



Navigating the Diamond Cluster

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Background

Before Covid:

- 50% of Diamond Users are MX
- 55% of Experimental Sessions are MX
- More than 75% of MX visits were remote



Since then added UDC to our offering

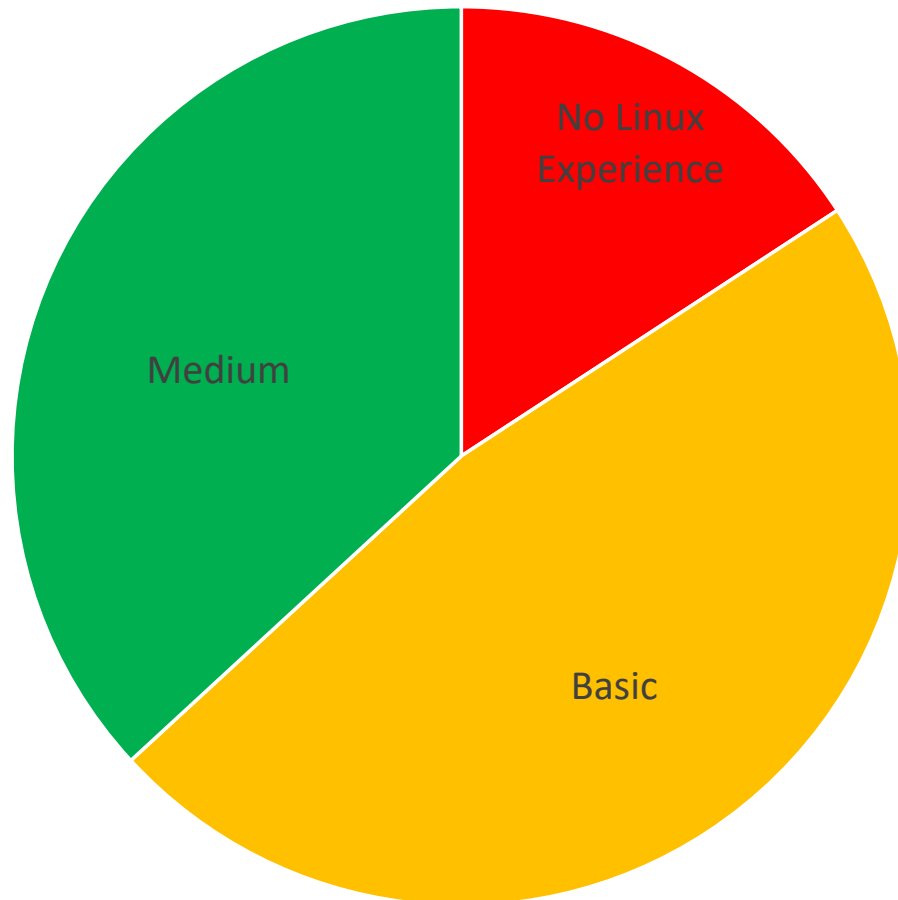
- UDC is “Unattended Data Collection” which doesn’t need any User interaction once they have put their data collection parameters into ISPyB, before shipping their crystals
- But now we don’t have Users on site, it’s harder to interact with them and train them – hence doing courses like this.
- Therefore please take the opportunity to network with members of the Diamond team

Lots of monitors to control a beamline...



- GDA
- ISPyB
- Diffraction Image Viewer
 - e.g. ADXV
- Machine Status Page

The Audience...



Multiple ways to get to the same destination...



You have to be precise



Fed IDs and Passwords

- You all have a Fed ID and password.
- If needed, Diamond staff can tell you what your Fed ID is, but not what your password is
- We can only request that a password is reset – and that is within UK office hours
- You will use this to log in to NX sessions (this talk) and ISPyB sessions – so make sure it works

NoMachine – Enterprise Client

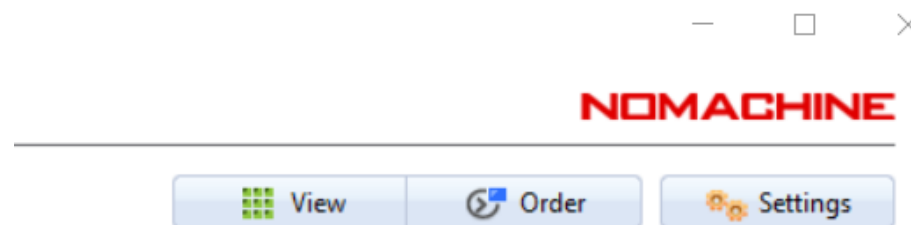
→ your route in to Diamond




- Download to your machine -
<https://www.nomachine.com/product&p=NoMachine%20Enterprise%20Client>


OR

- Make sure it is the latest version in Settings



Checking for updates in settings

 NoMachine

 Player settings



Input
Keyboard, mouse and menu



Appearance
Themes, languages and fonts



Transfers
File transfer preferences



Security
Proxy, log files, network browsing



Folders
Settings, recordings and transferred files



Updates
Software update preferences

Player updates

NOMACHINE
ENTERPRISE CLIENT

Product: NoMachine Enterprise Client

Version: 7.1.3

Platform: Windows

Copyright 2002, 2021 © NoMachine


Select how NoMachine must handle software updates.

☒ Automatically check for updates

Check now

☐ Install updates in background

First Time Users/Computers

 NoMachine - Connection to nx.diamond.ac.uk

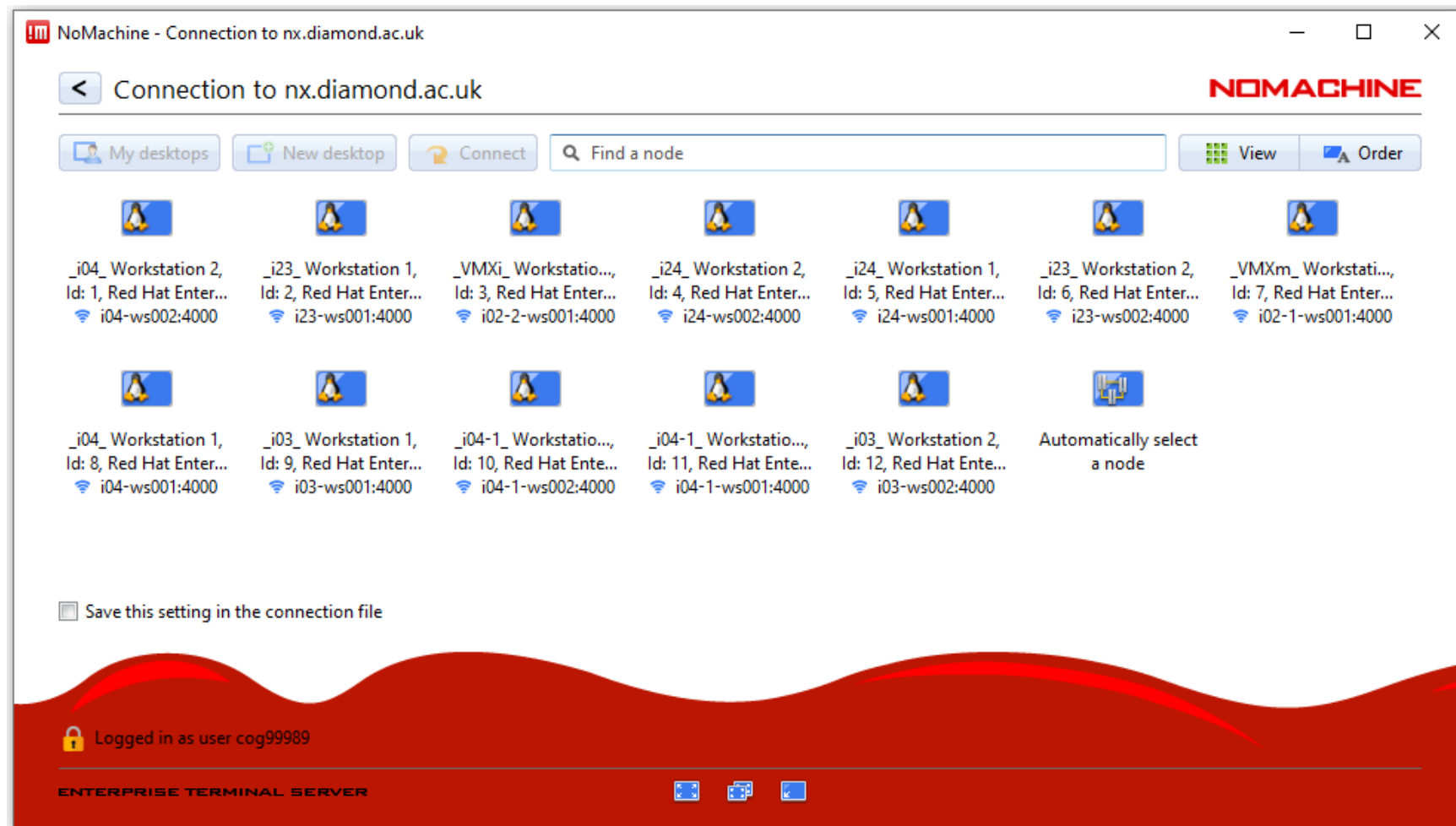


- Create a new connection using the protocol NX
- Set hostname to nx.diamond.ac.uk (ensure port is set to 4000)
- Use password authentication
- Don't use a proxy
- Give a name to the new connection, e.g. "Connection to nx.diamond.ac.uk"

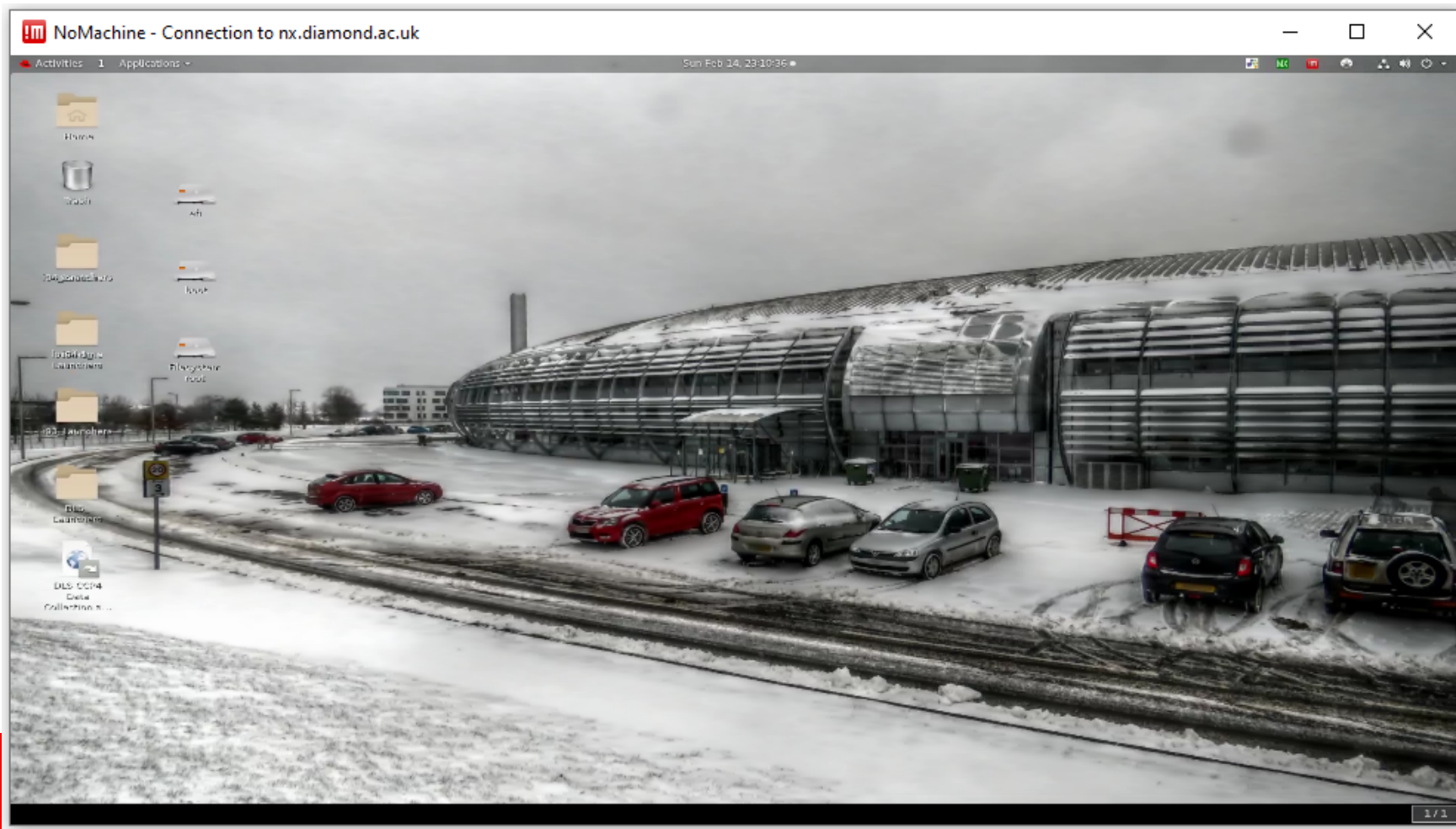
Create New Virtual Desktop



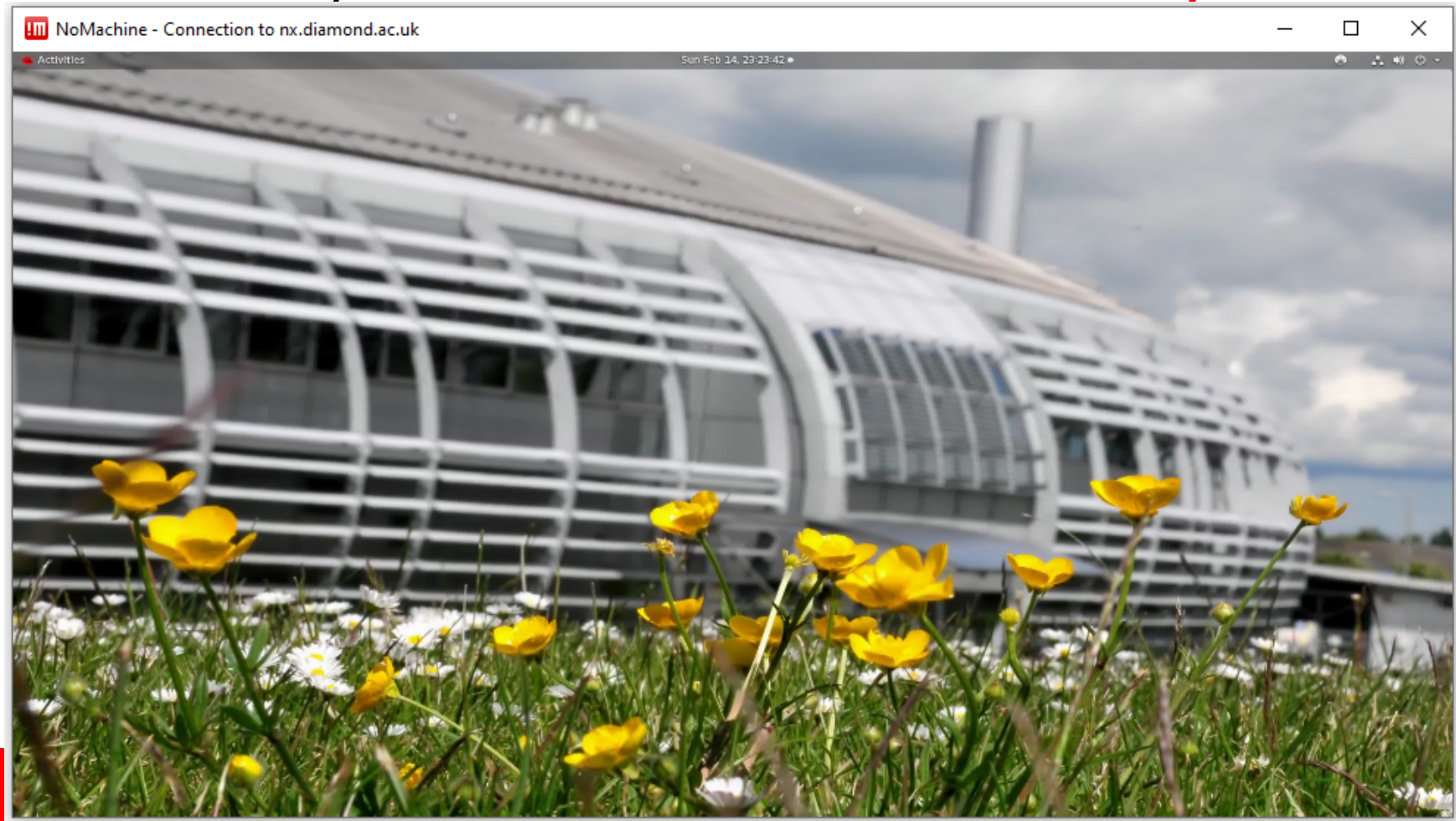
Connecting to NoMachine



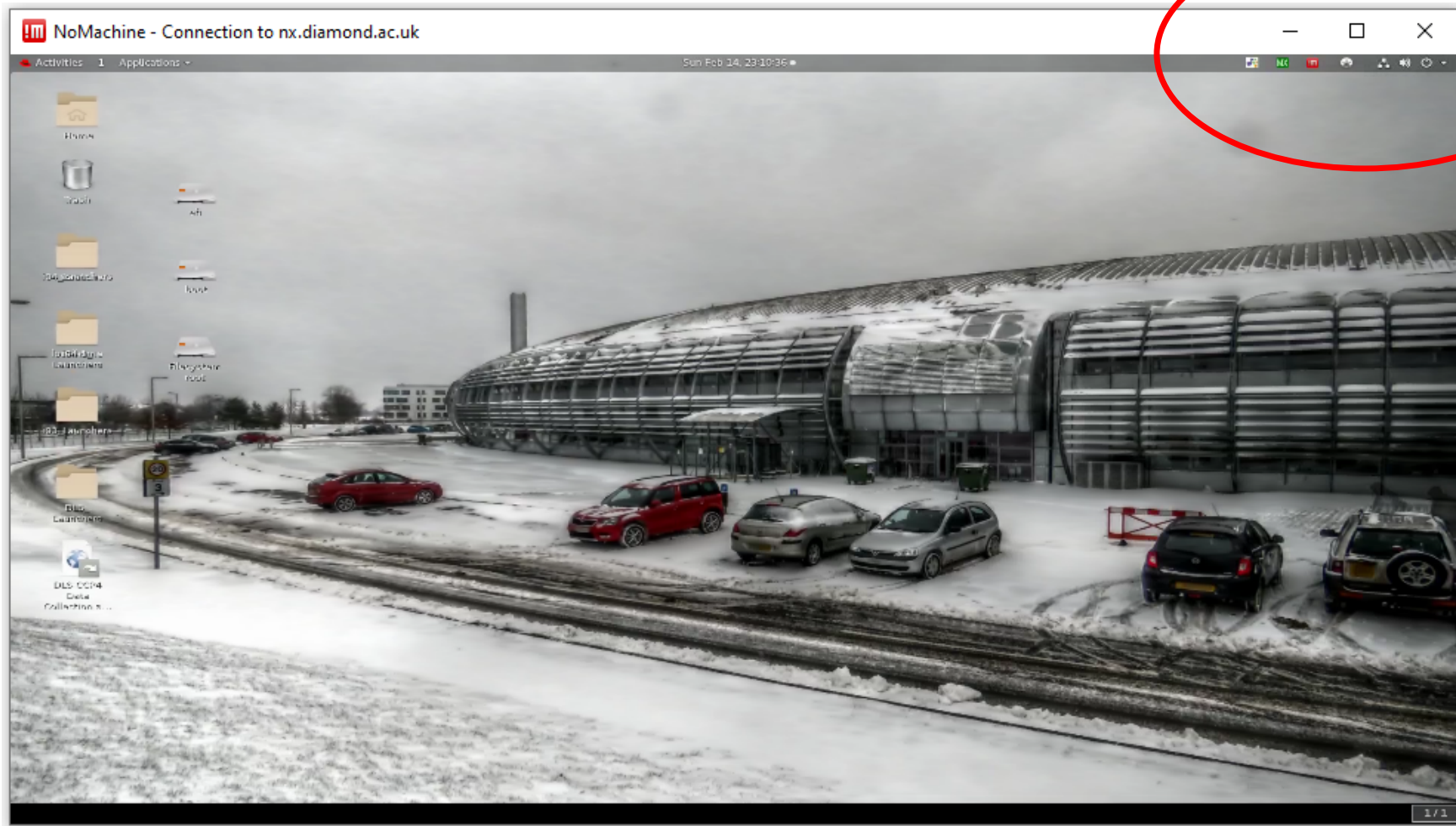
Connecting to a Beamline – **only for a visit**



Automatically select a node – all data processing

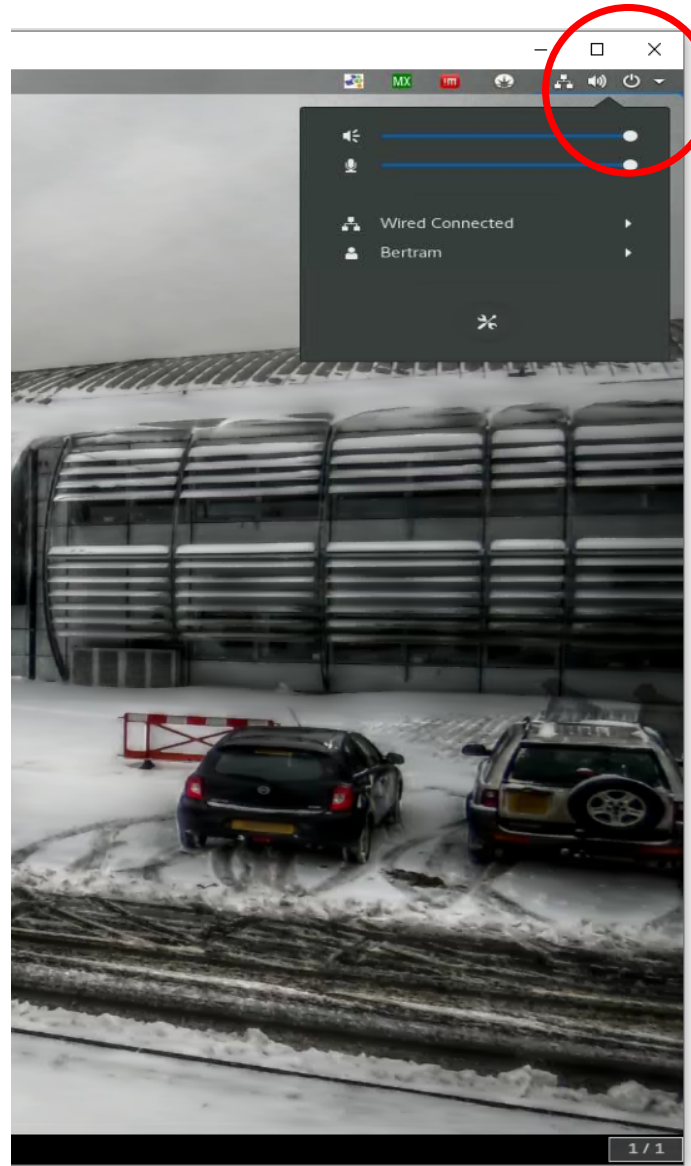
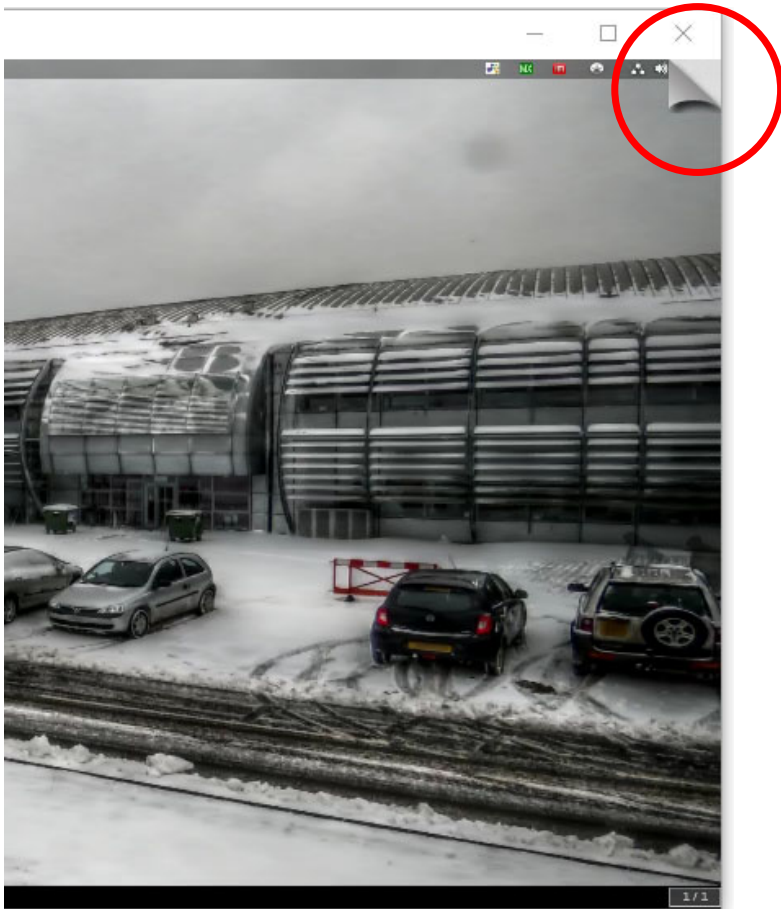


Beamline Navigation & Tools



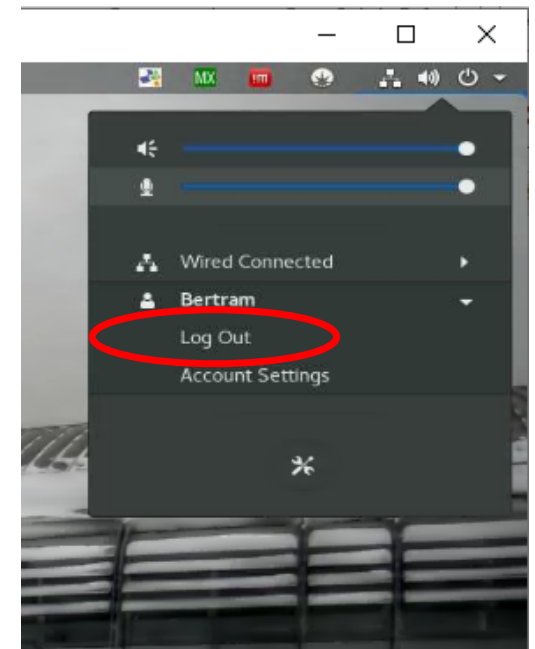
Logging Off

NX Settings – “corner peel”

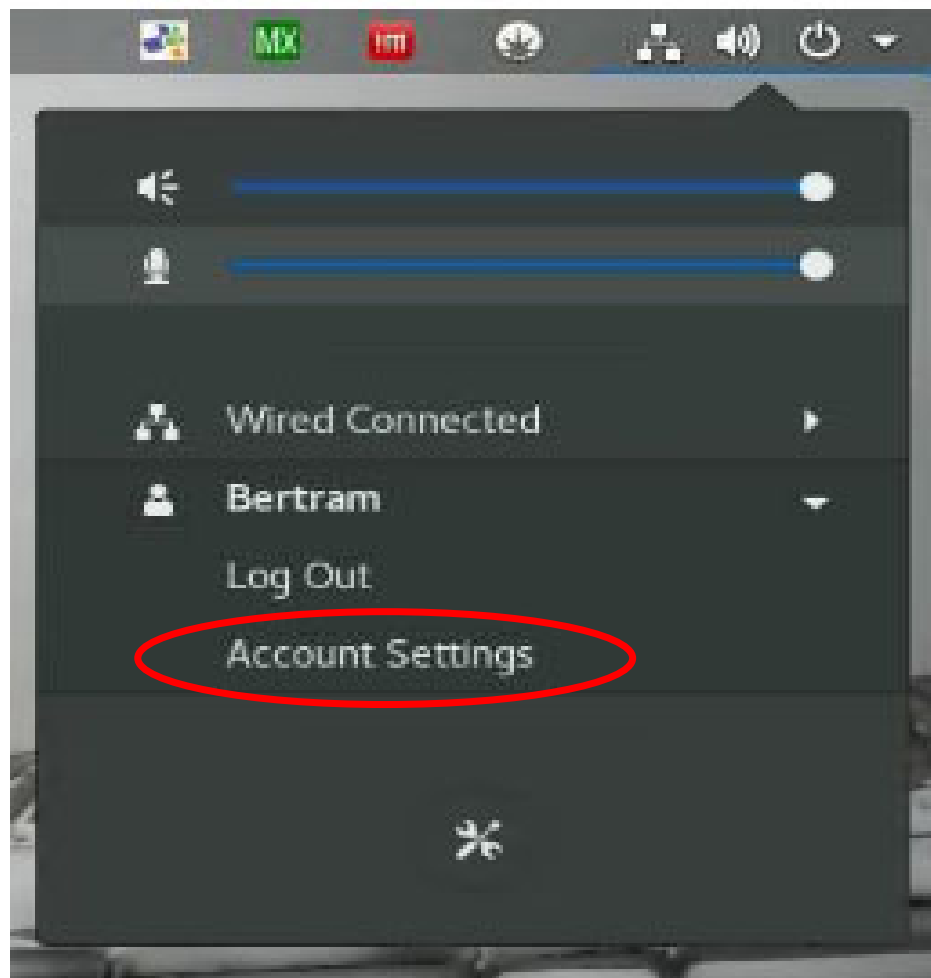


Log off:

- power button
- then click your name
- Then click “Log Out”

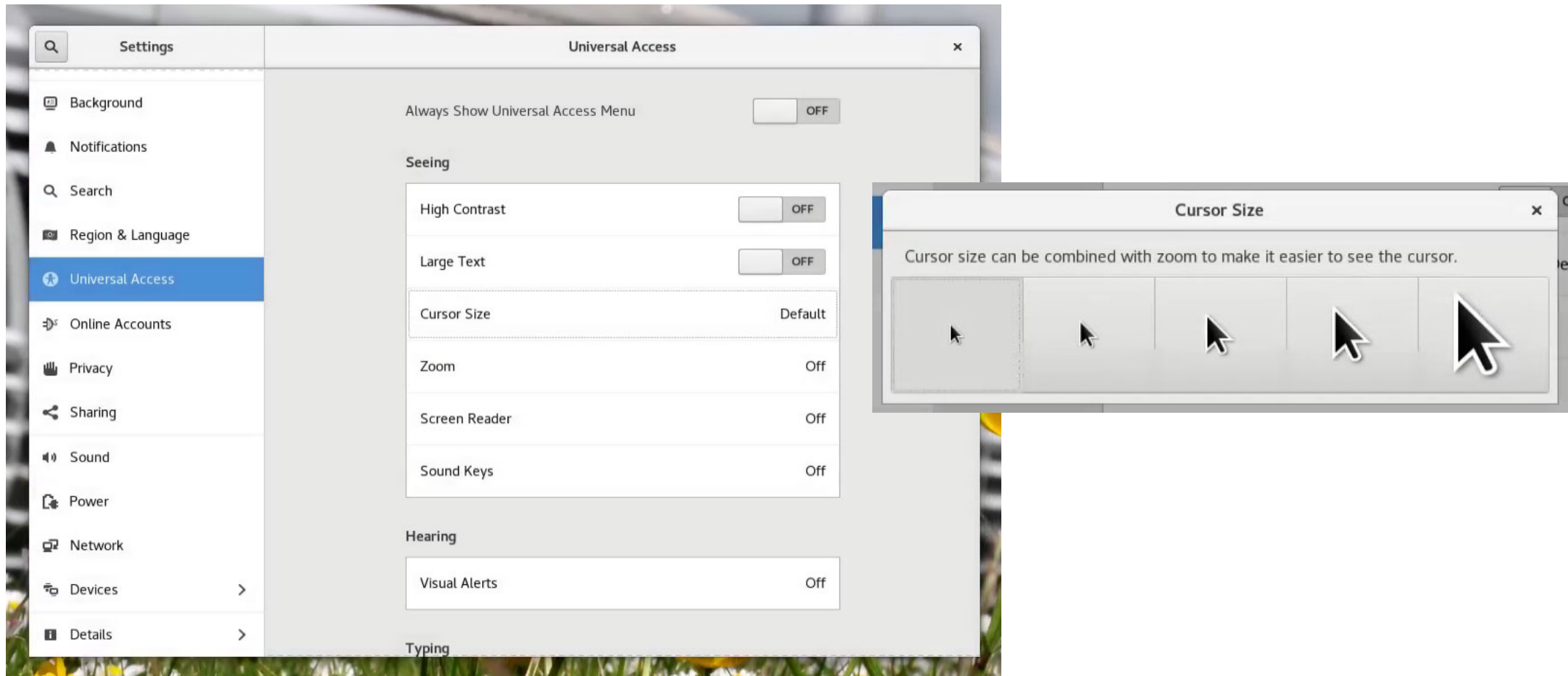


Account Settings



Universal Access

- use to increase the size of the cursor



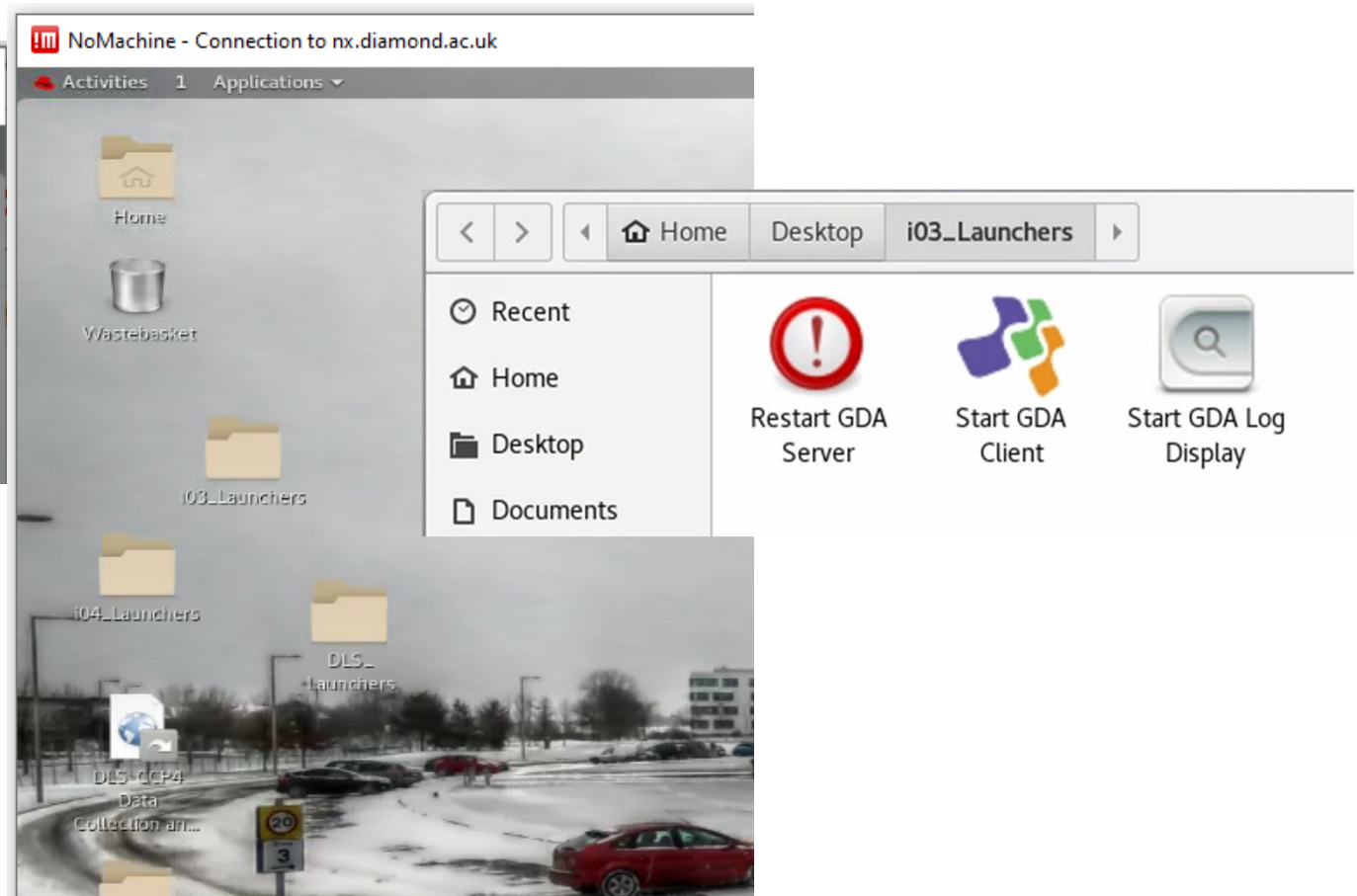
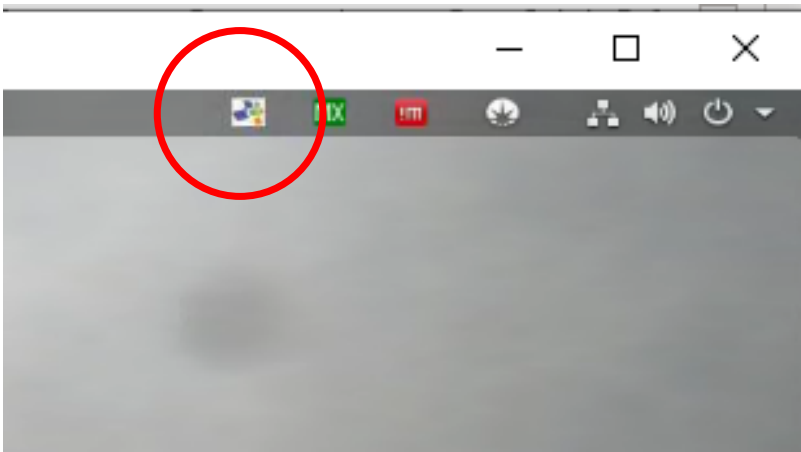
Nomachine Display Options



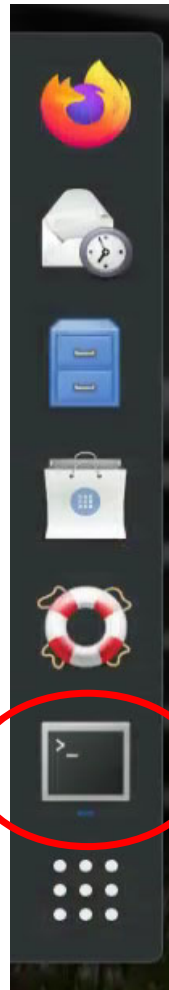
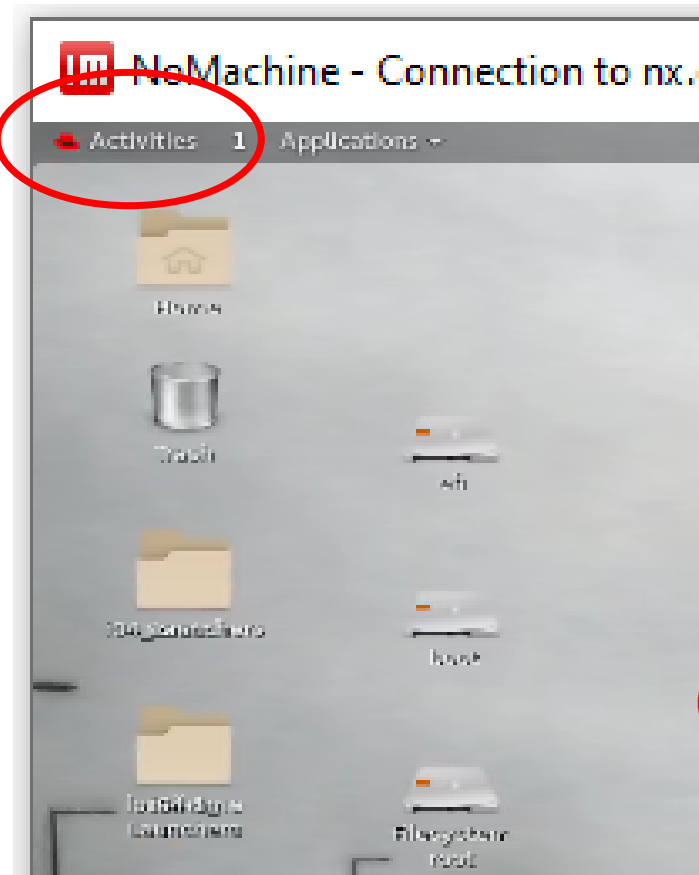
- “Enable viewport display” = Scrolling window (annoying)
- **“Scale to window” = Fits in window, everything shrinks when window shrinks**
- “Resize remote display” = Fits in window, icons remain large if window shrinks
- “Fullscreen” = window is maximised on current monitor
- “Fullscreen on all monitors” = windows are maximised on all monitors
- “Iconise” = minimise (ctrl + alt + M also works)
- “Settings”

Launch GDA (Generic Data Acquisition)

- used to control beamlines and collect data



Launch GDA from a terminal

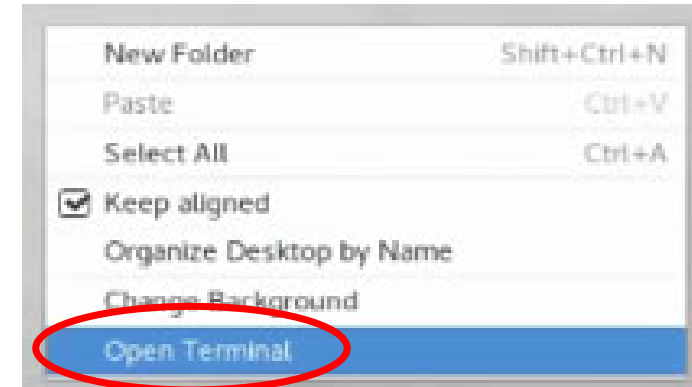


Start a terminal:

- Activities → Terminal
- Right-click → Open Terminal

In a terminal:

- **gdaclient** – start GDA client
- **gdalog** – start GDA log display
- **Gdaservers** – restart GDA servers



This Course - Identifiers

- All visits at Diamond happen under a Proposal – the Proposal for this course is **mx37045**
- For the purposes of teaching, we have already had a visit on this proposal for you to find some exemplar data – **mx33300-1**
- There will be additional visits for this course, such as for each of the beamline days (one for I03, one for I04 and one for I04-1), and to give you access to the tutorials etc., which will be numbered -2, -3, -4...

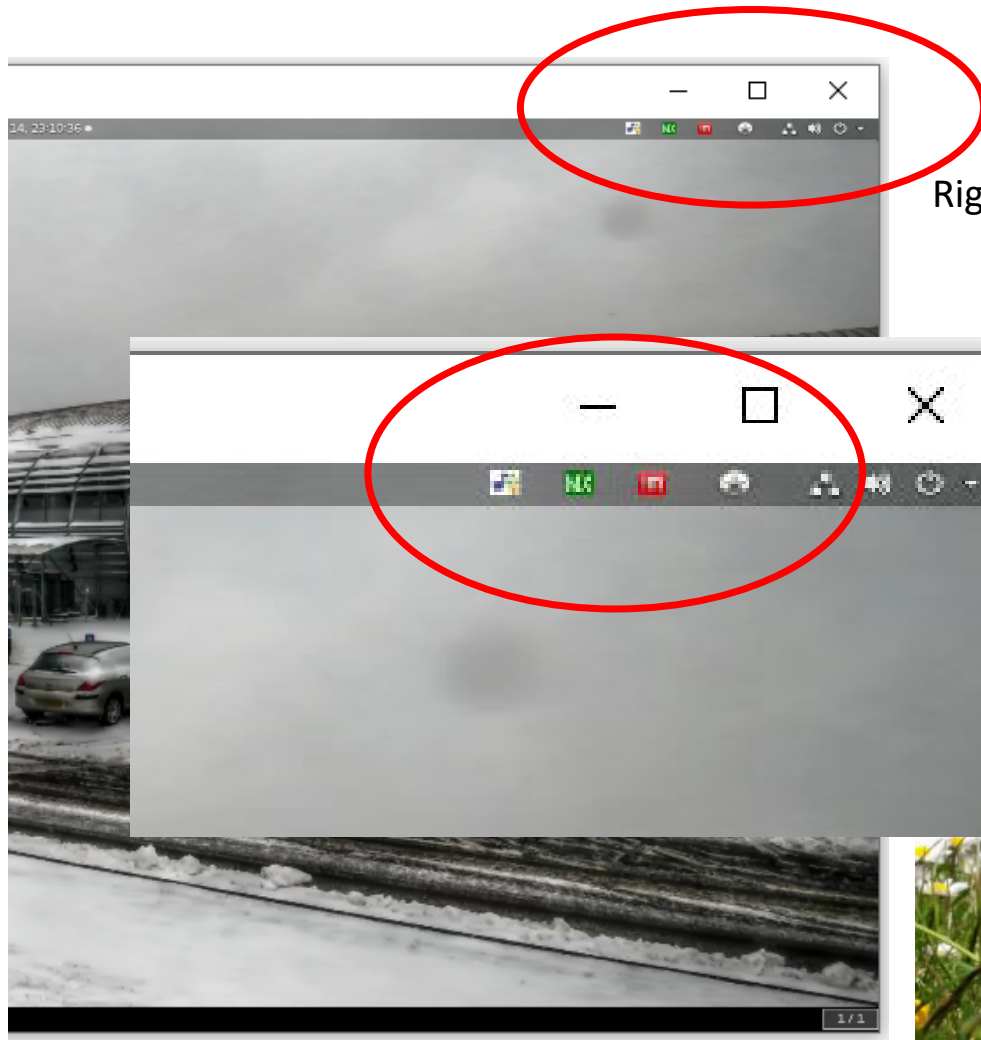
This Course - Identifiers

- mx37045-1 – today's visit for you to practice in & check access (I03)
- mx37045-2 – long visit (6th Nov – 6th Dec) to cover the whole course, with “data access only” for the participants to ensure access
- mx37045-3 – 27th Nov = beamline day on I03
- mx37045-4 – 27th Nov = beamline day on I04
- mx37045-5 – 27th Nov = beamline day on I04-1
- mx37045-6 – 27th Nov = beamline day on I24
- mx37045-7 – 27th Nov = beamline day on I23
- mx37045-8 – 27th Nov = beamline day on VMXm
- Visits for VMXi are actually crystallisation trays, not time-periods so these will be created for this

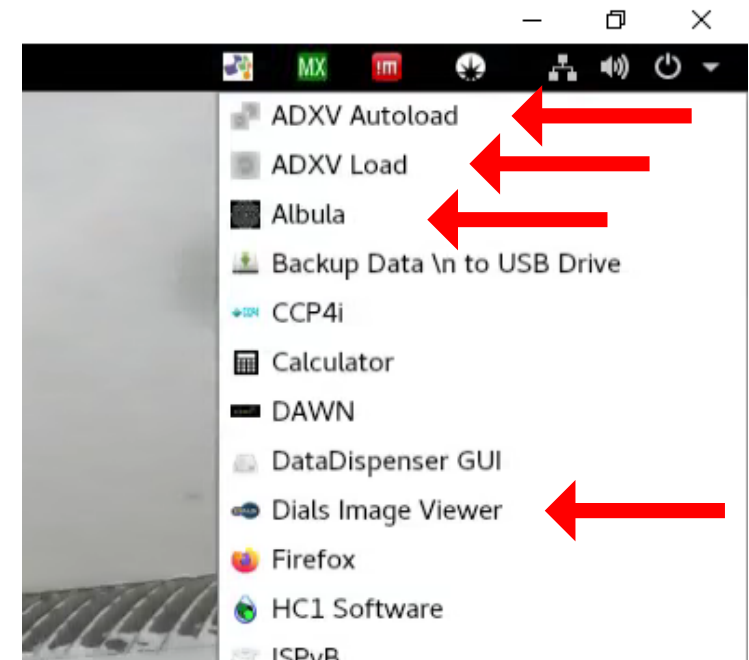
Data Collection Setup in GDA

- By default, data is stored in folders representing visits, with this structure:
- /dls/{beamline}/data/{year}/{visit number}
 - E.g. /dls/i03/data/2021/MX28204-5
- Then within that the default is:
 - /{proteinacronym}/{samplename}_{run_no}_{image_no}.cbf
- For large visits with multiple Users, or if you have multiple proteins, you can add **YourName/** to the left of the folder field
 - E.g. /dls/i03/data/2021/MX28204-5/**Felicity**/MyProtein/ProteinWT_1_3600.cbf

Image Viewers



Right-click



ISPyB View

Home

Calendar

Logout

diamond

Logistics

Stats

Fault Reports

Data Collections

i03

mx30951-8

Proposals

mx30951

Projects

Unit Cell Search

Feedback

Help (Off)

Data Collections for mx30951-8 on i03

This visit is inactive and will not auto update | Auto Refresh ☐ Refresh

Assign Containers

Summary

Auto Processing

Visit Stats

Users

Dewars

Sample Changer

Reprocessing

Beamline Status

Data Collections

Grid Scans

Full Collections

Auto Integrated

Processing Errors

Screenings

Edge Scans

MCA Spectra

Robot Actions

Sample Actions

Favourites

15

Page

<

<

1

2

3

4

5

6

7

8

9

>

>

18-11-2021 12:48:58 - gw/20211118/TestInsulin/ins_16/ins_16_2_master.h5

Sample: ins_16

Flux: 5.23e+11

Ω Start: -720.0°

Ω Osc: 0.10°

Ω Overlap: 0°

No. Images: 14400

Resolution: 1.51Å

Wavelength: 1.2399Å

Exposure: 0.004s

Transmission: 4.98%

Beamsize: 80x20µm

Type: SAD

Comment: (-209,332,-256) Xray centring boxes: ['27.2s (0s)', 340, '16.6s (0s)', 49]. Aperture: Large

Auto Processing

xia2 3dii: ✓

xia2 dials: ✓

fast_dp: ✓

autoPROC: ✓

xia2 multiplex: ✓

autoPROC+STARANISO: ✓

Downstream Processing

fast_ep: ✓

MrBUMP: 3x ✓

18-11-2021 12:48:33 - xraycentring/gw/20211118/TestInsulin/ins_16/ins_16_4_master.h5

Sample: ins_16

Ω Start: 300.0°

ϕ : 0° χ : -0.00038°

Resolution: 4.94Å

Wavelength: 1.2399Å

Exposure: 0.004s

Transmission: 31.17%

Beamsize: 20x20µm

Boxsize: 20x5µm

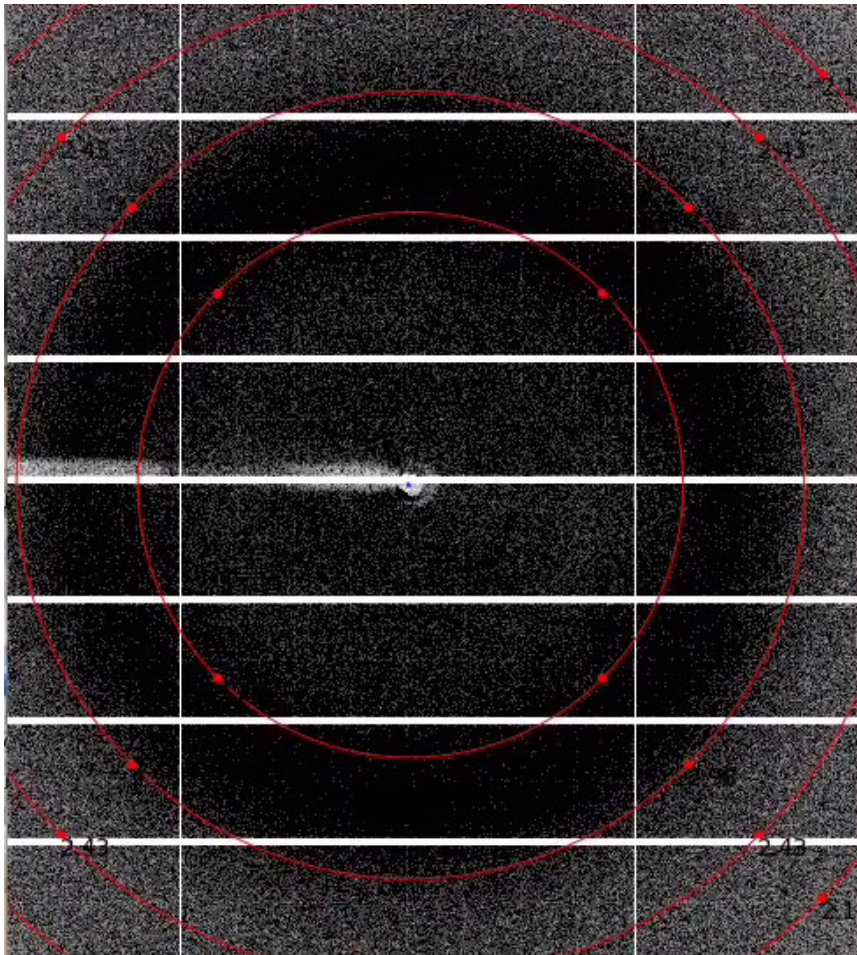
Comment: Xray centring - Diffraction grid scan of 1 by 80 images, Top left [421,123]. Bottom right [422,604]

Resolution: 0Å

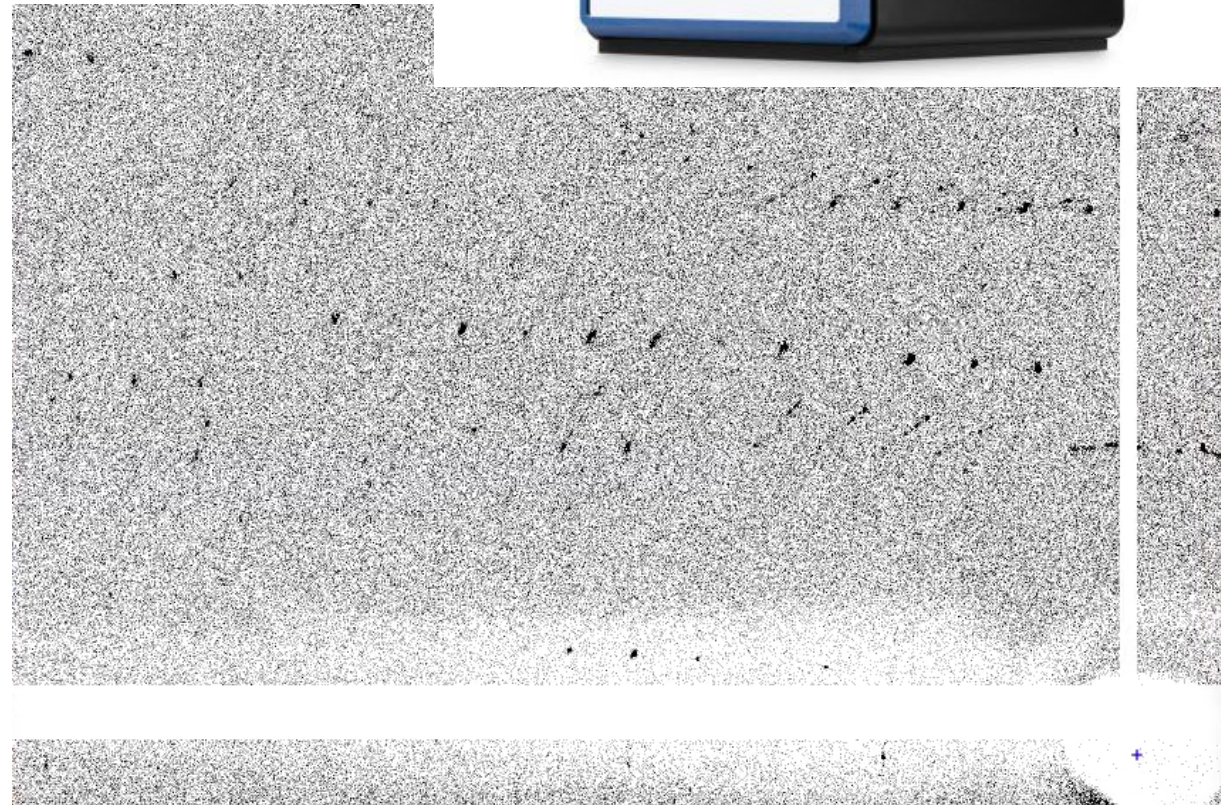
Click on the grid to load a diffraction image

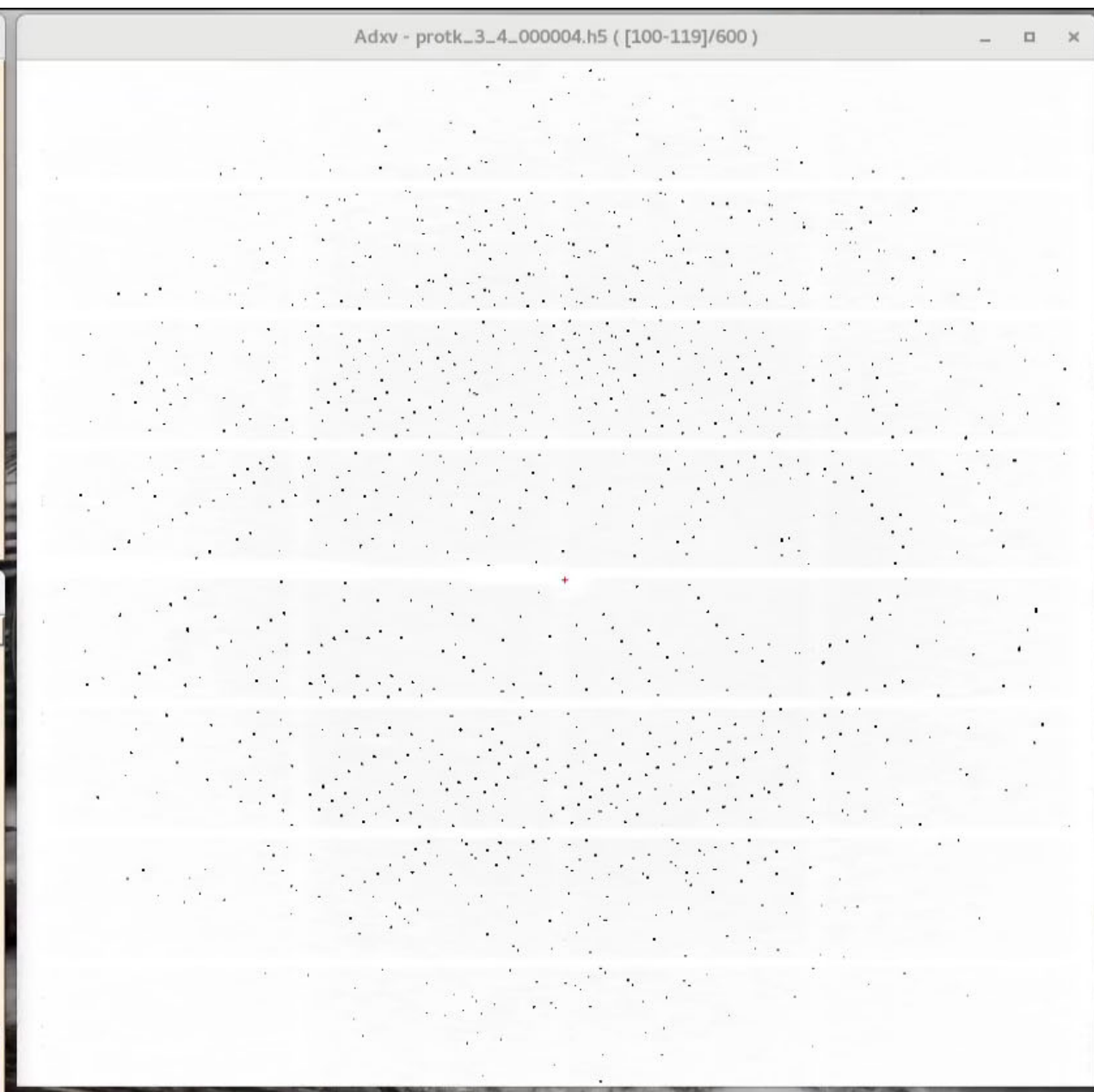
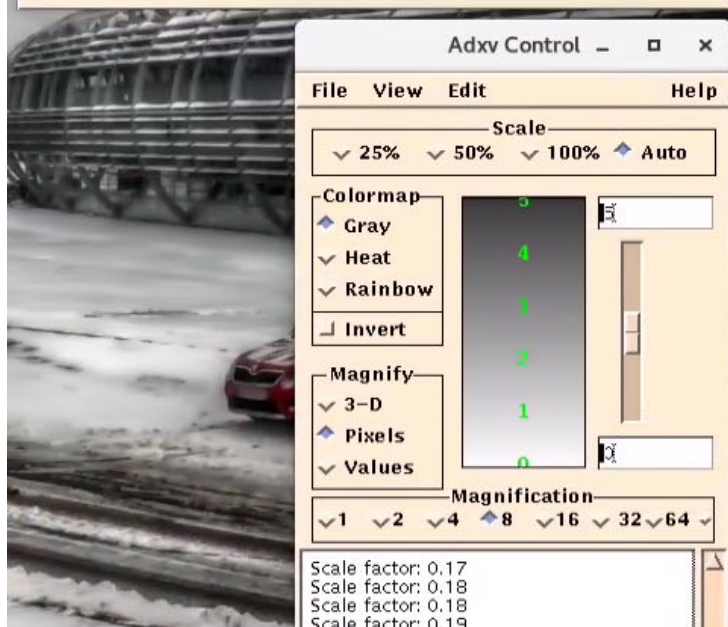
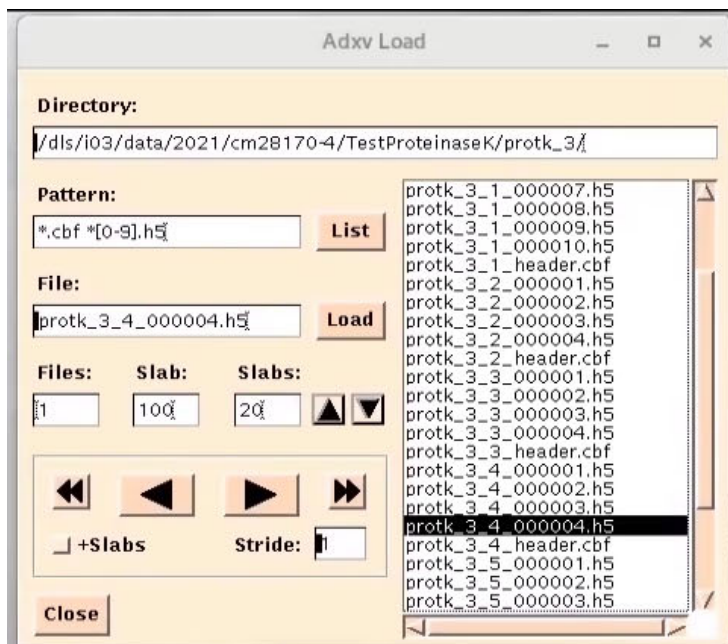
Threshold: ☐ Bragg

Dials Image Viewer or ADXV

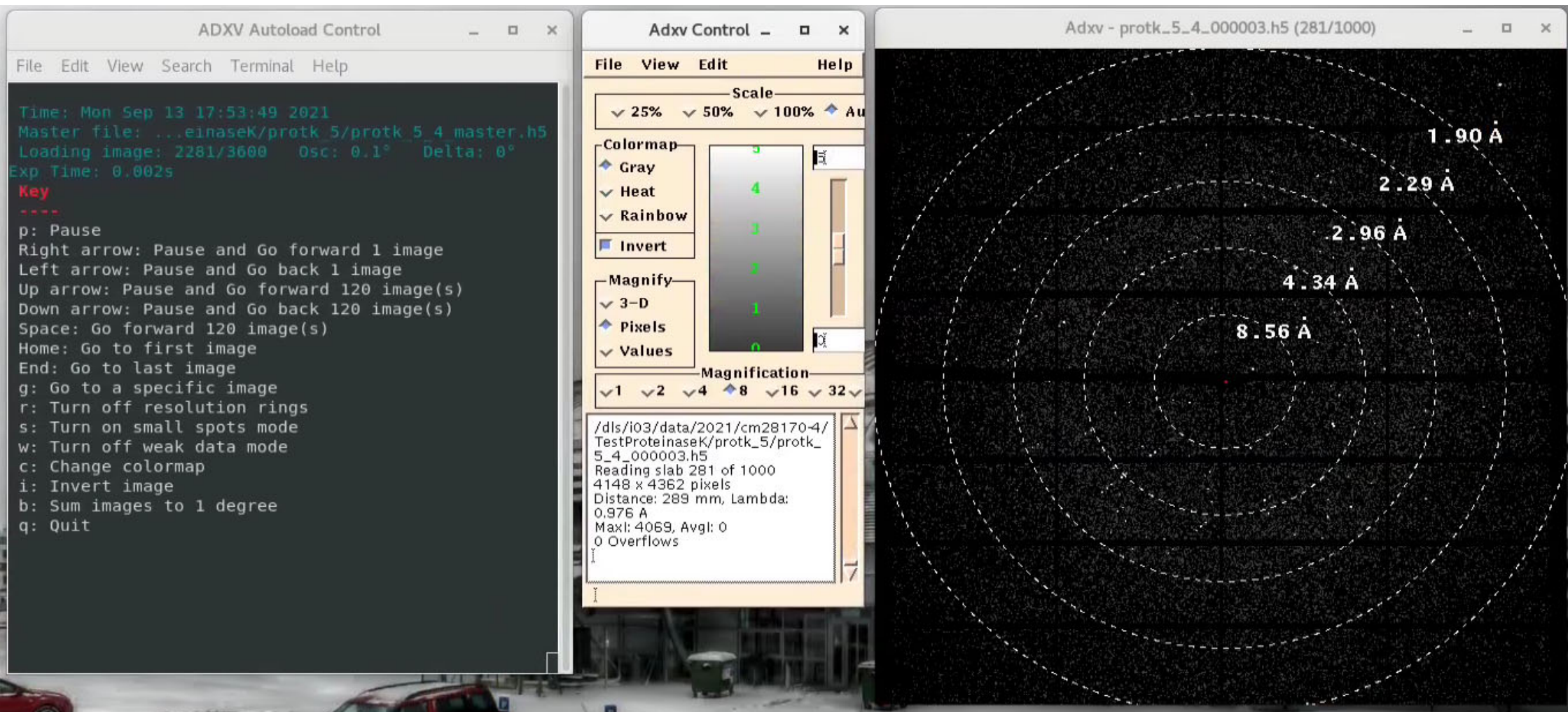


Not ISPyB



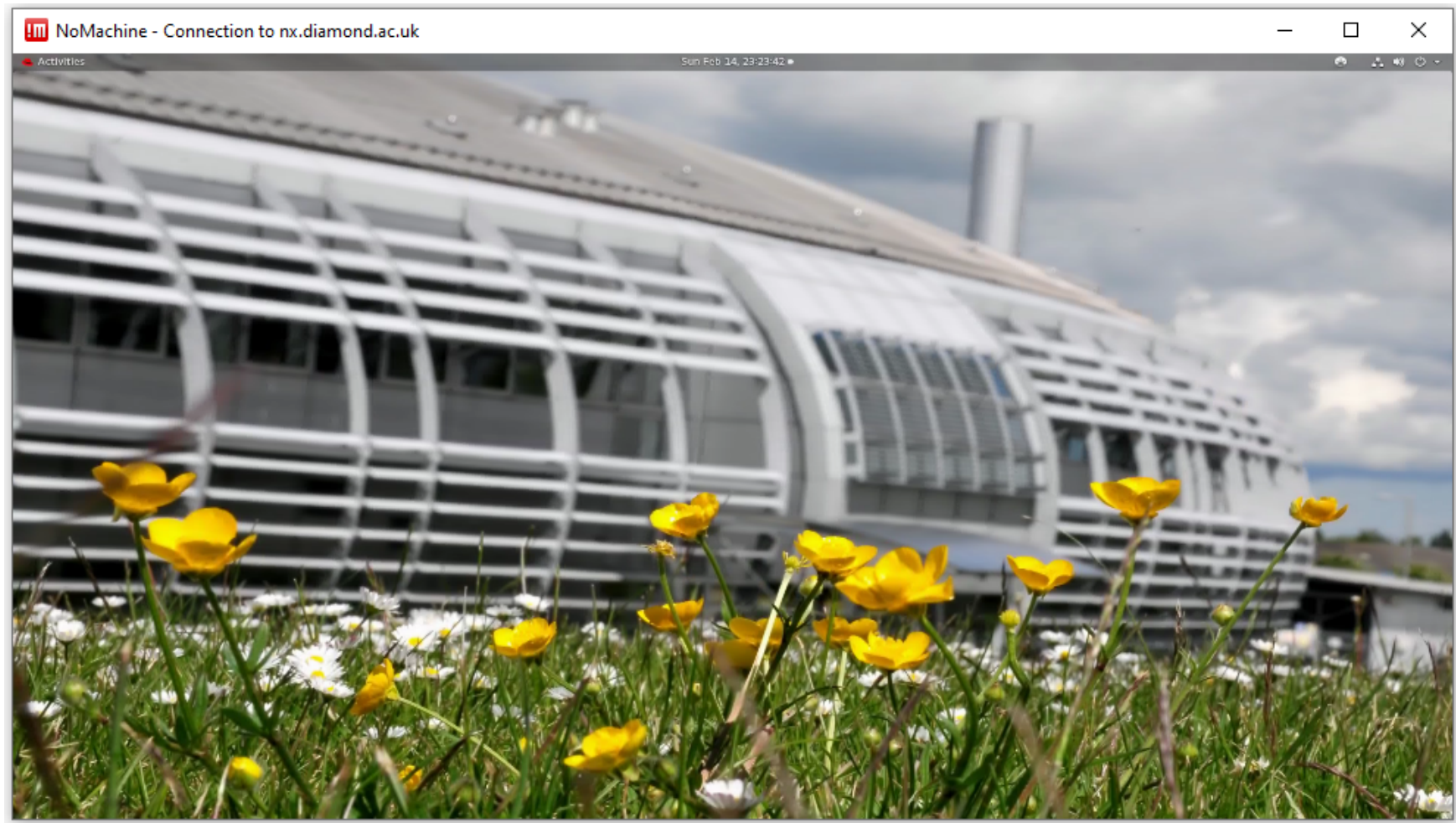


ADXV Autoload



Remote Data Processing

Remember: Work here, not on a beamline workstation



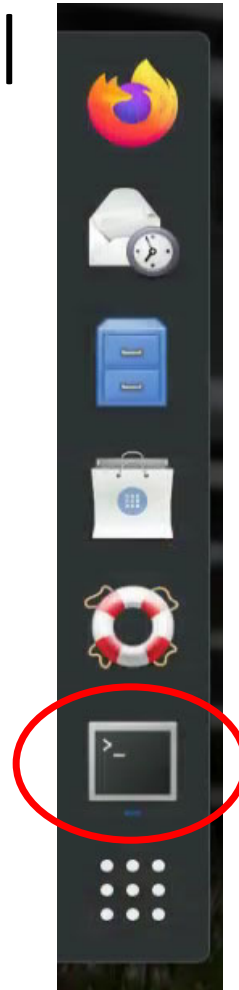
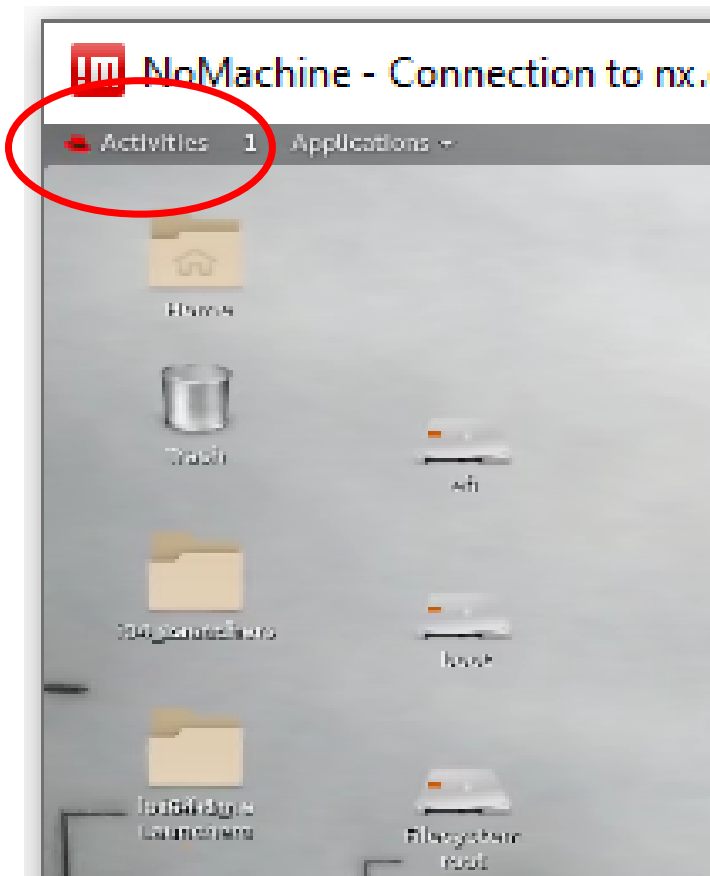
DON'T PROCESS DATA IN YOUR HOME DIRECTORY – IT IS TINY

WHEN IT GETS FULL YOU WON'T BE ABLE TO LOG IN TO DELETE THE
DATA THAT IS STOPPING YOU LOGGING IN AND IT CAUSES PROBLEMS

Error: Cannot create session directory: /home/abc12345/.nx/node/C-
cs05r-sc-serv-08.diamond.ac.uk-1023-
CC896785C4A9B79013D614E113768B6B

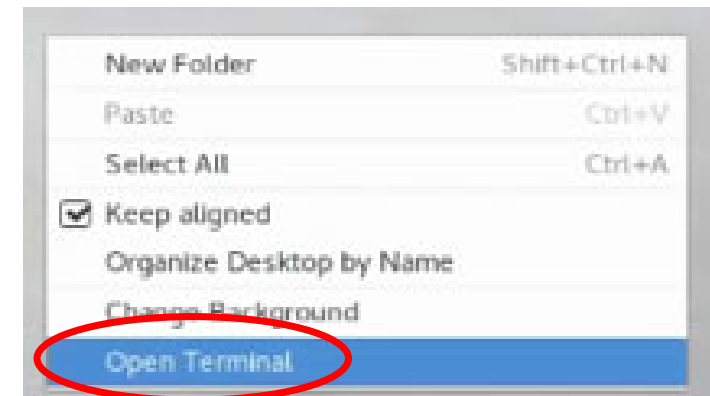
Error is: Disk quota exceeded

Launch a Terminal



Start a terminal:

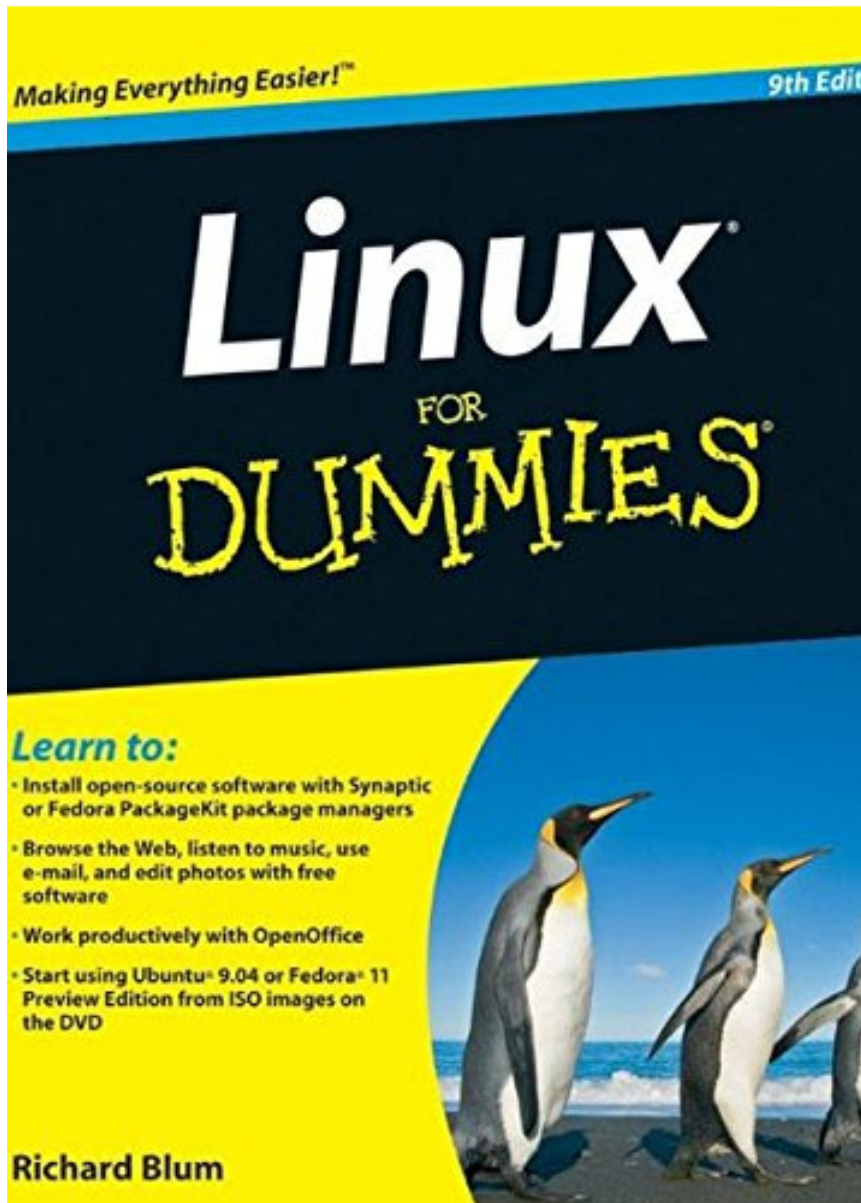
- Activities → Terminal
- Right-click anywhere (on beamline)
→ Open Terminal



Using the Command Line

- The Command line is more powerful than a GUI, and there will always be a Command line (not everything is packaged into a GUI)
- You can build on basic Command line work with scripts to run tasks more efficiently
- BUT get one character wrong and it won't work...





“Folders” = “Directories”

Linux Cheat-Sheet – on Slack

Linux cheat sheet and Diamond working directory

- man – gives manual
for command
- Grab someone for a tutorial
if you need it

NOTE: do NOT use spaces in file names

NOTE: commands are case sensitive

NOTE: Do not work in your home directory: /home/my_fedid !!!

NOTE: Location in file system

module load ccp4-workshop

Computer name	Location	User name	Prompt
Melanies-MacBook-Air	~	melanievollmar	\$
Melanies-MacBook-Air	Users	melanievollmar	\$
Melanies-MacBook-Air	/	melanievollmar	\$

Command	options	What it does
Help		
man	ls	Loads manual page for ls command
Navigation		
pwd		Print working directory → tells you where you are; which folder you are in
cd		Change directory; and gets

Linux - Continued

NOTE: do NOT use spaces in file names

NOTE: commands are case sensitive

NOTE: Do not work in your home directory: /home/my_fedid !!!

NOTE: Location in file system

module load ccp4-workshop

Computer name	Location	User name	Prompt
↓	↓	↓	↙
Melanies-MacBook-Air:	~	melanievollmar	\$
Melanies-MacBook-Air:	Users	melanievollmar	\$
Melanies-MacBook-Air:	/	melanievollmar	\$

Linux man = Manuals

- Example **man ls**
- **Enter** = move down 1 line
- **Space** = move down 1 page
- **g** = move to the top of the page
- **G** = move to the bottom of the page (one of the few times you use a capital)
- **Q** = quit

Linux tree

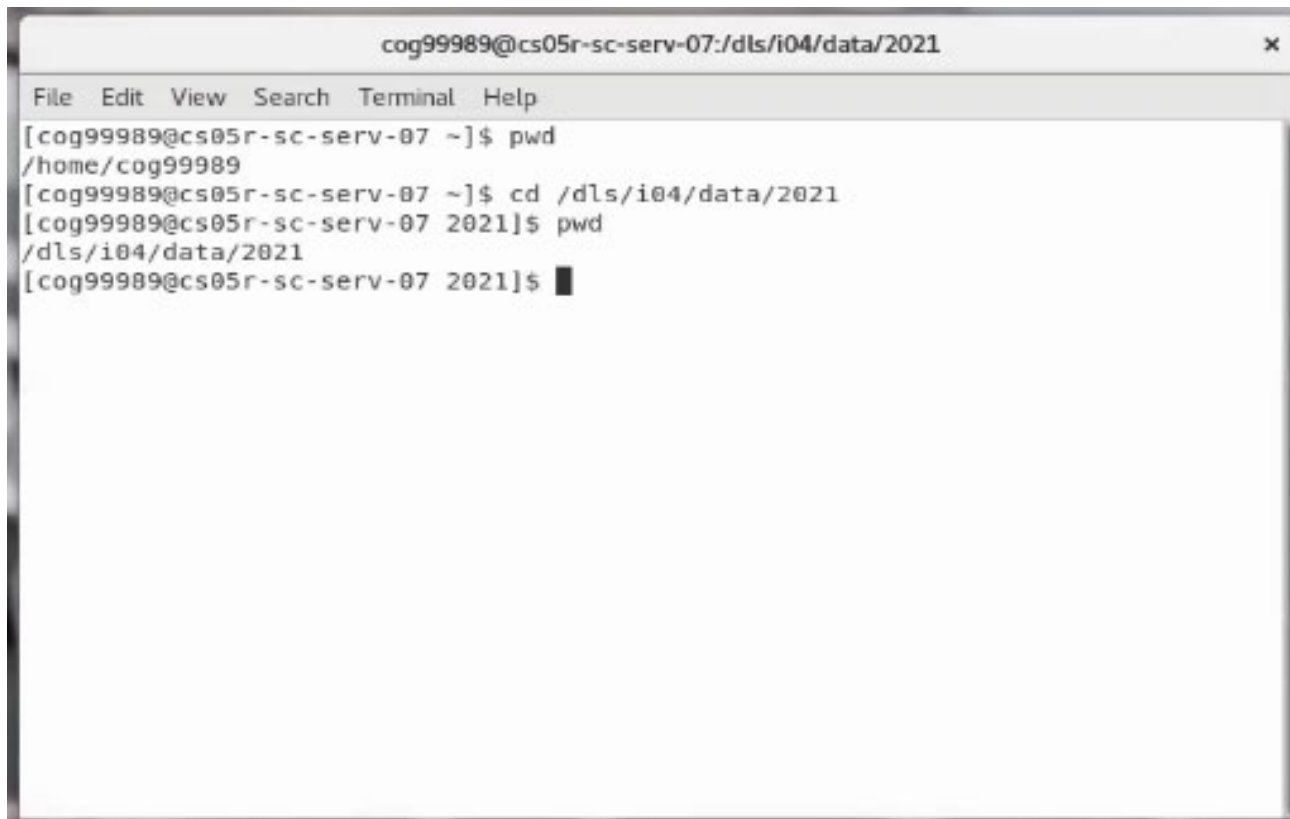
- tree -d

- tree

```
cog99989@cs05r-sc-serv-07:/dls/i04/data/2021/cm28182-1/TestInsulin
File Edit View Search Terminal Help
[cog99989@cs05r-sc-serv-07 TestInsulin]$ tree -d
.
├── ZincInsulinB3
├── ZincInsulinB4
└── ZincInsulinB5

3 directories
[cog99989@cs05r-sc-serv-07 TestInsulin]$ tree
.
├── ZincInsulinB3
│   ├── ZincInsulinB3_1_000001.h5
│   ├── ZincInsulinB3_1_000002.h5
│   ├── ZincInsulinB3_1_000003.h5
│   ├── ZincInsulinB3_1_000004.h5
│   ├── ZincInsulinB3_1_header.cbf
│   ├── ZincInsulinB3_1_master.h5
│   ├── ZincInsulinB3_1_meta.h5
│   ├── ZincInsulinB3_1.nxs
│   ├── ZincInsulinB3_2_000001.h5
│   ├── ZincInsulinB3_2_000002.h5
│   ├── ZincInsulinB3_2_000003.h5
│   └── ZincInsulinB3_2_000004.h5
```

Linux pwd

A terminal window titled 'cog99989@cs05r-sc-serv-07:/dls/i04/data/2021'. The window has a menu bar with 'File', 'Edit', 'View', 'Search', 'Terminal', and 'Help'. The terminal shows the following commands and output:

```
[cog99989@cs05r-sc-serv-07 ~]$ pwd
/home/cog99989
[cog99989@cs05r-sc-serv-07 ~]$ cd /dls/i04/data/2021
[cog99989@cs05r-sc-serv-07 2021]$ pwd
/dls/i04/data/2021
[cog99989@cs05r-sc-serv-07 2021]$
```

- pwd = Print Working Directory
- By default you start in your home directory **BUT DON'T WORK IN IT** (apart from the basic Linux tutorial)
- cd /dls/{beamline}...

Navigating to data

```
cog99989@cs05r-sc-serv-07:/dls/i04/data/2021/cm28182-1 x
File Edit View Search Terminal Help
[cog99989@cs05r-sc-serv-07 ~]$ cd /dls/i04/data/2021
[cog99989@cs05r-sc-serv-07 2021]$ ls
cm28182-1  in27057-6  mx19880-86  mx23694-52  mx25680-14  sw26339-9
cm28218-4  in27057-7  mx19884-13  mx24948-59  mx28114-1   sw26366-12
cm28218-5  in27060-1  mx19946-389 mx25108-29  mx28114-2   sw26527-11
in20015-87 in27061-5  mx20303-41  mx25108-30  mx28114-3   sw26527-12
in20015-88 in27062-5  mx21426-84  mx25108-31  nr27313-11  sw26527-13
in20015-89 in27062-6  mx21426-85  mx25108-32  nt28182-1   sw26527-14
in20015-90 in27062-7  mx21657-47  mx25402-34  nt28218-4   sw27105-6
in20015-91 in28247-1  mx23248-12  mx25402-35  nt28218-5   sw27105-7
in26774-63 mx19248-75 mx23269-47  mx25402-36  sw23392-19  sw28220-1
in26907-10 mx19880-85 mx23620-68  mx25402-38  sw24950-17
[cog99989@cs05r-sc-serv-07 2021]$ cd cm28182-1
[cog99989@cs05r-sc-serv-07 cm28182-1]$ ls
20210114      20210125  beamcentre
20210114_14_55_06.dat  20210126  beamline_setup
20210114_14_55_06.html 20210127  fluorescence_scans
20210114_14_55_06.mca  20210128  GDAUserOptions.xml
20210114_14_55_06.png  20210129  HG526_H3d2_2
20210114_14_58_37.dat  20210202  jpegs
20210114_14_58_37.html 20210203  processed
20210114_14_58_37.mca  20210204  processing
20210114_14_58_37.png  20210205  screening
20210114_15_36_18.dat  20210209  SeMet1.fluo
20210114_15_36_18.html 20210210  SeMet2.fluo
20210114_15_36_18.mca  20210211  spool
20210114_15_36_18.png  20210212  TestInsulin
20210114_15_41_47.dat  75383.dat  TestLysozyme
20210114_15_41_47.html 75384.dat  TestProteinaseK
20210114_15_41_47.mca 75385.dat  TestThermolysin
```

Deleting files – rm (ReMove)

- Proceed with caution
 - there is no recycle bin or undo
- `rm file.img`
 - Command will delete file.img
- You can also inadvertently delete files by over-writing them with a new file with the same name



Permissions

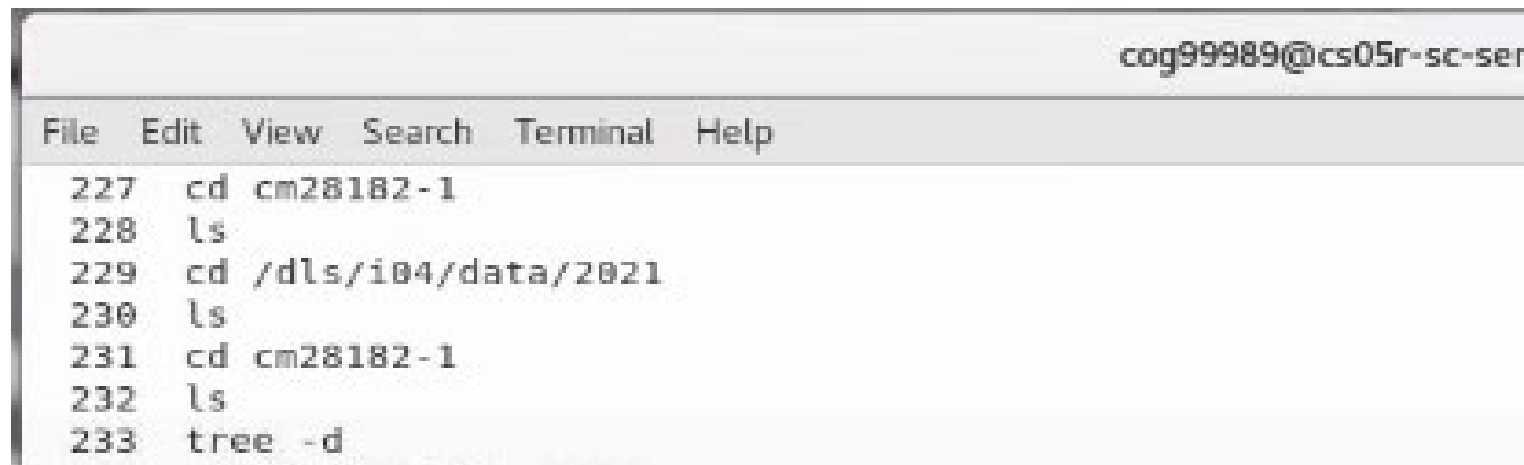
- `ls -l`

```
-rw-rw-r--. 1 cog99989 cog99989      74 Sep 18 2020 bashrc_local
drwxrwxr-x. 4 cog99989 cog99989    4096 Sep 23 15:04 cs-studio
drwxr-xr-x. 3 cog99989 cog99989    4096 Dec  4 2019 DepositFiles
drwxr-xr-x. 7 cog99989 cog99989    4096 Nov 21 09:25 Desktop
drwxr-xr-x. 3 cog99989 cog99989    4096 Aug 18 10:10 Documents
drwxr-xr-x. 2 cog99989 cog99989    4096 Aug 11 14:33 Downloads
drwxrwxr-x. 5 cog99989 cog99989    4096 Mar 10 2020 eclipse-workspace
```

- First character = file (-) or directory (d)
- Next 3 characters – permission of the owners
 - r = read permission
 - w = write permission
 - x = execute permission
- Characters 5-7 – permission of the group
- Characters 8-10 – permission of others

History

- history = gives history of most recent commands
 - Great if someone has shown you something, and you have forgotten what process they followed to do it!

A screenshot of a terminal window. The title bar at the top right shows the user 'cog99989@cs05r-sc-ser'. Below the title bar is a menu bar with 'File', 'Edit', 'View', 'Search', 'Terminal', and 'Help'. The main area of the terminal displays a list of commands with their corresponding line numbers: 227 cd cm28182-1, 228 ls, 229 cd /dls/i04/data/2021, 230 ls, 231 cd cm28182-1, 232 ls, and 233 tree -d.

```
cog99989@cs05r-sc-ser
File Edit View Search Terminal Help
227 cd cm28182-1
228 ls
229 cd /dls/i04/data/2021
230 ls
231 cd cm28182-1
232 ls
233 tree -d
```


Linux Tutorial – Navigating the Diamond Cluster

AIMS

The aim of this tutorial is to get a novice Linux User up to speed at navigating the Diamond cluster and getting started with data processing. Feel free to skip over anything that you already know and remember that there is often more than one way to achieve the same process.

Remember that commands are case-sensitive and are almost always in lower-case. In this tutorial, anything that is for you to type is written in bold such as the **tree** command here.

Please experiment! (we are scientists after all) – if you accidentally set off something that takes a long time, all you need to do is **Ctrl + C** and that will halt the current command. If you can suggest ways to improve this tutorial, please don't hesitate to contact me – felicity.bertram@diamond.ac.uk

TO START

Once in an NX session, open a terminal, either by:

- Clicking on “Activities” in the top left corner of the screen, and then clicking on the Terminal icon which is the 5th option down (a black box with a >_ in it – hover over an icon and it will tell you what it is
- right-clicking anywhere on the background screen, and selecting “Open Terminal” from the menu that appears – though this option may only work on beamline computers

See my slides from my presentation for more information about how you do this.

FINDING YOUR DATA

To find your data, you need to navigate away from your home directory. To do this, you will need to use the “Change Directory” command, which is:

cd

In its simplest form, you can just navigate to where your data is, in this instance by typing:

cd /dls/i04-1/data/2021/mx29507-1 (note there is a space between the cd and the file path)

However, you will come across much more complex paths than this, and if you type one character wrongly, it won't work, and will return a “No such file or directory” message. Therefore, you want to be able to explore folder by folder. To move up one folder, in this instance from /home/your Fed ID you need to type:

cd .. (once again there is a space between the cd and the ..)

If you then use the **pwd** command again, it will tell you that you are now in /home (go on, try it). If you want to see what is in the /home folder then you can use the **ls** command once again (in this instance it will list all Fed IDs currently using that node). We want to go up again, so type **cd ..** once again. This should mean that when you use the **pwd** once again, the location is simply /. This is also called “root” as it is the top of the directories.

Remembering that the path for any data collected at Diamond is /dls/{beamline}/data/{year}/{visit number} you now want to navigate into /dls. To do this type:

cd dls (cd /dls also works)

pwd → this will show that you are in /dls now, not /

ls → this will show what folders there are in /dls – most are a list of lots of beamlines, not just MX

• “-” means “-l” (long listing) and “-a” means “-la” (long listing, including hidden files)

AUTOCOMPLETE

To set yourself up for the next step, type `cd ..` to take you back to `/dls/i04-1/data/2021`

When you are navigating, if you start to type an option, you can do a few letters, and then press tab to autocomplete. So if you start typing:

`cd mx29` and then press **[Tab]**

It will start to autocomplete – but I’ve set this up as a trick question as there are two proposals in that folder which start *mx29* – they are *mx29502-2* (not yours) and *mx29507-1* (yours). You can see these in the folder by using the `ls` command. Therefore the autocomplete will only take you as far as `cd mx2950` so if you hit **[Enter]** after that

CLEAR

If your terminal becomes clogged up with all this practicing, then you can wipe the slate clean with:

`clear`

You will find everything has vanished, and you can start again. But not from the beginning, as if you do `pwd` again, you will find that you are still in the folder that you had just navigated to. You just don’t have all the mess of switching around.

HISTORY

This command is particularly useful if someone has just shown you how to do something, and you need more time to make notes on it. Or if you have just used the `clear` command and want to check back on what you just did. Typing the command:

`history`

Produces a list of the history of commands on that session. Note that if you are working hard, you’ll end up with a very long list of commands. Therefore, you can use:

`history 10`

This gives you the most recent 10 commands (you can use any number here, where I have used 10)


Retrieve your data and take it home





- Better to download it within 40 days
- **Globus** – main option, datasets over 20 GB
- **FTP** – File Transfer Protocol, only for datasets under 20 GB
- **SFTP** – Secure File Transfer Protocol, if your institution firewall blocks FTP, only for datasets under 20 GB
- **rsynch** - Good for Unix-like systems like Linux - only recommended for experienced rsync users
- <https://www.diamond.ac.uk/Users/Experiment-at-Diamond/IT-User-Guide/Not-at-DLS/Retrieve-data.html>

Retrieve your data and take it home

- After 40 days...
- Your data will now be in the archive and need to be restored from tape
- Download files using Diamond's TopCAT software
- <https://www.diamond.ac.uk/Users/Experiment-at-Diamond/IT-User-Guide/Not-at-DLS/Retrieve-data.html>
- Note that files will be found here instead of the normal link:
 - /dls/staging/dls/\$instrument/data/\$year/\$visit
 - Not /dls/{beamline}/data/{year}/{visit number}


Have a look now...


 Help



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Types (2) ▾

Start date 

End date 

Search

For example "x-ray diffraction" or protein AND acid. See all [search options](#).


 Only the top 100 results will be displayed for each type










Display as cards

Clear filters

Visit 8

Dataset 0



Title Include 	Visit ID Include 	Name Include 	DOI Include 	Dataset Count	Beamline Include 	Start Date From...  To... 	End Date From...  To... 
▼ DLS/CCP4 worksh...	MX37045-1	MX37045		0	i03	2023-11-06	2023-12-06
▼ DLS/CCP4 worksh...	MX37045-2	MX37045		0	i04	2023-11-06	2023-11-07
▼ DLS/CCP4 worksh...	MX37045-3	MX37045		0	i03	2023-11-27	2023-11-28
▼ DLS/CCP4 worksh...	MX37045-4	MX37045		0	i04	2023-11-27	2023-11-28
▼ DLS/CCP4 worksh...	MX37045-5	MX37045		0	i04-1	2023-11-27	2023-11-28
▼ DLS/CCP4 worksh...	MX37045-6	MX37045		0	i24	2023-11-27	2023-11-28
▼ DLS/CCP4 worksh...	MX37045-7	MX37045		0	i23	2023-11-27	2023-11-28
▼ DLS/CCP4 worksh...	MX37045-8	MX37045		0	i02-1	2023-11-27	2023-11-28



Any questions...?

