

Optimising the Diamond experience from a user's perspective

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Optimising the Diamond experience from a user's perspective

Data collection strategy:

- Maximizing efficiency
- Minimizing time commitment
- Remote data collection...

...from here

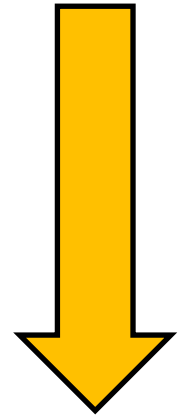
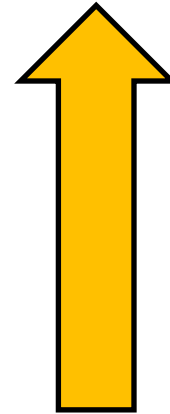
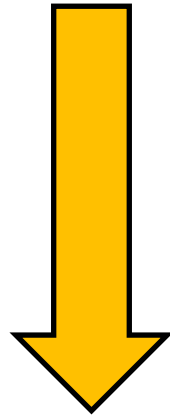
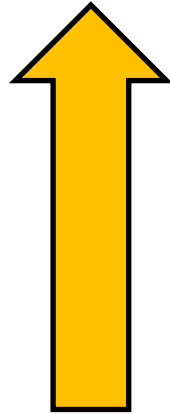


“Routine” data collection:

- 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...

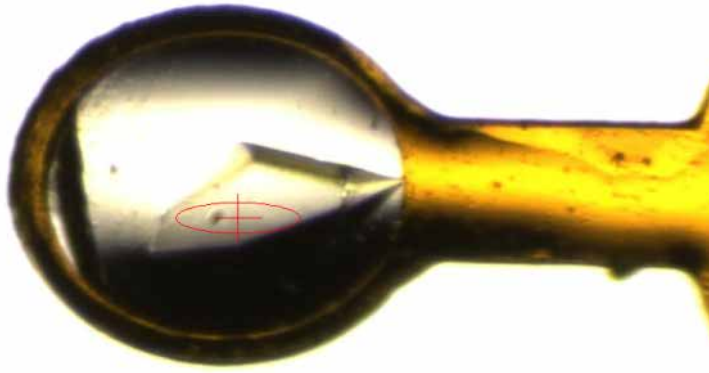
Data collection philosophy...



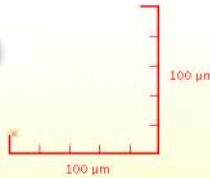
Remote collection



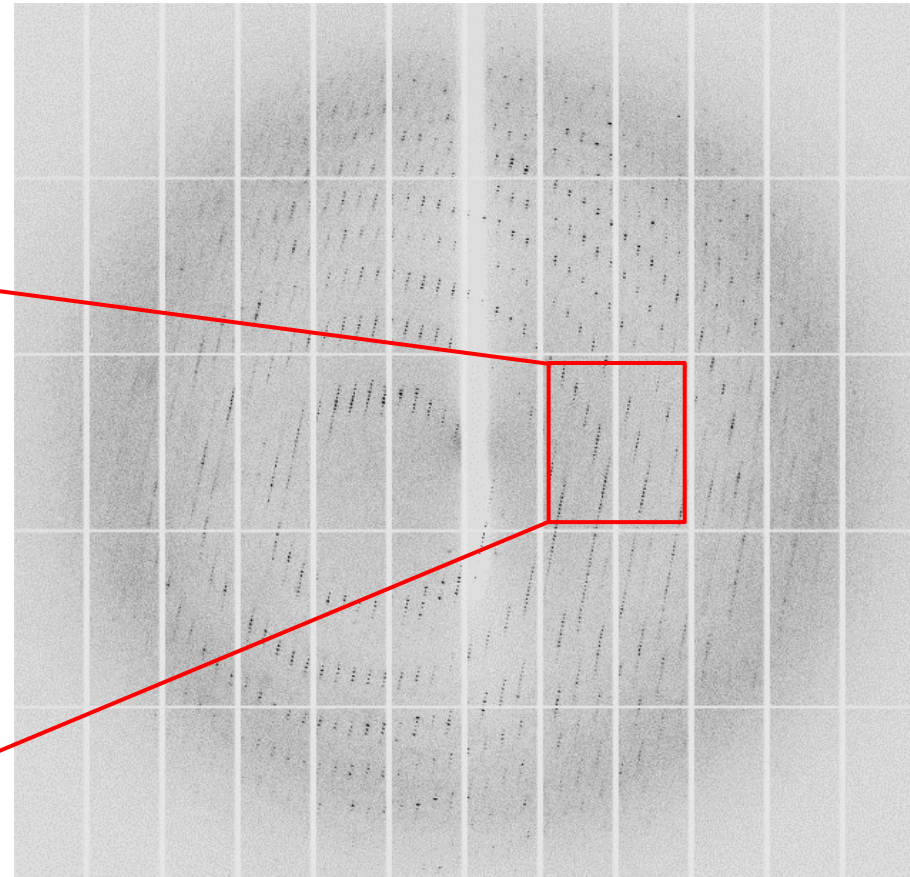
Some real data...



Crystal cooled in loop



Diffraction pattern recorded from crystal at Diamond



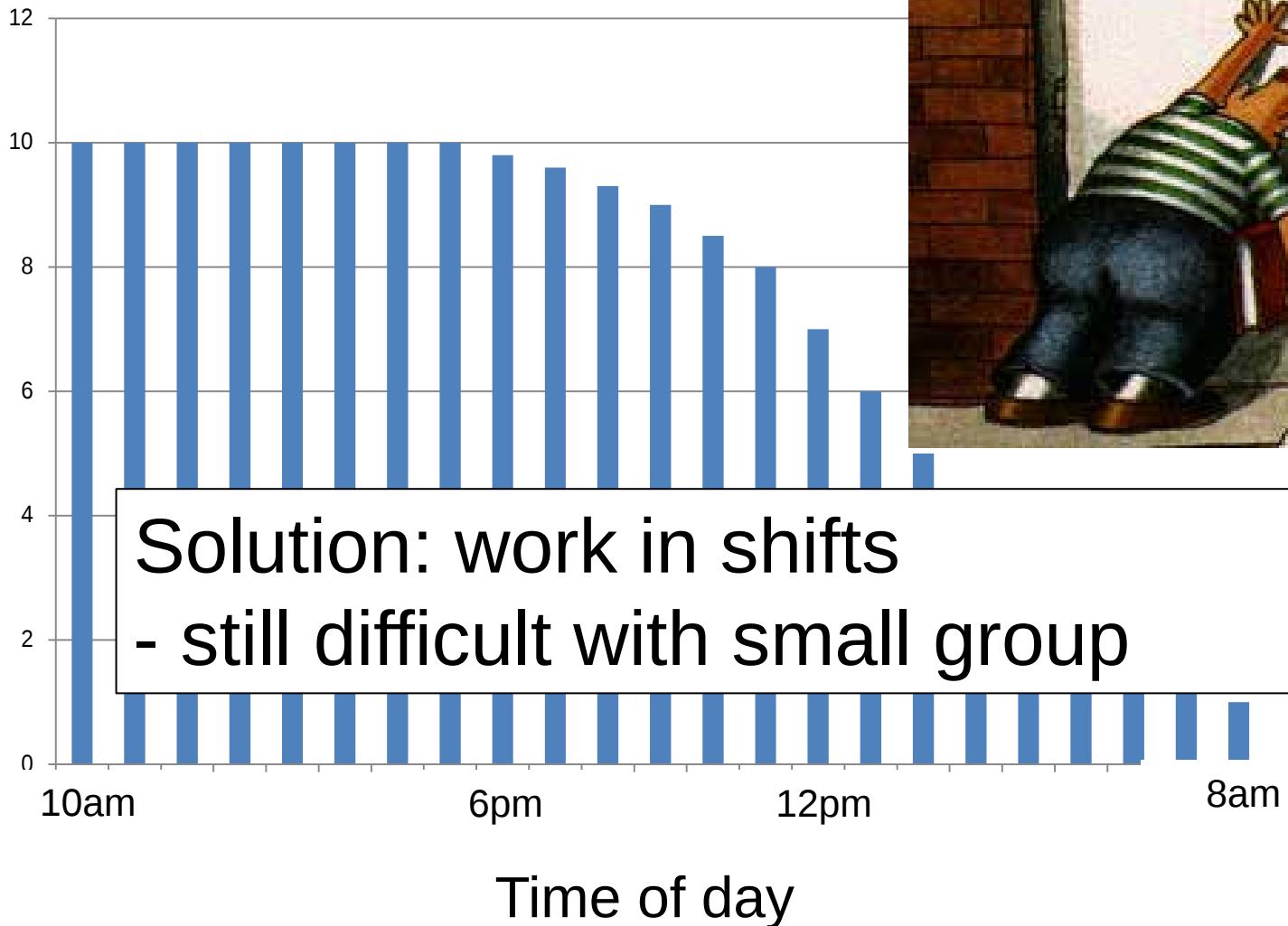
Beam size: 82.0 $\times$ 21.0 μm

Some fictitious data...

A day at the beamline...



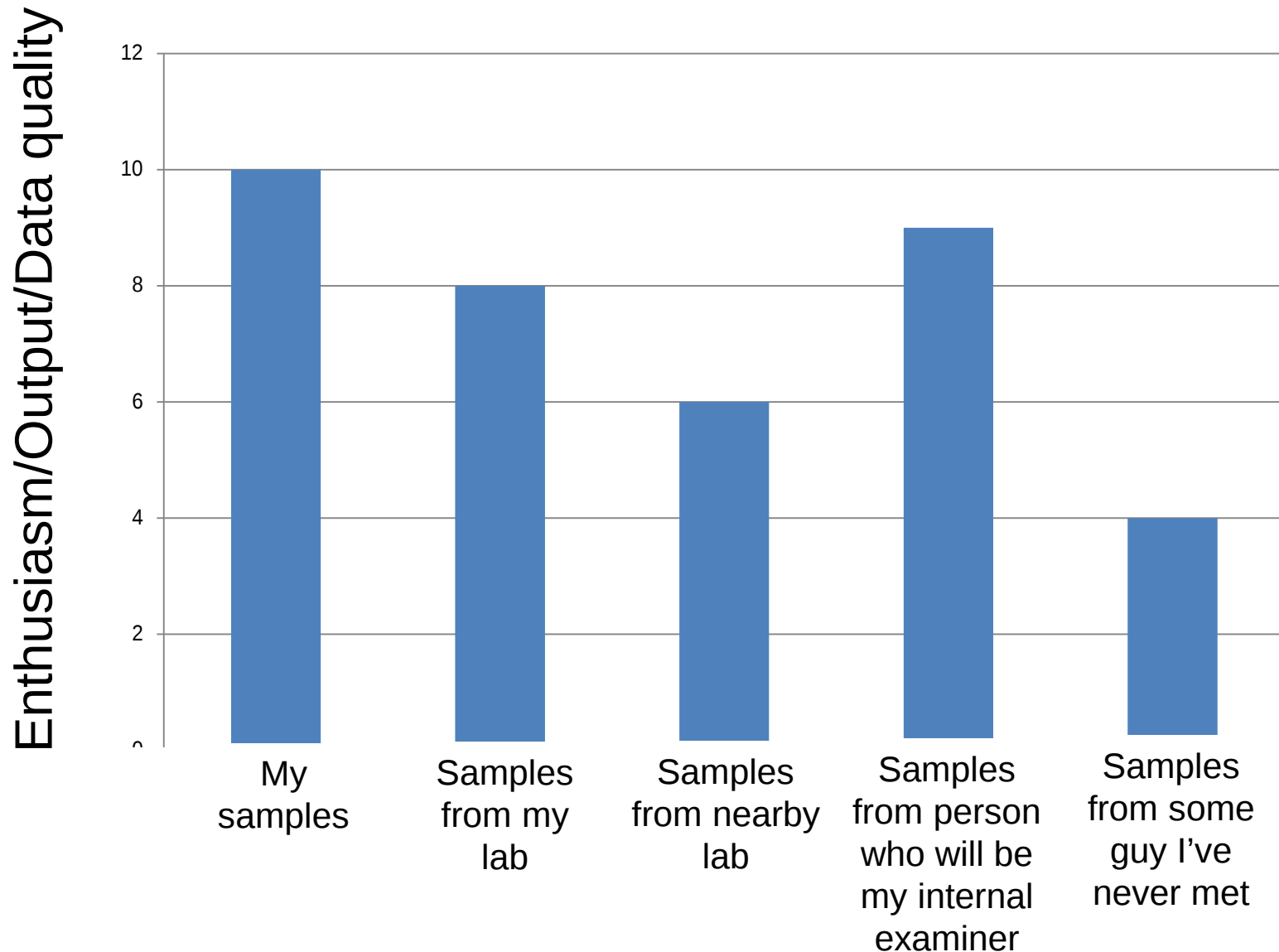
Data quality



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:

Ø everyone collects data from their own crystals



Ø 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?

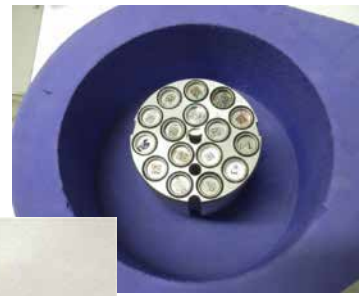
- 1 experienced user can cope, but better with 2
- any number of new users



Setting the scene for MX experiments

For routine data collection at 100 K:

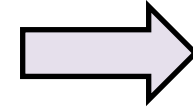
- Samples prepared and cryo-cooled in home lab
- Transported to DLS in dry shipping dewars
- Samples mounted robotically
- Data collection controlled through GDA GUI
- Only manual operation at DLS: loading/unloading pucks
 - up to 144 or 160 samples can be loaded at once (depending on beamline)
 - may 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

Id: Paste from Spreadsheet

Shipment: test

Dewar: Dewar1

Puck Name: test



Location	Protein Acronym	Sample Name	Specgroup	Barcode	Comment
1	/ys	/ys1	1		
2	/ys	/ys2	2		
3	/ys	/ys3	3		

Getting started...

Macromolecular Crystallography

MX ▼ I02 I03 I04 I04-1 I23 I24 VMXi Membrane Protein Laboratory Staff Research Contacts

 Beamlines / MX / I02 / I02 Manual / Remote Access

In This Section

I02 Manual

[Preparing for Beamtime](#)[New-ISPyB](#)[Old-ISPyB](#)[Shipping Samples](#)[Sample Holders](#)[Sample Changer](#)

Remote Access

[Connection to Diamond cluster](#)[Linux and Mac OS X systems](#)[Windows system](#)[Known Remote Access](#)[Issues](#)[Speed test](#)[Webcams](#)

Remote Access

IMPORTANT NOTICE

We have (15-Aug to 13-Sep 2014):

- updated the NX servers from 3.5 to 4
- replaced NX client with NX player on Linux work stations
- updated RHEL 5 to RHEL 6 on beamline Linux work stations

Please check [our dedicated pages](#) to test your connection with the new configuration!

Introduction to Remote Access

The MX beamlines at Diamond ([I02](#), [I03](#), [I04](#), [I04-1](#) and [I24](#)) have been highly automated. When combined with intuitive software, comprehensive manuals (both [written](#) and [videos](#)) and highly experienced local support staff it is possible to provide remote access experiments at all these beamlines for the novice through to expert users. Most experiments are feasible remotely with minor exceptions such as [humidity control](#) or those at [biological containment level III](#).

Requirements

To carry out remote access experiments to Diamond we recommend:

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!

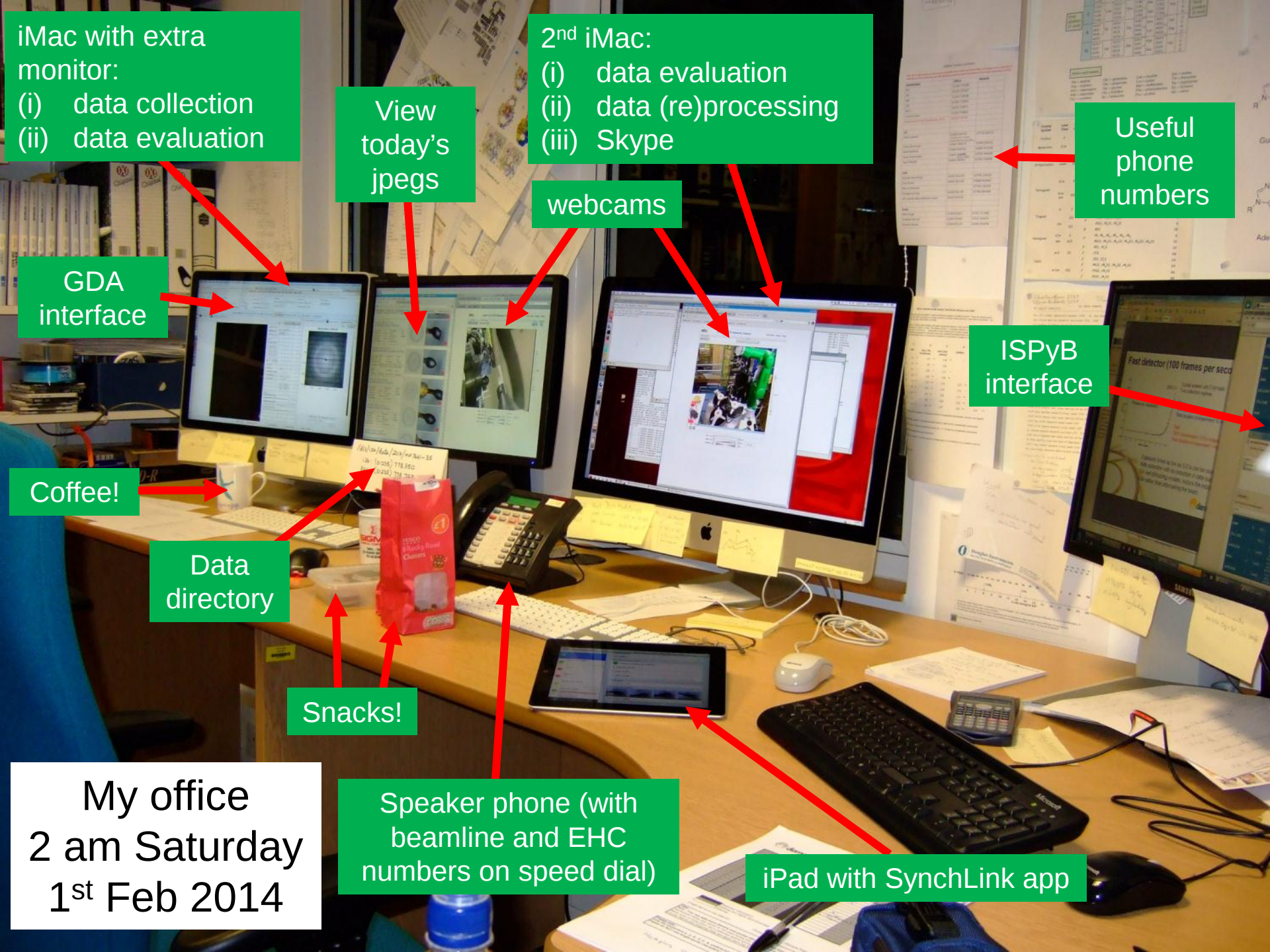
Data
directory

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 screenshot displays the EEMaX website interface. The top navigation bar includes links for 'Front Page', 'People', 'Bookmarks', and 'Recent Changes'. A search bar is located on the right. The main content area shows a beamtime entry for MX9475-18, scheduled from 10:00 Mon 1 Dec 2014 to 09:00 Tue 2 Dec 2014, with a deadline of 13 Nov. Below this, there are sections for 'DML', 'MJB', 'AMH', 'IC', 'CD', and 'MAH', each containing details about local users, arrival/departure dates, remote users, contact numbers, pucks/time, and comments. An Outlook reminder window is overlaid on the right side of the page. The reminder is titled '1 Reminder' and contains the following information: 'Start time: 16 December 2014 21:00', 'Location: N/A', and a table with the subject '*BEAMTIME* MX9475-19: 5 HRS - I02 from 21:00 Tue 16 Dec 2014 to 02:00 ...' and a due date of 13 days. The reminder window also includes buttons for 'Dismiss All', 'Open Item', 'Dismiss', and 'Snooze'.

Welcome, David Lawson
(edit, settings | settings | logout)

Front Page Edit Info Talk

Search: []

contact numbers (contact name/landline/mobile):
pucks/time:
comments:
Priority (H/M/L): NOT REQUIRED

MX9475-18: 23 HRS - I03 from 10:00 Mon 1 Dec 2014 to 09:00 Tue 2 Dec 2014 - DEADLINE: 13 Nov

DML
local users (dietary requirements):
arrival/departure dates and times:
remote users: Lawson, S
contact numbers (contact name/landline/mobile):
pucks/time: 4 pucks/ 8 h
comments:
Priority (H/M/L): M

MJB
local users (dietary requirements):
arrival/departure dates and times:
remote users: Banfield, T
contact numbers (contact name/landline/mobile):
pucks/time: 3, 6hrs
comments:
Priority (H/M/L): M

AMH
local users (dietary requirements):
arrival/departure dates and times:
remote users:
contact numbers (contact name/landline/mobile):
pucks/time:
comments:
Priority (H/M/L): NOT REQUIRED

IC
local users (dietary requirements):
arrival/departure dates and times:
remote users: Tom Clark
contact numbers (contact name/landline/mobile):
pucks/time: 3-4 pucks, 6 hrs
comments:
Priority (H/M/L): M

CD
local users (dietary requirements):
arrival/departure dates and times:
remote users: Yinghong G
contact numbers (contact name/landline/mobile):
pucks/time: 5 pucks/6 hrs
comments:
Priority (H/M/L): M

MAH
local users (dietary requirements):
arrival/departure dates and times:
remote users:
contact numbers (contact name/landline/mobile):
pucks/time:
comments:

1 Reminder

***BEAMTIME* MX9475-19: 5 HRS - I02 from 21:00 Tue 16 Dec 2014 to 02:00 ...**

Start time: 16 December 2014 21:00
Location: N/A

Subject	Due in
BEAMTIME MX9475-19: 5 HRS - I02 from 21:00 Tue 16 Dec 2014 to 02:00 ...	13 days

Dismiss All Open Item Dismiss

Click Snooze to be reminded again in:

5 minutes before start [v] Snooze

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

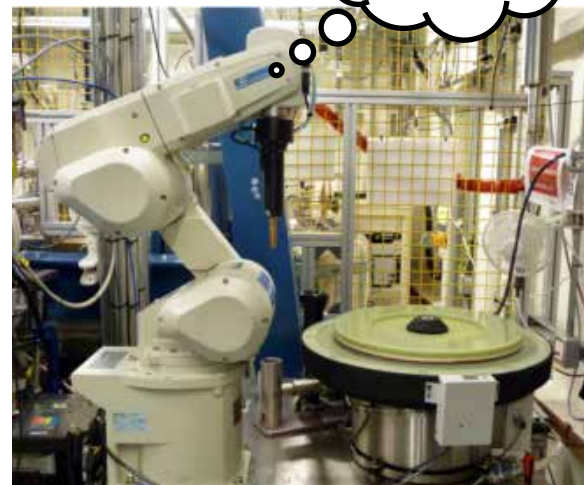
“I need preliminary data for my grant application!”



“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

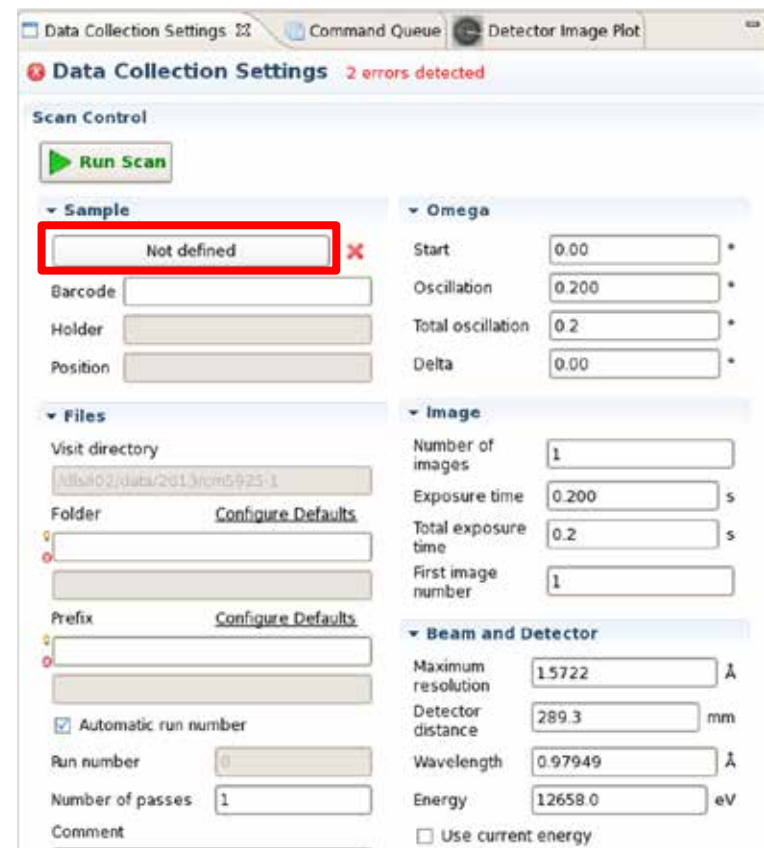
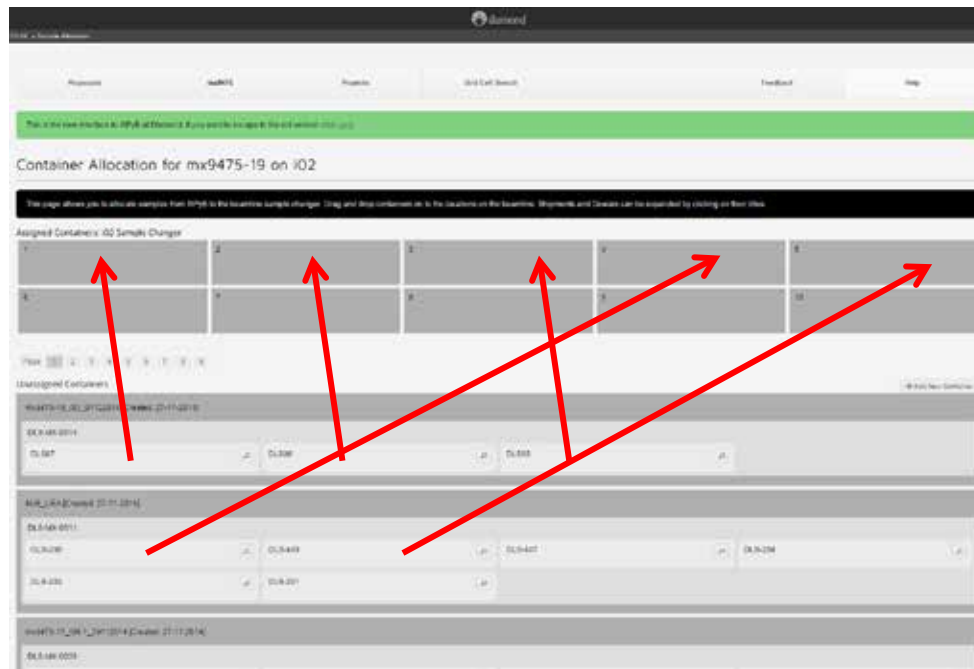
2 - 4 days before:

- 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
- 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
232.261

Refill
130.903

Hutch
Locked

Port Shutter
Open

Expt Shutter
Open

Fast Shutter
Closed

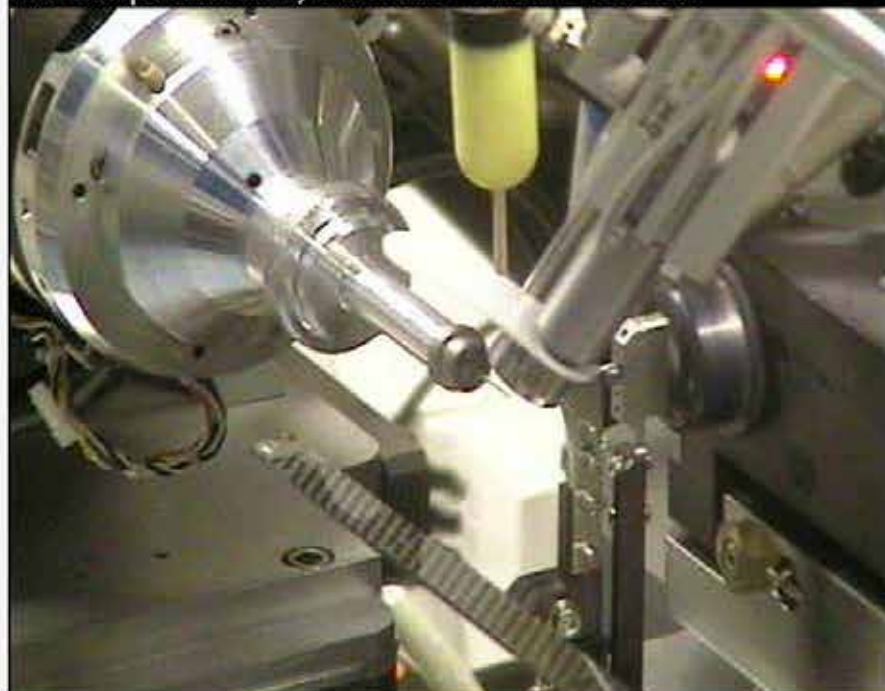
Wavelength
0.976254

Transmission
100

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

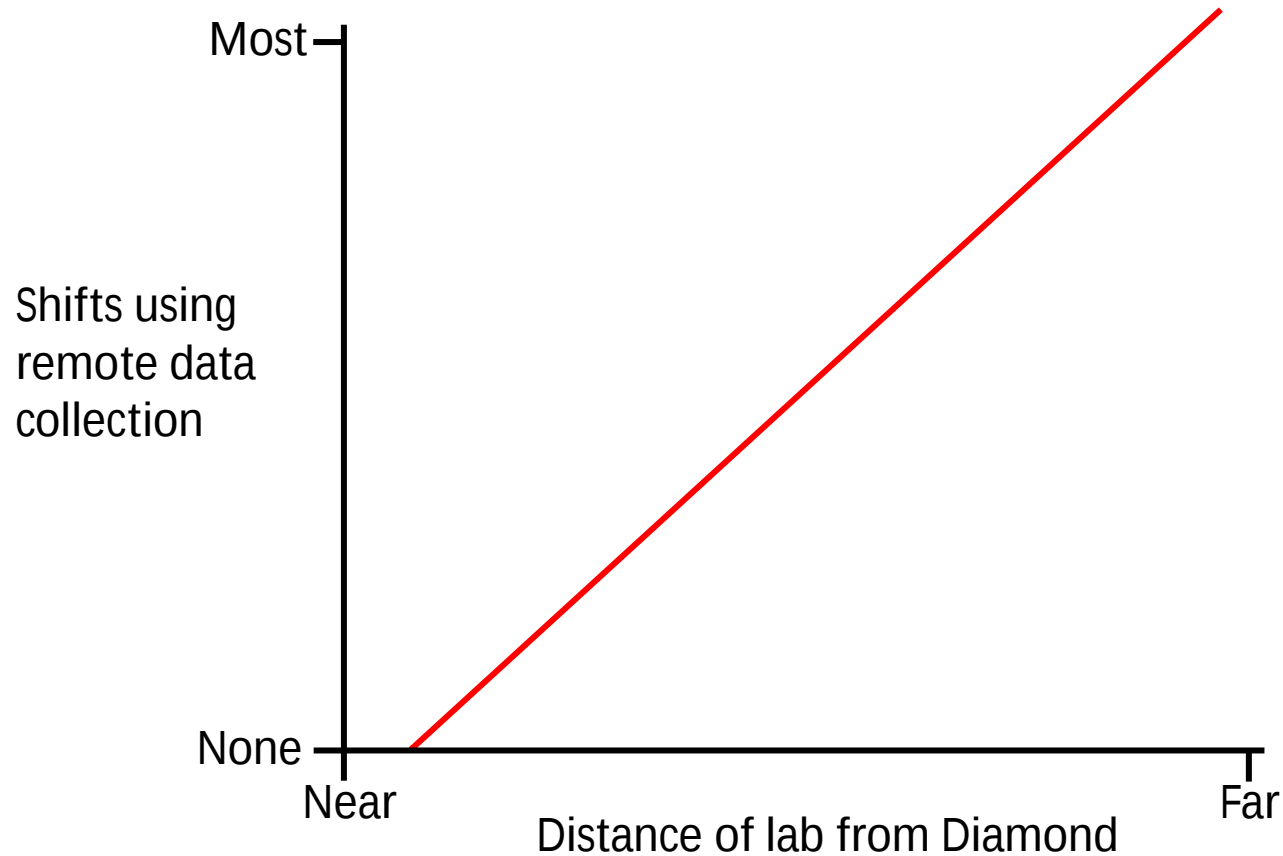


i03 Sample Position, Mon Dec 1 2014 10:07:50





How remote is “remote”?



People can be set in their ways...



Let go Luke...

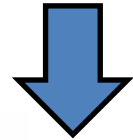


...use remote!

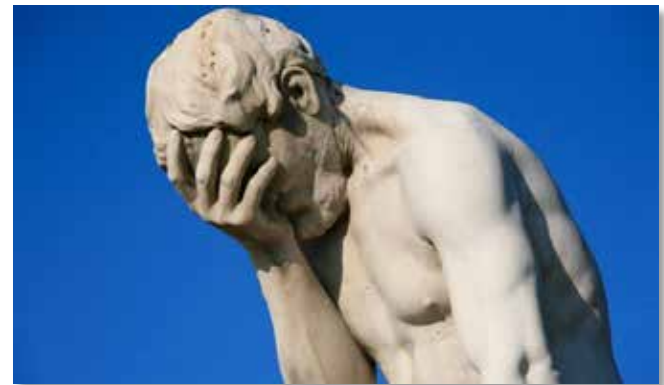
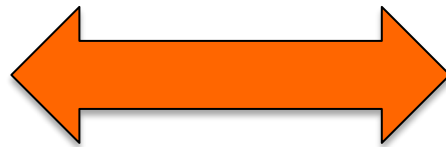
I know what
you're getting
for Christmas.

How?

Because I felt
your
presents!



=



When things go wrong...

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

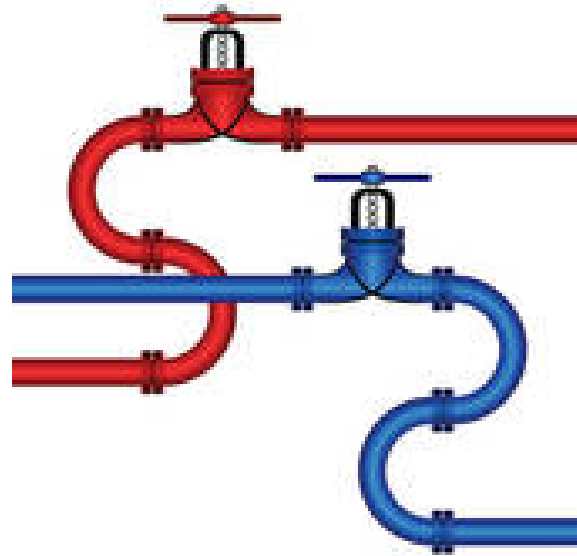
Advantages of remote data collection:

- Beamtime is fully used
- Users collect data on their own crystals
- Most/all of the users stay at home labs
 - Ø time commitment is low for remote users
 - Ø stakeholders can observe data collection
 - Ø 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



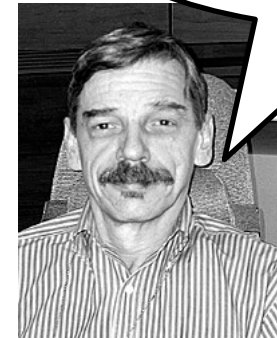
Goals for my beamtime...



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!)

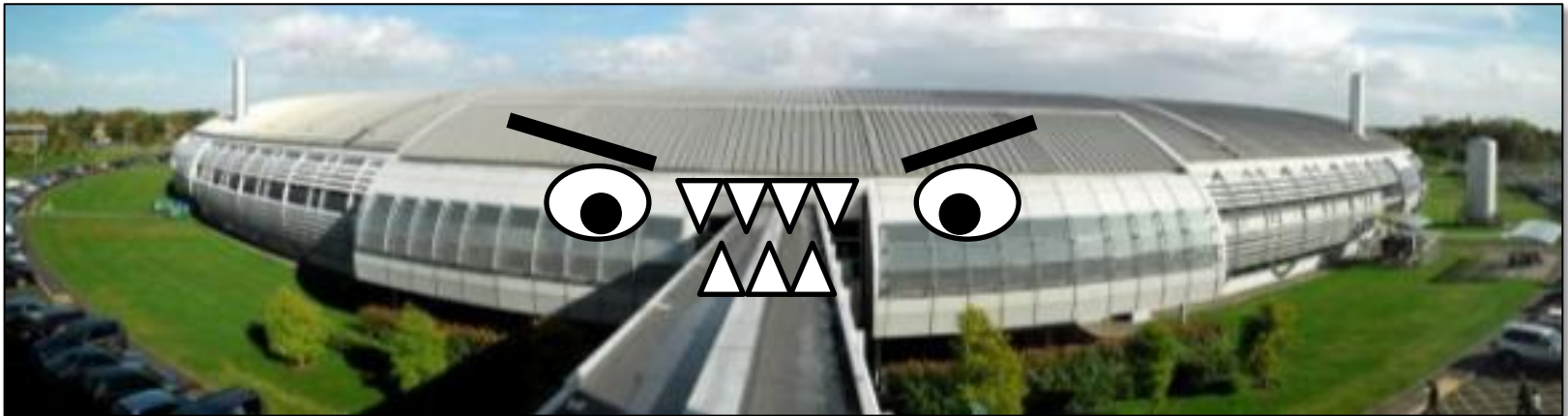


Zbyszek
Dauter

“Data collection is
the last
experimental step!”

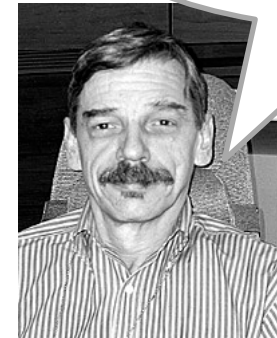
Ask yourself:

- Do you spend a long time re-processing data at home?
- Does the next visit come along before you have analyzed all the data from the previous trip?
- Is Diamond an insatiable monster that eats all your crystals?



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



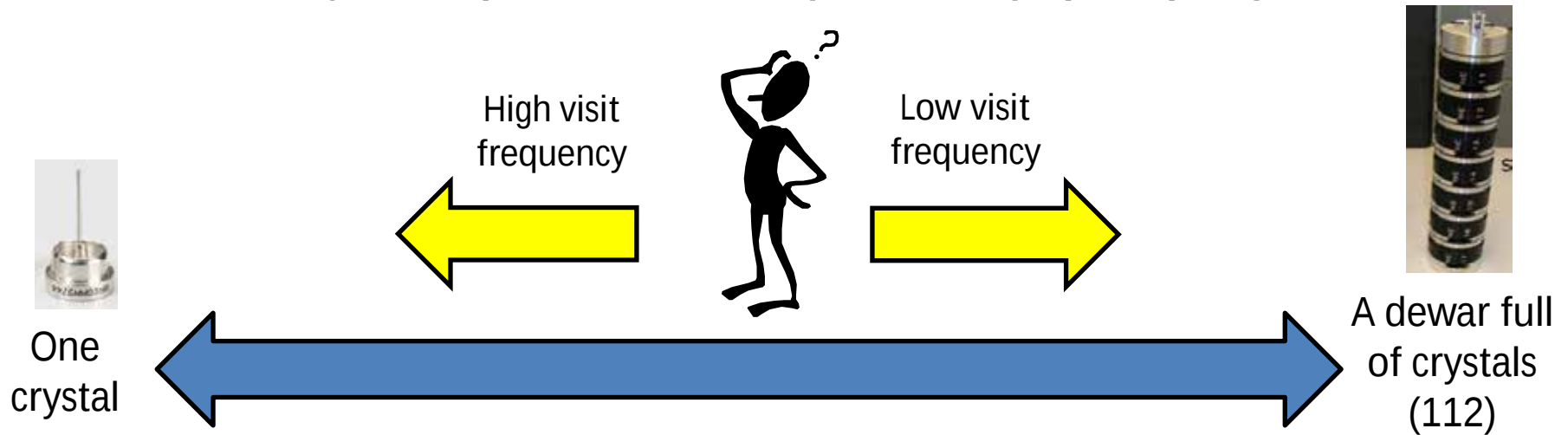
“Data collection is
the last
experimental step!”

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

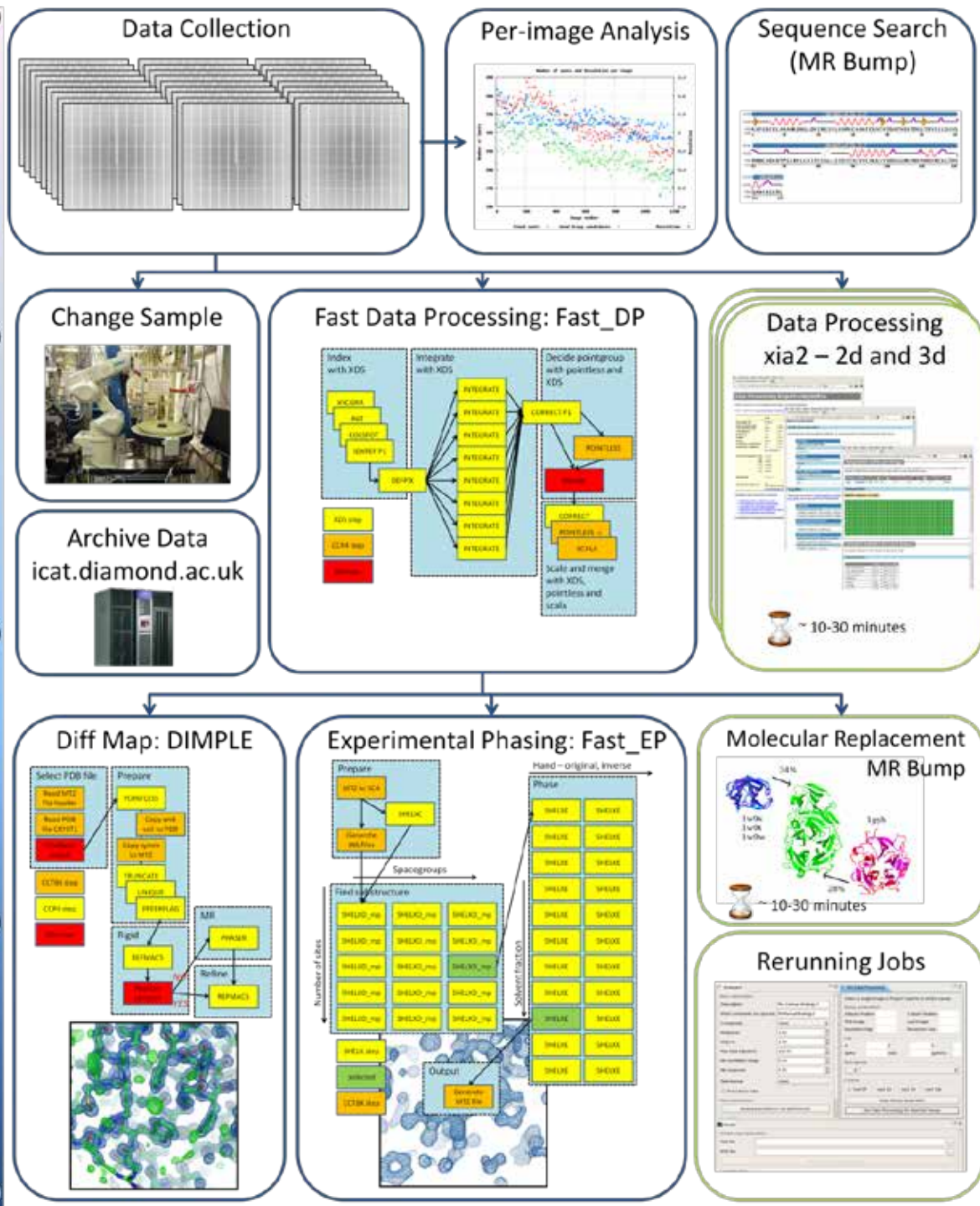
To recap...

- 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

Sample
info.

ISPyB database

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...

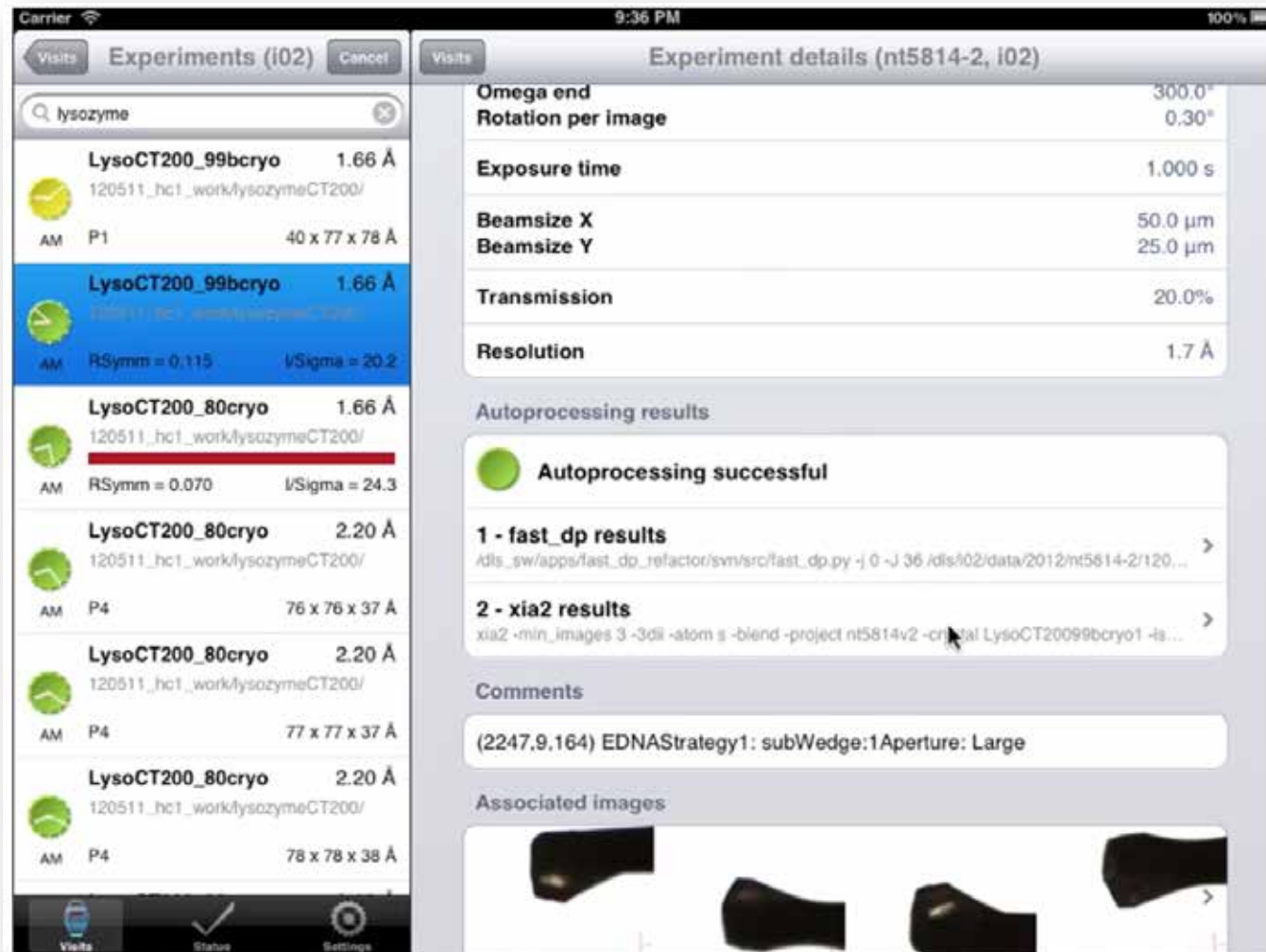


During beamtime:

- (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...

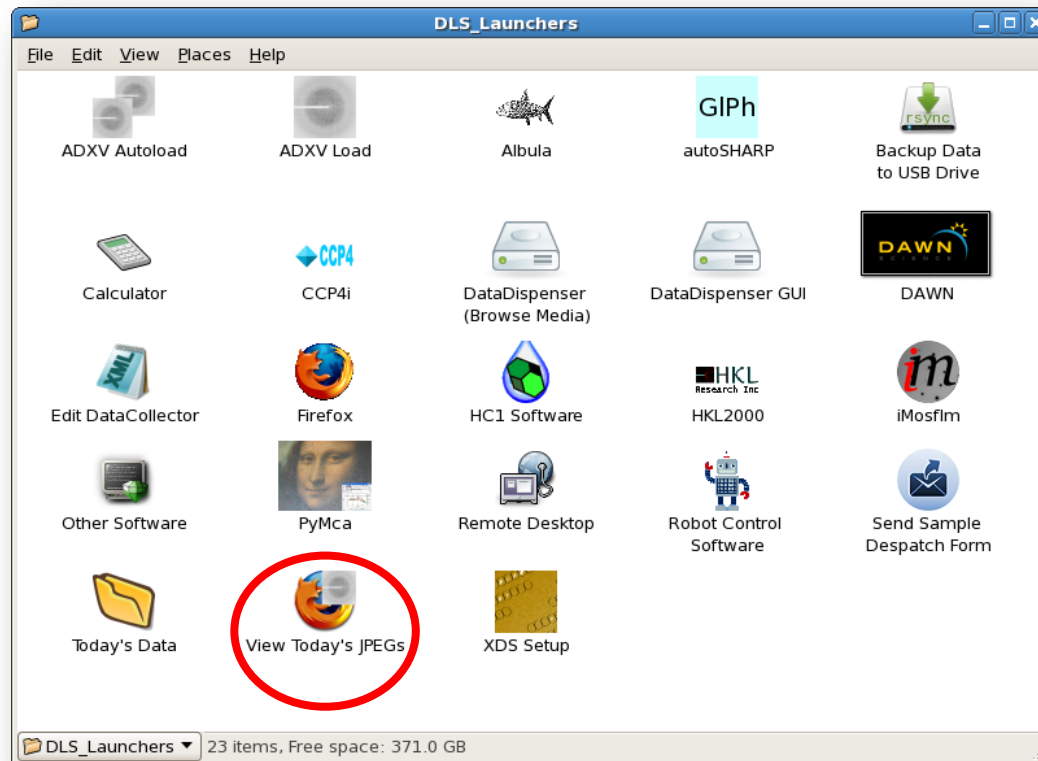
Keeping track of your data:

- 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

file:///C:/Users/ndy35357/Desktop/ds/03/data/2013/mx7641-23/jpegs/index.html

Webcams mx7641-27 mx7641-23

Sat May 4, 2013 - 21:24:53
[BBA_GISM_4/BBA_GISM_4_MIS4_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_dp 😊	MrBUMP 😊	DIMPLE 😊

Sat May 4, 2013 - 21:21:23
[BBA_GISM_4/BBA_GISM_4_MIS4_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_MIS1_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_dp 😊	MrBUMP 😊	DIMPLE 😊

Sat May 4, 2013 - 21:11:23
[BBA_M1M_3/BBA_M1M_3_MIS1_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_MIS1_2_####.cbf](#)

No. Images:	3	Resolution:	1.50Å
Exp. Time:	0.2	Trans:	50.16%
Omega Osc:	0.2°	Wavelength:	0.9763Å

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

15:58 Friday 2013-05-04

Keeping track of your data:

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

02-05-2014 12:37:21 - JIC/ADH4/ADH4-9/ADH4_M759_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: ☒ Xia2: ☒

Space Group	A	B	C	a	β	γ
P 2 ₁ 2 ₁ 2	102.18	112.20	37.12	90.00	90.00	90.00

☒ Merge ☒ Data ☒ Process Data

Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity
overall	2100040	140145	1.30 - 23.32	0.071	24.0	91.7	14.2	90.4	7.1
innerShell	30103	1968	5.81 - 23.32	0.061	59.0	95.4	15.2	99.1	8.8
outerShell	25217	5665	1.30 - 1.33	0.607	2.5	45.2	4.5	41.3	2.0

Downstream Processing

Fast EP: ☒ Dimple: ☒

Fast EP

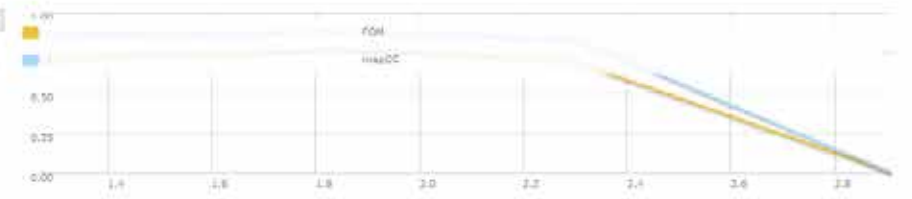
Figure of Merit: 0.726
Pseudo-free CC: 74.0%

☒ Data / Model Viewer

☒ LPSQMT2 file

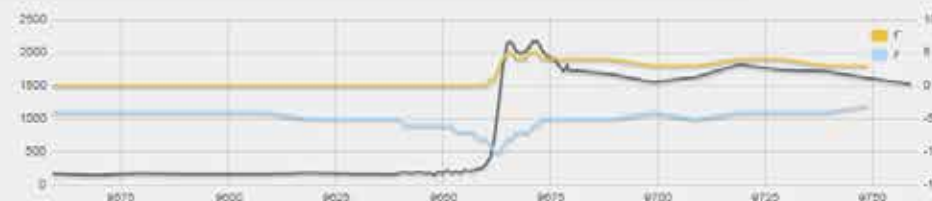
☒ Data file

#	X	Y	Z	Occ
1	4.001	55.507	19.743	1.000
2	26.457	34.571	1.295	0.845
3	19.209	7.042	11.593	0.693
4	6.537	3.166	16.611	0.684
5	0.444	47.030	27.339	0.100

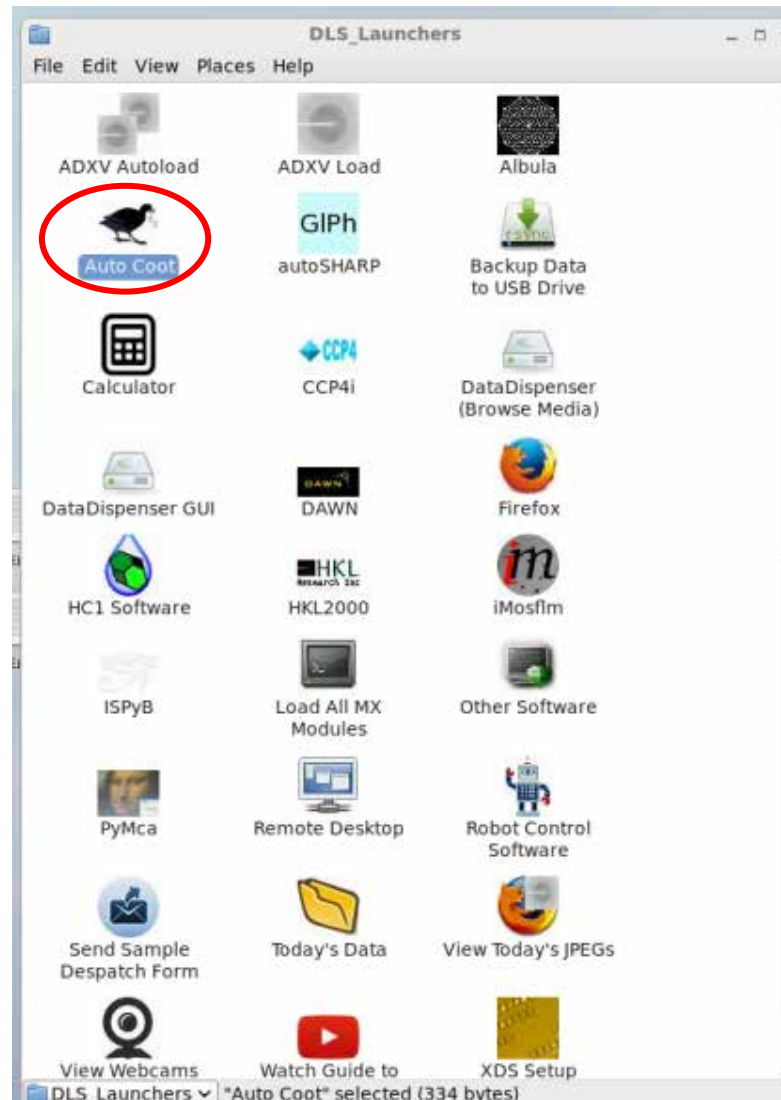


02-05-2014 12:15:21 - Zn Edge Scan

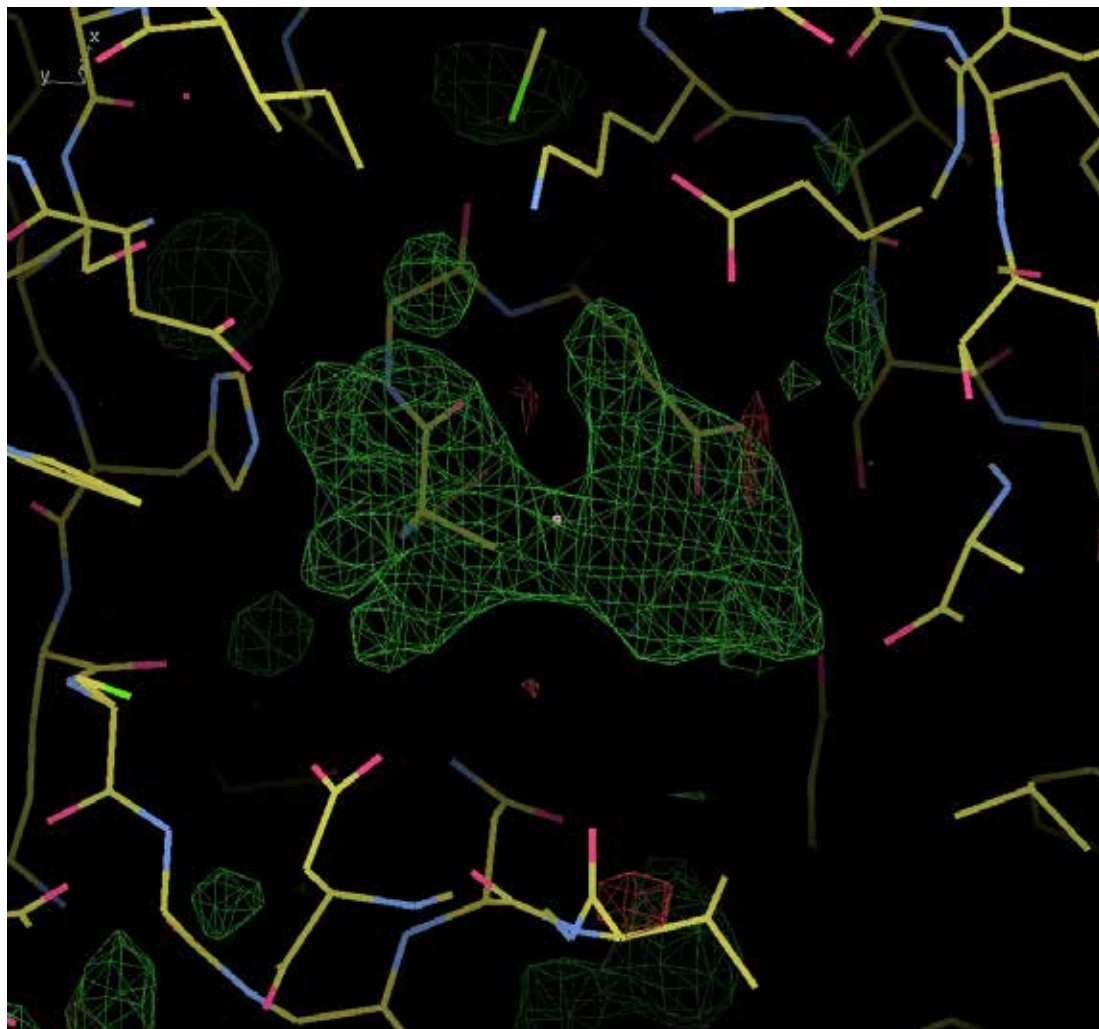
Sample: ADH4_9	Scan File: ADH4_9_Zn_edgescan1.fluo
E(Peak): 9671eV (1.2820Å)	f: 5.23 / f: -6.73e
E(In): 9663eV (1.2831Å)	f: 3.15 / f: -10.45e
Exposure: 1s	Transmission: 0.40%
Comment: Click to edit	



Looking at maps:



Dimple (difference map pipeline)



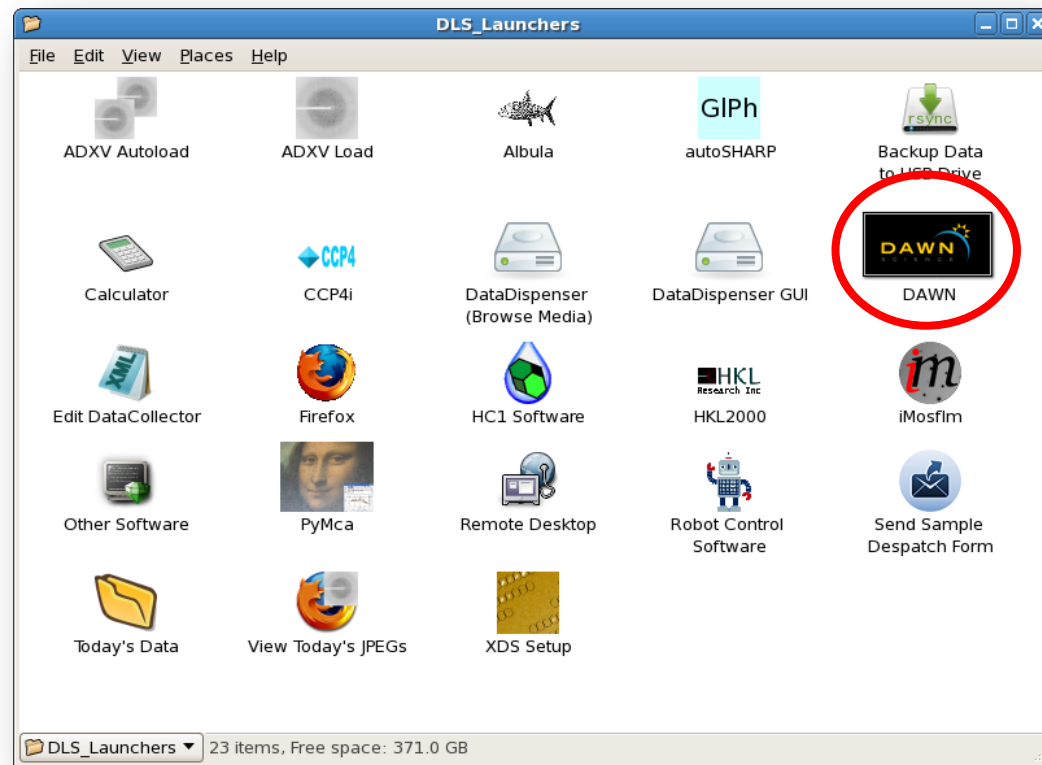
Step	Approx. time (mins)
Data collection	2
Fast_dp	2
Dimple	1
1 st image -> map	5

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

[illegible]

Keeping track through local wiki

X-ray Data Collection [\[edit\]](#)

Diamond [\[edit\]](#)

- Instructions for remote data collection
- Use of Dave's iMac (n61205) during remote data collection
- Diamond homepage [↗](#)
- MX beamlines home page [↗](#)
- Short-Shift-Timeline [↗](#)
- UAS [↗](#)
- ISPyB [↗](#)
- Summary of past Diamond trips (opens PDF file)
- All ISPyB data from past Diamond trips (opens PDF file)
- Jpegs from Diamond trips
- Crystals for Diamond
- Data collection spreadsheets
- Link to crystallography filestore
- Useful information
- X-ray Anomalous Scattering [↗](#)
- X-ray wavelength to energy converter [↗](#)
- X-ray Emission Lines [↗](#)
- EEMaX Wiki [↗](#)
- Welcome to the world of Crystallography! (lots of useful information) [↗](#)
- Instructions on how to process with xia2 on diamond computers

In-house [\[edit\]](#)

- Accessing data from the in-house facility
- Archiving procedure

Single PDF with
all ISPyB data

“View today’s jpegs” directories

Annotated Excel files from ISPyB

Values in parentheses are for the other resolution shell	
No. of crystals	1
Beamline	B27 Diamond Light Source
Wavelength (Å)	0.9795
Detector	ADSC Quantum 315 CCD
Crystal-to-detector distance (mm)	280.7
Exposure time per image (s)	0.1
Exposure time per image (h)	0.25
Room temperature (°C)	27.2
Total rotation range (°)	204.0
Resolution range (Å)	67.5 (30.7) (3.0)
Space group	$P6_3$
Unit-cell parameters (Å, °)	$a = 232.4, b = 769.6,$ $c = 142.22, \beta = 92.96$
Estimated completeness (%)	0.2
Total No. of measured intensities	67796 (5760)
Unique reflections	14600 (2500)
Multiplicity	4.6 (2.1)
Mean $I/\sigma(I)$	8.3 (2.6)
Completeness (%)	98.3 (95.1)
R_{meas}	0.127 (0.053)
R_{cyc}	0.147 (0.070)
$\sigma(I)$	0.094 (0.076)
Weighted R value (χ^2)	0.16

Chapter 4 • Structural Investigation of the Fas L/Protein

[illegible]

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....



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- Access to MX beamlines at Diamond
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