data sets per hour is good
 - includes screening for “best” crystal
 - ...and thinking!
- Most groups can’t generate enough crystals for more than 1 shift (8 hrs) – often 2 - 3 hrs is sufficient
 - therefore a visit is usually split between several groups...



If



+



= fast data collection

Then why not...

**SHOOT FIRST, ASK
QUESTIONS LATER!**

Think...

Test...

Think more...

(Test more...)

Shoot...

Think even more...



~~THE GOOD, THE BAD AND THE UGLY~~

Keeping pace with data collection...

data
analysis



data
collection



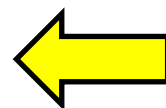
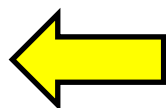
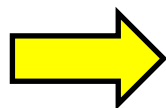
MX beamline tools

To recap...

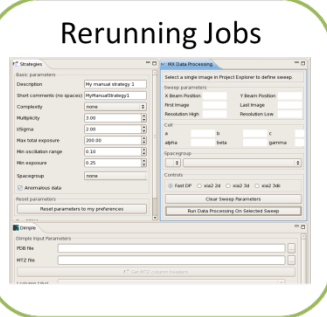
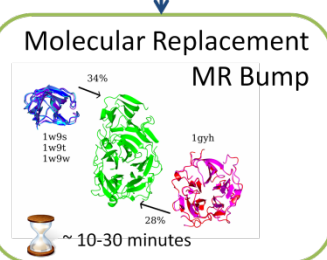
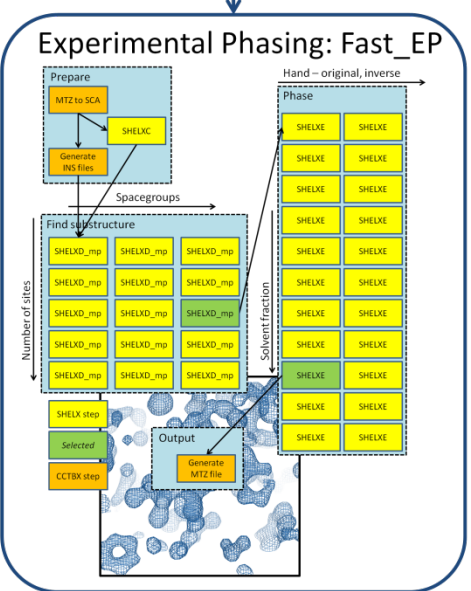
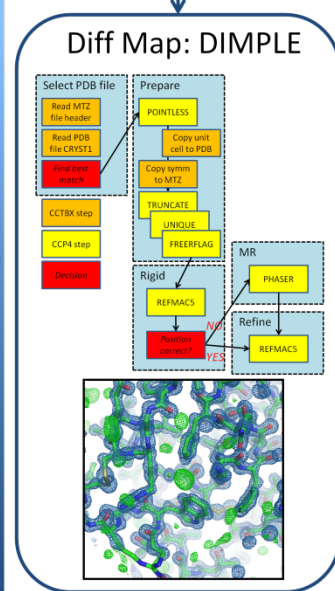
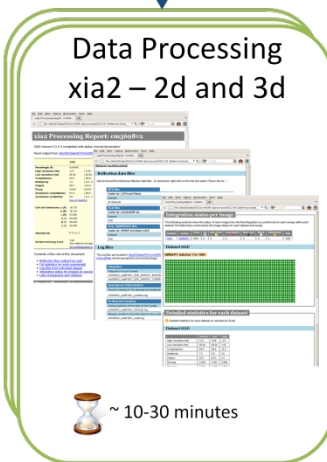
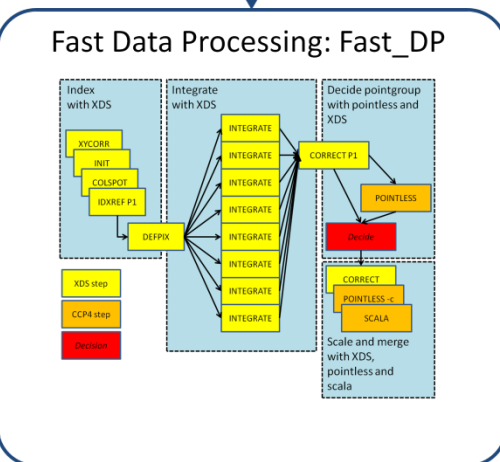
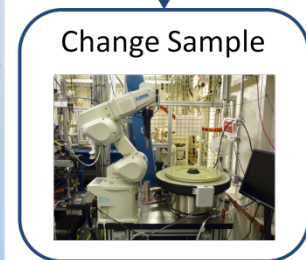
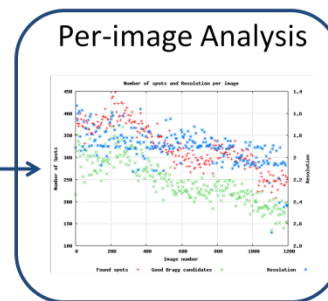
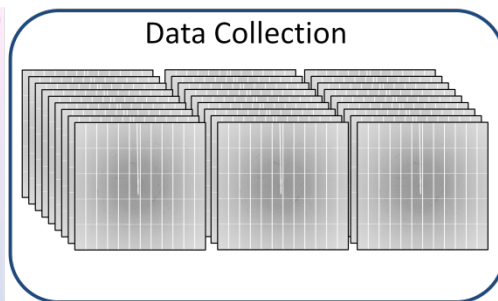
- Multi-centre BAG
- Extensive use of remote data collection
 - fully remote most of the time
 - otherwise mixture of local and remote users
- Most visits are shared between 2 or more groups
 - 2 - 8 hrs per group
- Therefore, need to be as efficient as possible

ISPyB database

Sample info.



Time / s
0
60
120
180
240



To make efficient use of beamtime:

1. *Before beamtime:*

- (Load crystals into pucks)
- Enter sample information into ISPyB
- Upload PDBs for Dimple into ISPyB
- Upload sequences for MrBUMP into ISPyB
- Decide on running order for samples (may change later...)

2. *During beamtime:*

- Use automated software tools to **rapidly** inform decision-making process
- Re-run jobs if necessary
- Revise running order/strategy based on processing results

3. *After beamtime:*

- Data already triaged
- Focus only on promising stuff - less follow-up work
- Better informed for next trip...

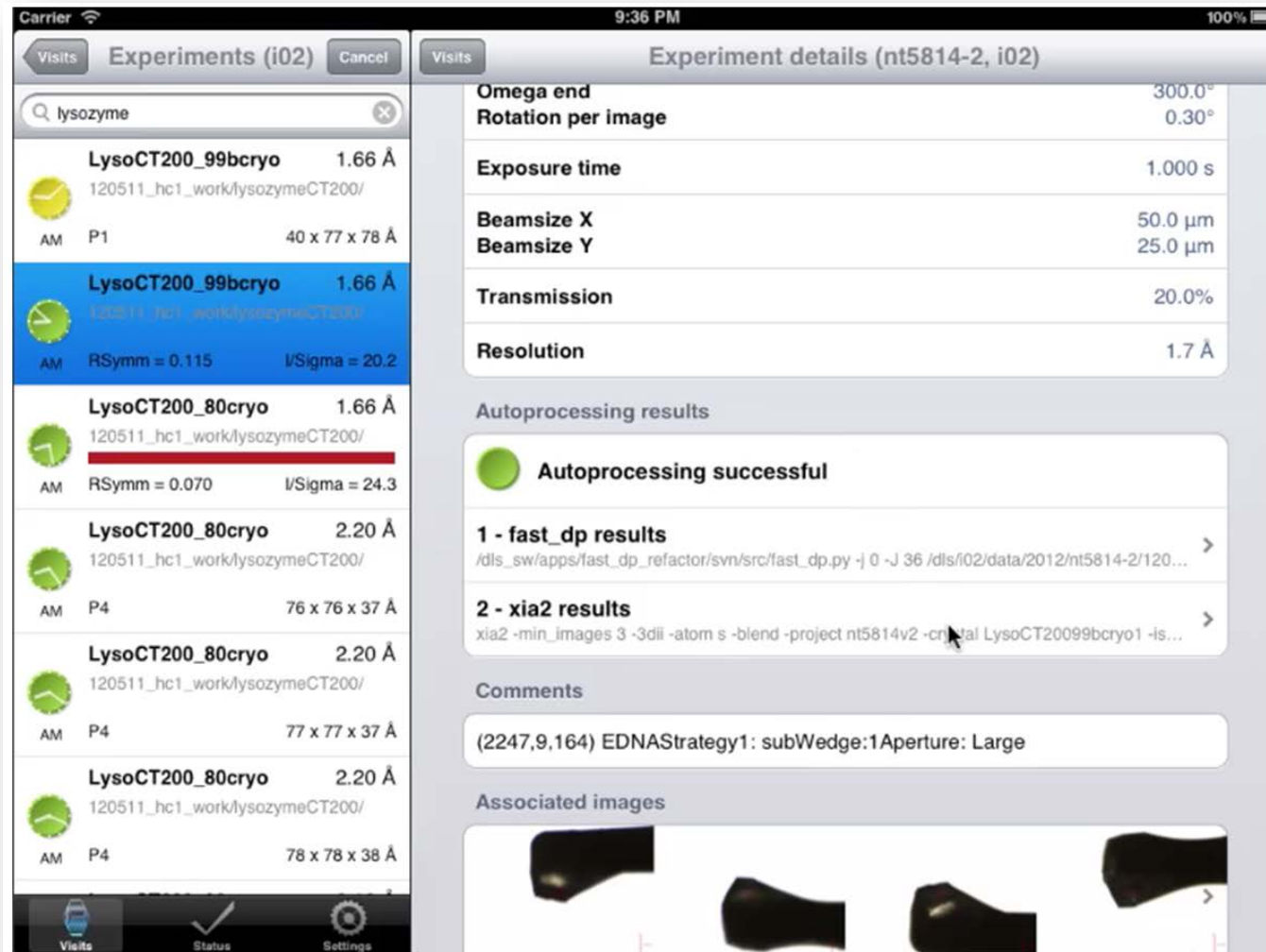


During beamtime:

- (use ISPyB)
- Select required sample from drop-down menu
 - no need to enter sample information or specify sample location
 - less likely to get the wrong sample
- Collect test images
- Decide on strategy based on EDNA/prior knowledge/requirements/
(time available)
 - collect/don't collect/revisit later (if time allows)
- Collect data set
- Analyse data on the fly
 - let the automated tools take the strain (fast_dp, fast_ep, Dimple, MrBUMP...)
 - **BUT – remember to sense check the output!**
 - re-run jobs if necessary (e.g. to set space group, resolution, exclude images...)
 - (may revise sample running order/strategy based on processing results)
- Move onto next sample...

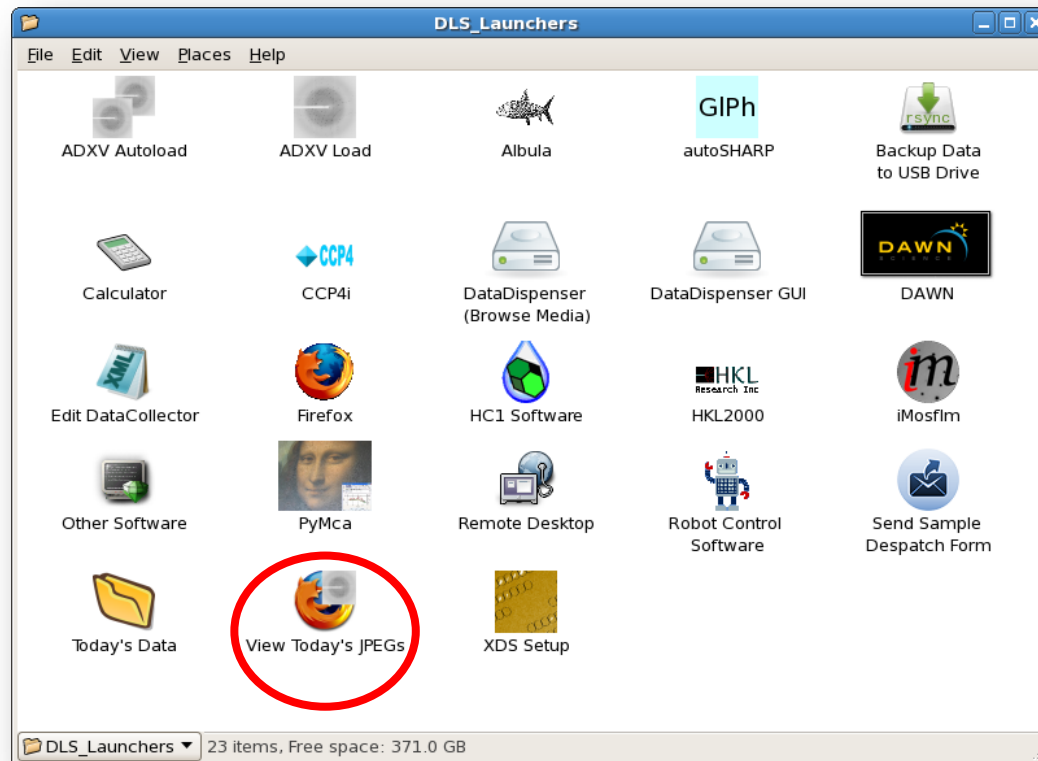
Keeping track of your data:

- Using SynchLink App
 - need iPad/iPhone



Keeping track of your data:

- Using SynchLink App
 - need iPad/iPhone
- Using “View Today’s jpegs” launcher



View Today's jpegs

mx7641-23 - Mozilla Firefox
 NX - ndy35357@cs04r-sc-serv-46.diamond.ac.uk/4:1172 - DLSproc

file:///dls/i03/data/2013/mx7641-23/jpegs/index.html

Webcams mx7641-27 mx7641-23

Sat May 4, 2013 - 21:24:53 BBA_G1SM_4/BBA_G1SM_4_M1S4_2_####.cbf			
No. Images:	1200	Resolution:	1.60Å
Exp. Time:	0.2s	Trans:	50.16%
Omega Osc:	0.15°	Wavelength:	0.9763Å
Comments:	(-233,25,-255) Aperture: Medium		
Fast_dp Status:	✓	Xia2 Status:	✓✓✓
Running:	Fast_ep 😊	MrBUMP 😊	DIMPLE 😊

Sat May 4, 2013 - 21:21:23 BBA_G1SM_4/BBA_G1SM_4_M1S4_1_####.cbf			
No. Images:	3	Resolution:	1.50Å
Exp. Time:	0.2s	Trans:	50.16%
Omega Osc:	0.2°	Wavelength:	0.9763Å
Comments:	(-233,25,-255) Aperture: Medium		
EDNA Status:	✓	Mosfilm Status:	✓

Sat May 4, 2013 - 21:14:38 BBA_M1M_3/BBA_M1M_3_M1S1_4_####.cbf			
No. Images:	1200	Resolution:	1.50Å
Exp. Time:	0.2s	Trans:	50.16%
Omega Osc:	0.15°	Wavelength:	0.9763Å
Comments:	(-2019,-626,164) Aperture: Medium		
Fast_dp Status:	✓	Xia2 Status:	✓✓✓
Running:	Fast_ep 😊	MrBUMP 😊	DIMPLE 😊

Sat May 4, 2013 - 21:11:23 BBA_M1M_3/BBA_M1M_3_M1S1_3_####.cbf			
No. Images:	3	Resolution:	1.20Å
Exp. Time:	0.2s	Trans:	50.16%
Omega Osc:	0.15°	Wavelength:	0.9763Å
Comments:	(-2019,-626,164) Aperture: Medium		
EDNA Status:	✓	Mosfilm Status:	✓

Sat May 4, 2013 - 21:07:17 BBA_M1M_3/BBA_M1M_3_M1S1_2_####.cbf			
No. Images:	3	Resolution:	1.50Å
Exp. Time:	0.2s	Trans:	50.16%
Omega Osc:	0.2°	Wavelength:	0.9763Å



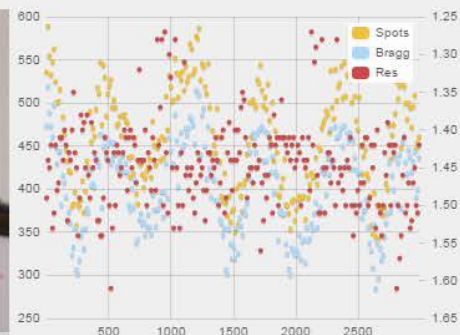
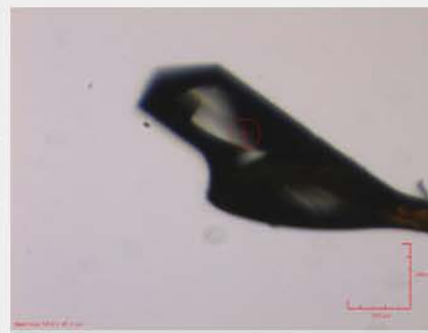
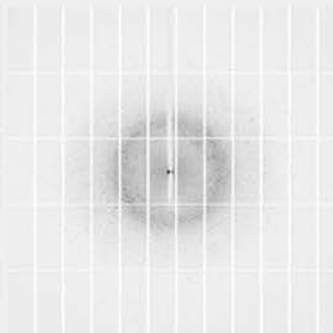
save the jpegs directory on your home computer
 - can then access most of this content locally...

Keeping track of your data:

- Using SynchLink App
 - need iPad/iPhone
- Using “View Today’s jpegs” launcher
- Through ISPyB web interface (SynchWeb)

02-05-2014 12:37:21 - JIC/ADH4/ADH4-9/ADH4_M7S9_6_###.cbf

Sample: ADH4-9
 Ω Start: 190.0°
 Ω Osc: 0.15°
 Ω Overlap: 0°
No. Images: 3000
Resolution: 1.50Å
Wavelength: 1.2820Å
Exposure: 0.040s
Transmission: 3.00%
Beamsize: 50x45µm
Type: Data Collection
Comment: (-445,10,360)



Auto Processing

Fast DP: ☒ Xia2: ☒

Fast DP: ☒ XIA2 3dai ☒ XIA2 3daii ☒ XIA2 2da

Space Group: **A** **B** **C** **α** **β** **γ**
P 21 21 2 102.18 112.20 57.12 90.00 90.00 90.00

↓ MTZ file **↓ Log file** ↓ Lookup Cell

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity
overall	2100048	148145	1.30 - 23.32	0.071	24.0	91.7	14.2	90.4	7.1
innerShell	30183	1988	5.81 - 23.32	0.061	59.0	98.4	15.2	99.1	8.8
outerShell	25217	5665	1.30 - 1.33	0.607	2.5	48.2	4.5	41.3	2.0

Downstream Processing

Fast EP: ☒ Dimple: ☒

Fast EP

Figure of Merit: 0.726
Pseudo-free CC: 74.88

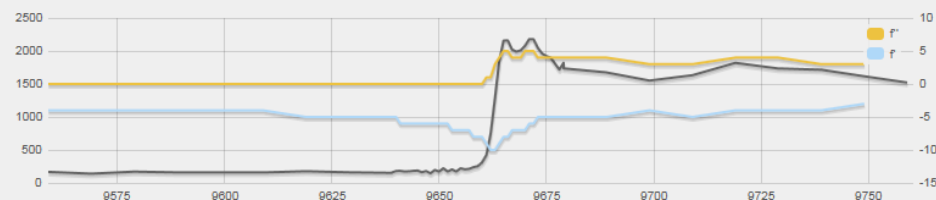
↓ Map / Model Viewer ↓ PDB/MTZ file ↓ Log file

#	X	Y	Z	Occ
1	4.081	51.507	19.743	1.000
2	29.957	24.573	1.395	0.845
3	19.209	7.842	11.593	0.693
4	6.537	3.166	16.611	0.684
5	8.444	42.030	27.339	0.108



[mx9475-2] 02-05-2014 12:15:21 - Zn Edge Scan

Sample: ADH4-9 Scan File: ADH4_9_Zn_edgescan1.fluo
E(Peak): 9671eV (1.2820Å) f': 5.23 / f'': -6.73e
E(Inf): 9663eV (1.2831Å) f': 3.15 / f'': -10.45e
Exposure: 1s Transmission: 0.40%
Comment: Click to edit



xia2 Processing Report: mx9475v2

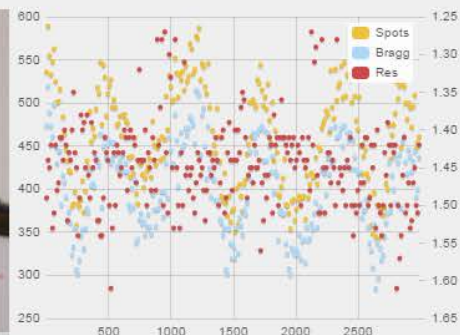
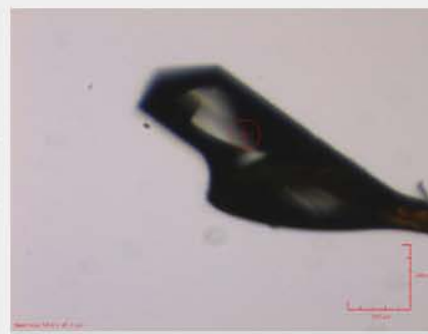
XIA2 version 0.3.6.3 completed with status 'normal termination'

Read output from /dls/i04/data/2014/mx9475-2/processed/JIC/ADH4/ADH4-9/ADH4_M7S9_6_/xia2/3da-run

SAD		
Wavelength (Å)	1.28202	
High resolution limit	1.30	(5.81 - 1.30)
Low resolution limit	23.32	(23.32 - 1.33)
Completeness	91.7	(98.4 - 48.2)
Multiplicity	14.2	(15.2 - 4.5)
I/sigma	24.0	(59.0 - 2.5)
R _{merge}	0.060	(0.048 - 0.486)
Anomalous completeness	90.4	(99.1 - 41.3)
Anomalous multiplicity	7.1	(8.8 - 2.0)
See all statistics		
Unit cell dimensions: a (Å)	102.180	
b (Å)	112.200	
c (Å)	57.120	
α (°)	90.000	
β (°)	90.000	
γ (°)	90.000	
Spacegroup	P 2 ₁ 2 ₁ 2	
Sfcheck twinning score	2.16	
Your data do not appear to be twinned		
All crystallographic parameters..		

02-05-2014 12:37:21 - JIC/ADH4/ADH4-9/ADH4_M7S9_6_###.cbf

Sample: [ADH4-9](#)
 Ω Start: 190.0°
 Ω Osc: 0.15°
 Ω Overlap: 0°
No. Images: 3000
Resolution: 1.50Å
Wavelength: 1.2820Å
Exposure: 0.040s
Transmission: 3.00%
Beamsize: 50x45µm
Type: Data Collection
Comment: (-445,10,360)



Auto Processing

Fast DP: Xia2:

Fast DP: [XIA2 3da](#) [XIA2 3daii](#) [XIA2 2da](#)

Space Group: **A** **B** **C** **α** **β** **γ**
P 21 21 2 102.18 112.20 57.12 90.00 90.00 90.00

[Download MTZ file](#) [Download Log file](#) [Lookup Cell](#)

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity
overall	2100048	148145	1.30 - 23.32	0.071	24.0	91.7	14.2	90.4	7.1
innerShell	30183	1988	5.81 - 23.32	0.061	59.0	98.4	15.2	99.1	8.8
outerShell	25217	5665	1.30 - 1.33	0.607	2.5	48.2	4.5	41.3	2.0

Downstream Processing

Fast EP: Dimple:

Fast EP

Figure of Merit: 0.726
Pseudo-free CC: 74.88

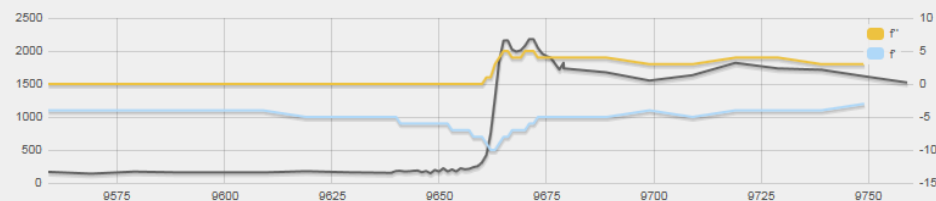
[DMap / Model Viewer](#) [Download MTZ file](#) [Download Log file](#)

#	X	Y	Z	Occ
1	4.081	51.507	19.743	1.000
2	29.957	24.573	1.395	0.845
3	19.209	7.842	11.593	0.693
4	6.537	3.166	16.611	0.684
5	8.444	42.030	27.339	0.108



[\[mx9475-2\]](#) 02-05-2014 12:15:21 - Zn Edge Scan

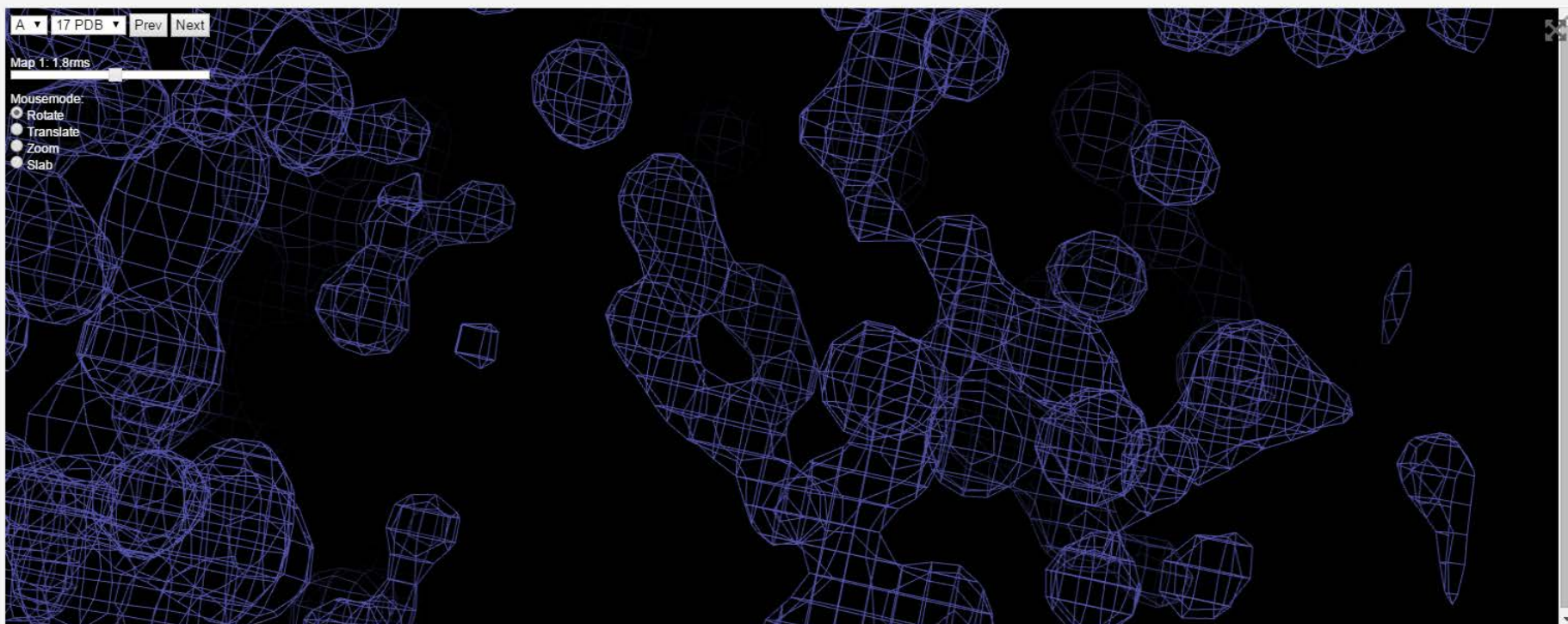
Sample: [ADH4-9](#) Scan File: [ADH4_9_Zn_edgescan1.fluo](#)
E(Peak): 9671eV (1.2820Å) f'' : 5.23 / f' : -6.73e
E(Inf): 9663eV (1.2831Å) f'' : 3.15 / f' : -10.45e
Exposure: 1s Transmission: 0.40%
Comment: [Click to edit](#)



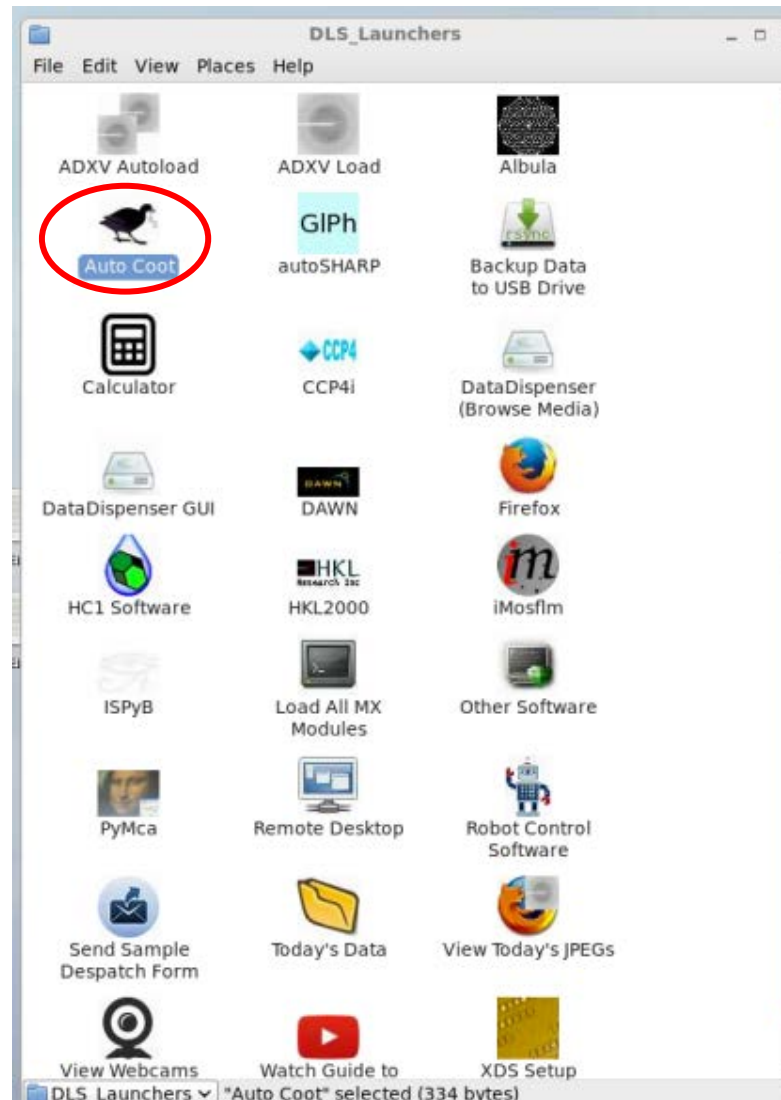
This is the new interface to ISPyB at Diamond. If you want to escape to the old version click [here](#)

mx9475-2: JIC/ADH4/ADH4-9/ADH4_M7S9_6

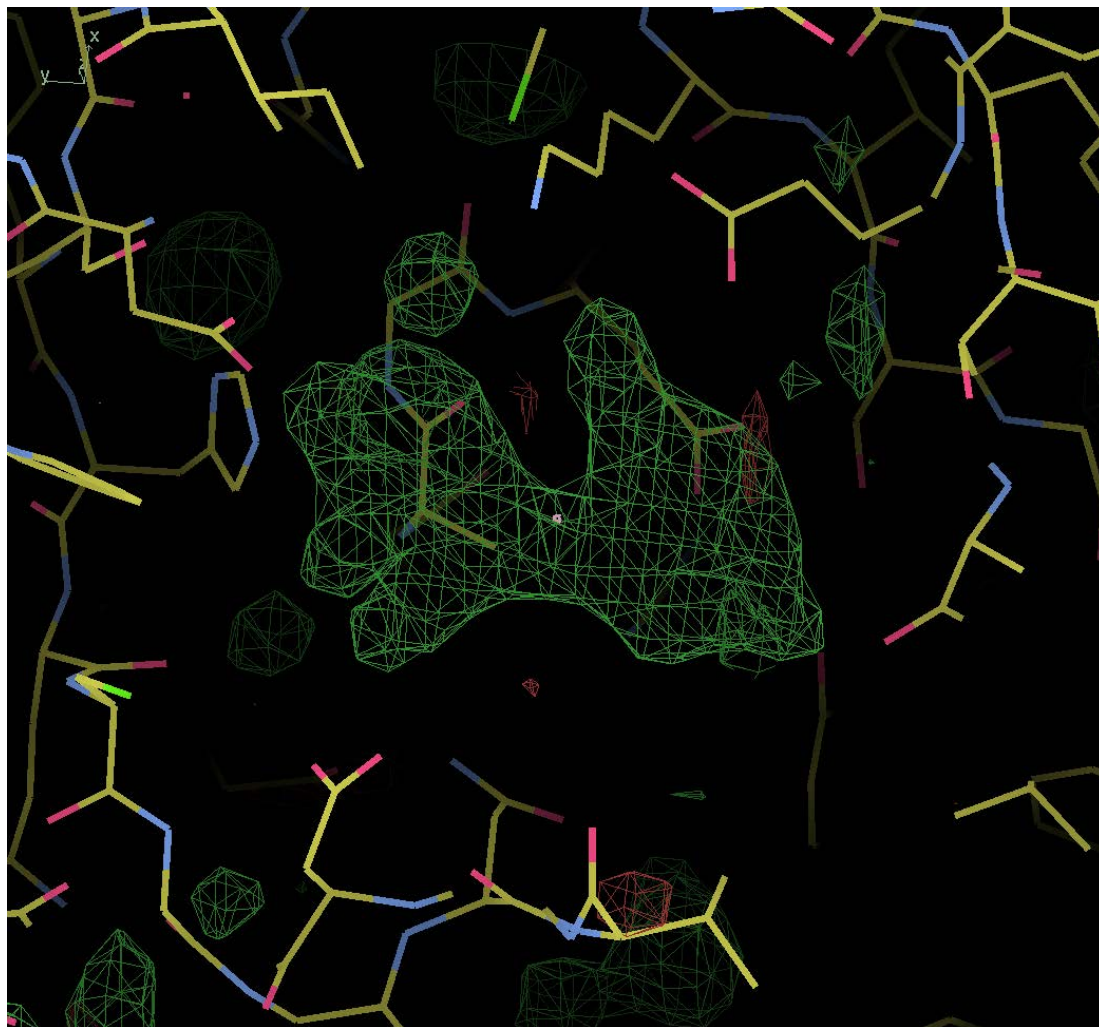
This page is an interactive map and model viewer. You can rotate the view using left mouse. Mousewheel zooms in and out. You can navigate through residues by pressing space or shift+space. Toggle fullscreen with the icon in the top right. CTRL+ left click to translate



Looking at maps:



Dimple (difference map pipeline)



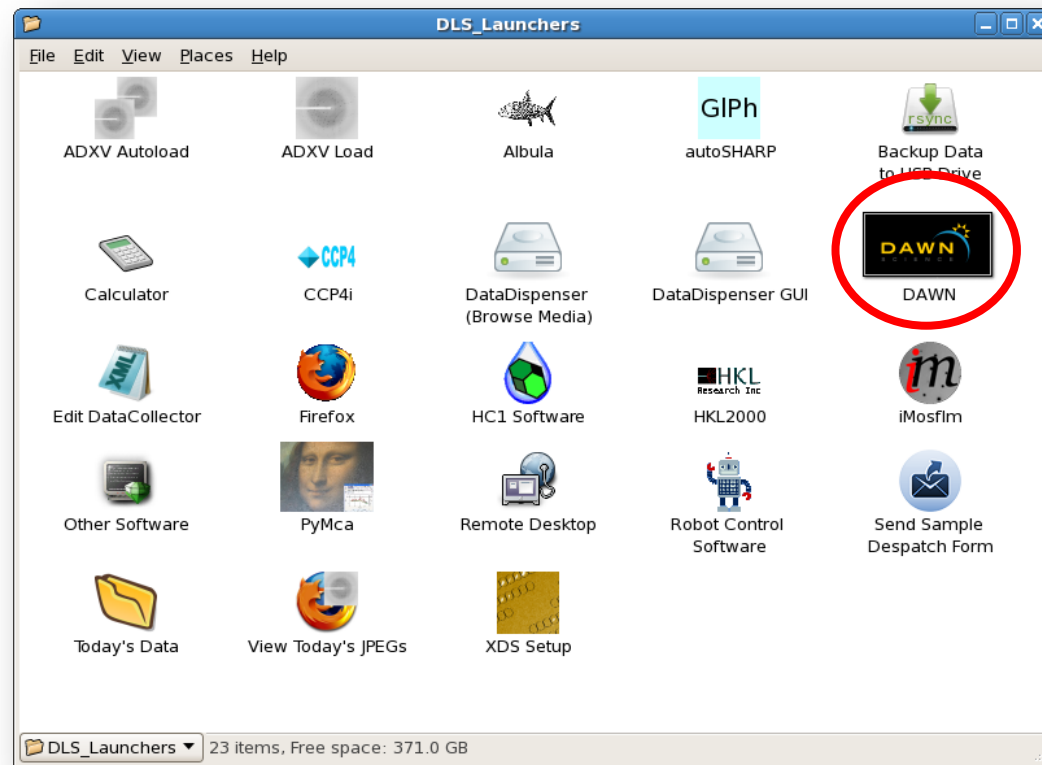
Step	Approx. time (mins)
Data collection	2
Fast_dp	2
Dimple	1
1 st image -> map	5

Get the “answer” whilst working on the next crystal...
...assuming no jobs fail!

NB. Sense check the result e.g. are R-values reasonable?

Re-running jobs:

- Most pipelines will run from the command line
- Fast_dp and Xia2 will also run through the DAWN GUI:

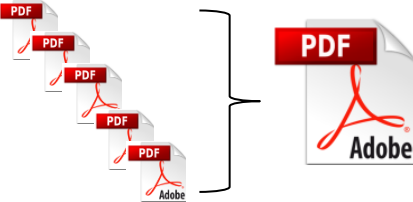


By end of visit:

- Each data set should be characterised as:
 - useful/may be useful/not useful
- Some data sets may be re-processed to your satisfaction
- You may have interpretable experimental maps
- You may have preliminary structures
- You **will** have less follow-up work to do!

After your beamtime:

- Re-process “useful” and “may be useful” datasets if necessary
- Use Diamond computers through the NXclient:
 - using latest versions of software
 - no local installation of pipelines required
 - likely to be much faster than your workstation
- Copy results home (best way?)
- With help of ISPyB database:
 - keep track of data collections
 - document your results and conclusions



This is the new interface to ISPyB at Diamond. If you want to escape to the old version

Visits for mx9475

This page lists the visits available to the

Show 10 entries

Start Date

End Date

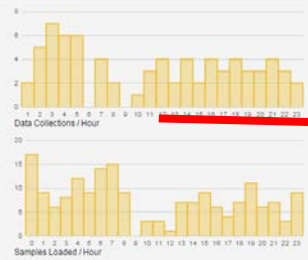
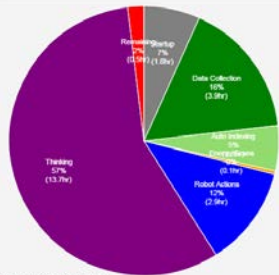
21:00 01-08-2014 02:00 02-08-

21:00 01-08-2014 02:00 02-08-



Started: 02-05-2014 09:00 Ended: 03-05-2014 09:00 Beamline: i04 Length: 10.0m

Data Collections: 313 (74 / 179) Collections Stopped: 5 Energy Scans: 1 MCA Spectra: 1 Samples Loaded: 182



mx9475-2 on i04 at 0

Sample	Images	Res	λ	Ω Osc	Spacegroup	Unit Cell	Process Resolution
ADH4-9	5	300	1.2	0.9795 0.10	P 21 21 2	101.85, 112.21, 57.09 57.09 - 1.26 57.09 - 5.63 1.29 - 1.26	
ADH4-9	5	300	1.5	1.2820 0.50	P 21 21 2	102.18, 112.20, 57.12 57.12 - 1.3 90.00, 90.00, 90.00	
ADH4-9	3000	1.5	1.2820 0.15	P 21 21 2		102.18, 112.22, 57.15 57.15 - 1.31 90.00, 90.00, 90.00	
ADH4-9	3000	1.5	1.283 0.15	P 21 21 2		102.22, 112.25, 57.15 57.15 - 1.31 90.00, 90.00, 90.00	
ADH4-9	2000	2.4	2.0000 0.15	P 21 21 2		102.28, 112.32, 57.20 57.20 - 2.01 90.00, 90.00, 90.00	
KI_NRC1_45	63	3.0	2.0000 0.00				
KI_NRC1_45	12	3.0	2.0000 0.00				
ADH4-9	5	3.0	2.0000 0.50				
KI_NRC1_45	35	3.0	2.0000 0.00				
KI_NRC1_45	18	3.0	2.0000 0.00				
KI_NRC1_45	5	3.0	2.0000 0.50				
KI_NRC1_45	3800	3.0	2.0000 0.20	P 6		111.06, 111.06, 54.21 54.21 - 6.19 90.00, 90.00, 120.00	
KI_NRC1_50	56	3.0	2.0000 0.00				
KI_NRC1_50	15	3.0	2.0000 0.00				
KI_NRC1_50	5	3.0	2.0000 0.50				
KI_NRC1_50	3800	3.0	2.0000 0.20	P 62		110.66, 110.66, 53.97 53.97 - 6.3 90.00, 90.00, 120.00	
KI_NRC1_54	5	3.0	2.0000 0.50				
KI_NRC1_53	24	3.0	2.0000 0.00				
KI_NRC1_53	12	3.0	2.0000 0.00				

Diffraction grid scan of 9 by 7 images
(-439,16,280)
Diffraction grid scan of 7 by 5 images
Diffraction grid scan of 3 by 6 images
(-246,62,406)
Diffraction grid scan of 7 by 8 images
Diffraction grid scan of 3 by 5 images
(-232,66,216)
Diffraction grid scan of 6 by 4 images
Diffraction grid scan of 3 by 4 images

to edit	173
to edit	73
to edit	257
to edit	50
to edit	51
to edit	85
to edit	0
to edit	102
to edit	313

i03 Dr Graeme Winter Click to edit
b21 Dr Katsuaki Inoue Click to edit
i04-1 Dr Keith Henderson Click to edit
i04 Dr Pierpaolo Romano Click to edit

Summary - why use the automated tools?

- Faster sample changing (ISPyB)
 - essential for remote
- Informs the decision making process
 - make decisions sooner
 - revise strategy on the fly (e.g. recollect dataset x)
 - make better overall use of beamtime
- Easier to cope with a small team
- Reduces amount of post-beamtime follow-up work
 - reprocess with Xia2 (“routine” data)
- Simple to keep track of your samples and data (ISPyB)

Take home messages

- If you are not using remote data collection – why not?
- If you are not using ISPyB – why not?
- If you are not using the software tools/pipelines – why not?
- If you don't have a life – you know why....

