Remote access to eBIC systems for data collection, analysis, session monitoring and data download

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Revision summary:	1) Change of folder structure 2) Information added on new security measures (only allowed 3 failed password attempts now before account is locked)
Comments to:	Lorna Malone
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Introduction

This document is intended as a guide for trained eBIC users to assist them in accessing eBIC systems using NoMachine (NX), initiating and montitoring on-the-fly processing via PATo and setting up their data download following a session at eBIC. The guide is principally aimed at the remote user but is applicable to on-site operation. The level of detail is targeted at a standard eBIC operator. The user is ultimately responsible for their use of eBIC and Diamond systems. If you are in doubt about an action you need to perform or are unable to progress, then please reach out to the eBIC Local Contact assigned to your session for assistance. Finally, please report any errors in this guide to your Local Contact or lorna.malone@diamond.ac.uk.

Please consult the following documentation for guidance on the set up of your data collection session: 'Remote EPU operation guide for eBIC microscopes' or 'Remote TOMO operation guide for eBIC microscopes'

Information box colour key

Information boxes are presented in green	Optional action instructions are presented in yellow
Terminal commands are presented in violet	

Getting prepared

Before your session you will need to ensure the following:
☐ You will be using a high speed and stable internet connection
☐ Check with your IT department that the traffic from NoMachine will not be blocked by any corporate firewall

You should also download (or update to the latest version) and set up the following:
☐ Microsoft Teams
☐ NoMachine

Finally, ensure that you know your fedID:
☐ Check your fedID (if you need any assistance or need to change your fedID password go to: https://www.diamond.ac.uk/Users/Experiment-at-Diamond/IT-User-Guide.html)

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1 Access eBIC microscopes using NoMachine

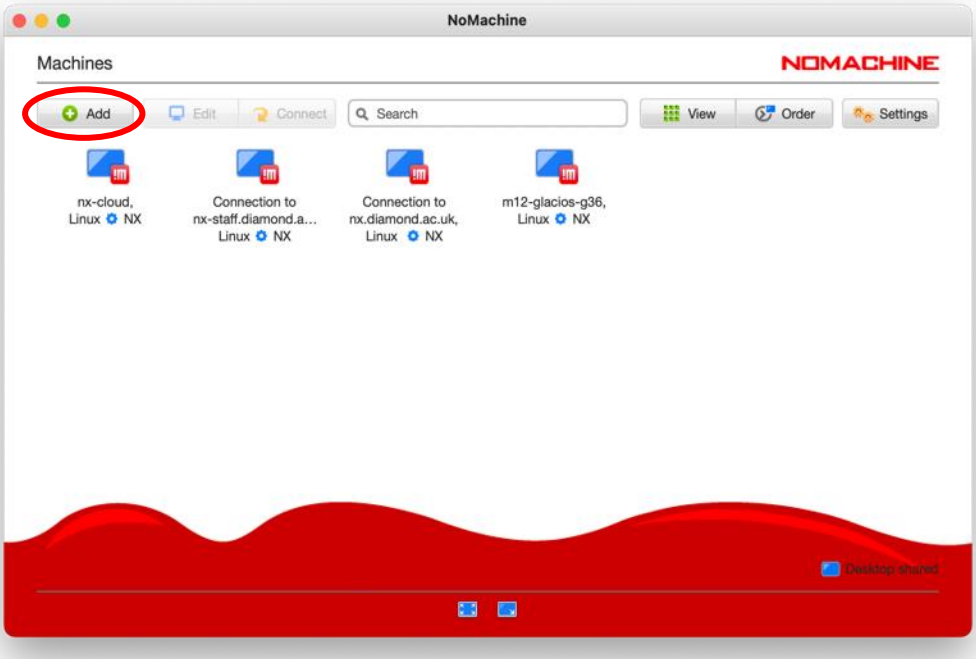
Remote access to eBIC microscopes is provided via NoMachine (nx-cloud.diamond.ac.uk). To access a microscope, users must connect to the microscope support PC via NoMachine and then connect to the microscope via Teamviewer on the support PC.

For security reasons, NoMachine only allows a single connection to the microscope at a time with any additional connections requiring approval from that user. To avoid creating remote access issues for others (e.g., eBIC staff, users for subsequent sessions etc.), you **MUST** close your nx connection if you leave the microscope for any reason.

Please also note that for security reasons NoMachine will only allow 3 unnsuccessful password entries before your account is locked, please ensure you know your password and that it is typing correctly in NoMachine – this is a particular issue for international keyboards and Mac keyboards where keyboards may not map correctly in NoMachine.

1.1 New nx-cloud connection

☐ Click ‘Add’ to create a new connection for using nx-cloud

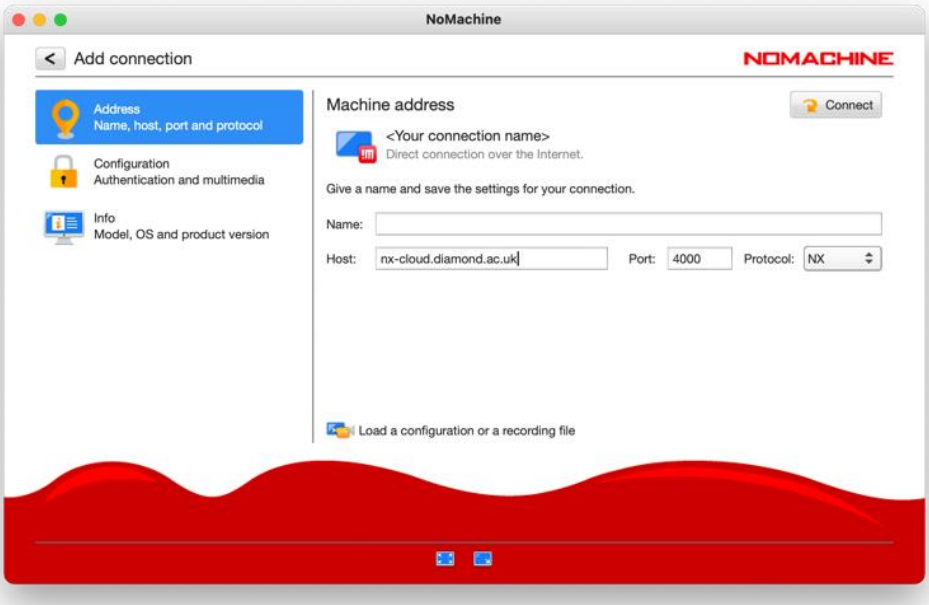


☐ Enter the host name ‘nx-cloud.diamond.ac.uk’

☐ Check the Port and Protocol settings

Note: *If NX does not progress to authentication it is likely that your firewall is blocking the port*

☐ Click ‘Connect’

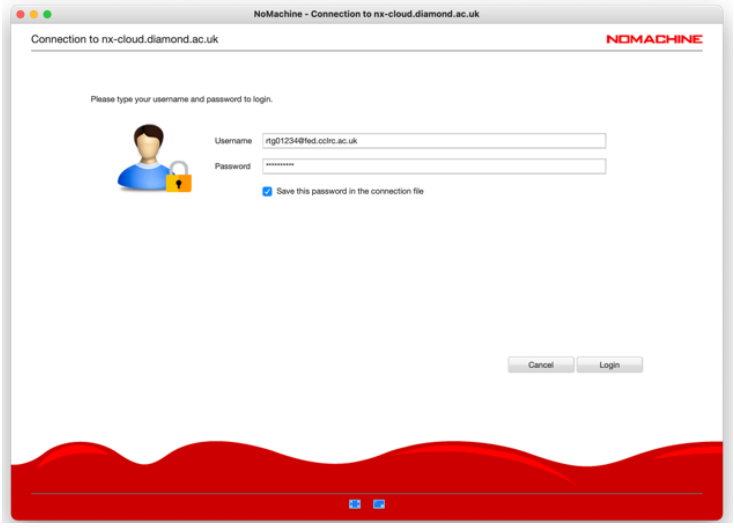


☐ Enter your FedID and password

You must enter the suffix '@fed.cclrc.ac.uk' (i.e. 'rtg01234@fed.cclrc.ac.uk')

☐ For convenience, we suggest selecting 'Save this password in the connection file'

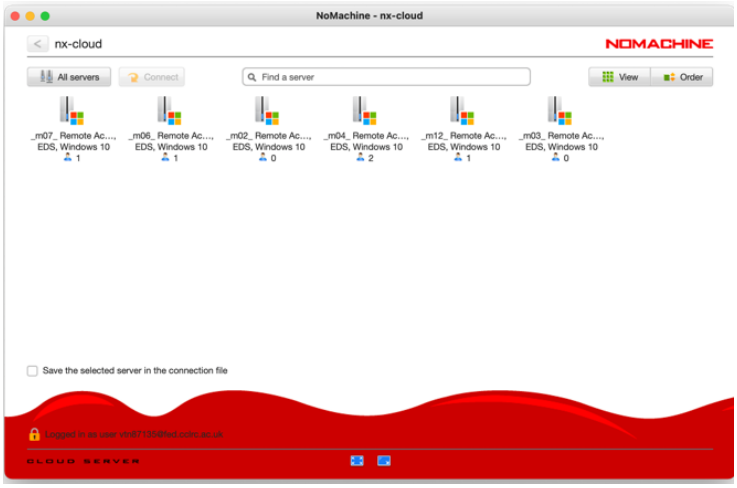
☐ Click 'Login'



Troubleshooting authentication errors:
Note that your account will be locked after 3 failed attempts, it will then require unlocking by the scientific computing and IT departments in Diamond. To prevent significant delays, please ensure that you know your password and that you are typing it correctly. You may manually type your password into the Username field to confirm it is correct, before manually typing into the Password field. This is particularly important for passwords containing special characters and users who have non-UK keyboards.

1.2 Connect to the remote support PC

☐ Double-click the remote support PC of the microscope you want to connect to



Each remote support PC is associated with a microscope. You will only see the remote support PC of the microscope that is scheduled for your session during your session. The names of the machines are as follows:

Krios I: m02
Krios II: m03
Krios III: m06
Krios IV: m07
Talos: m04

☐ A remote connection to the microscope support PC should open

Note: *If a connection does not open and you instead appear to be stuck waiting with a message saying 'waiting for the desktop user to authorise your connection' then contact your LC. For security reasons only one connection can be made to nx-cloud at a time – if the previous user has not properly closed their nx cloud connection then your LC will have to manually close this connection before you can connect.*

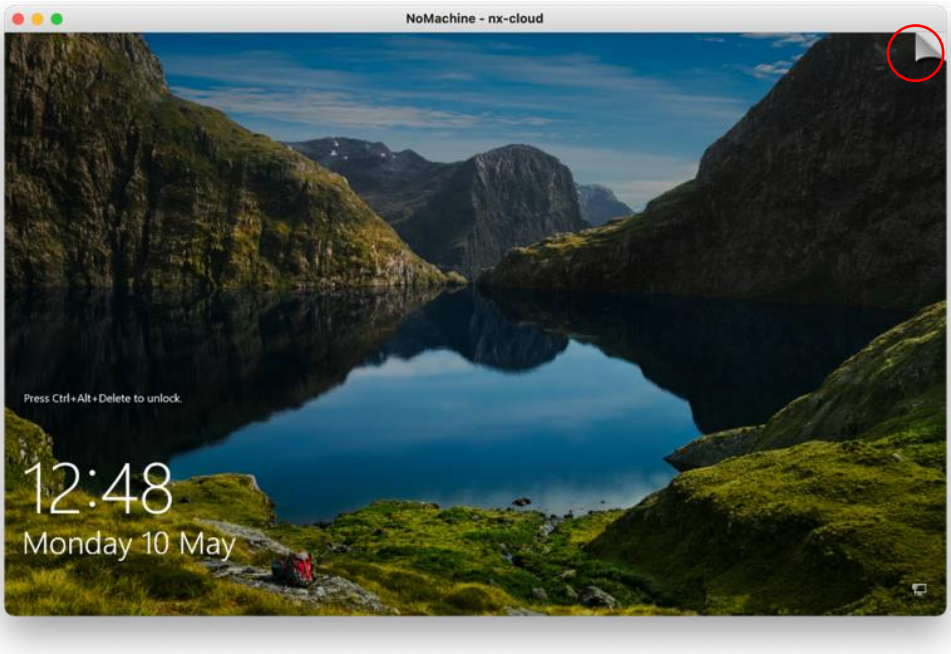
1.3 Log in to the remote support PC

☐ After a few seconds you should be able to see a windows login screen for the microscope support PC

☐ If you are asked to 'Press Ctrl+Alt+Delete to unlock' then use NX to send this command to the remote machine as follows:

☐ Press Ctrl+Alt+0 (Win) or Ctrl+Option+0 (Apple) on your keyboard to access NX options

Note: *You may also access the NX options by hovering your mouse in the top right corner and clicking the 'page turn' graphic that appears.*

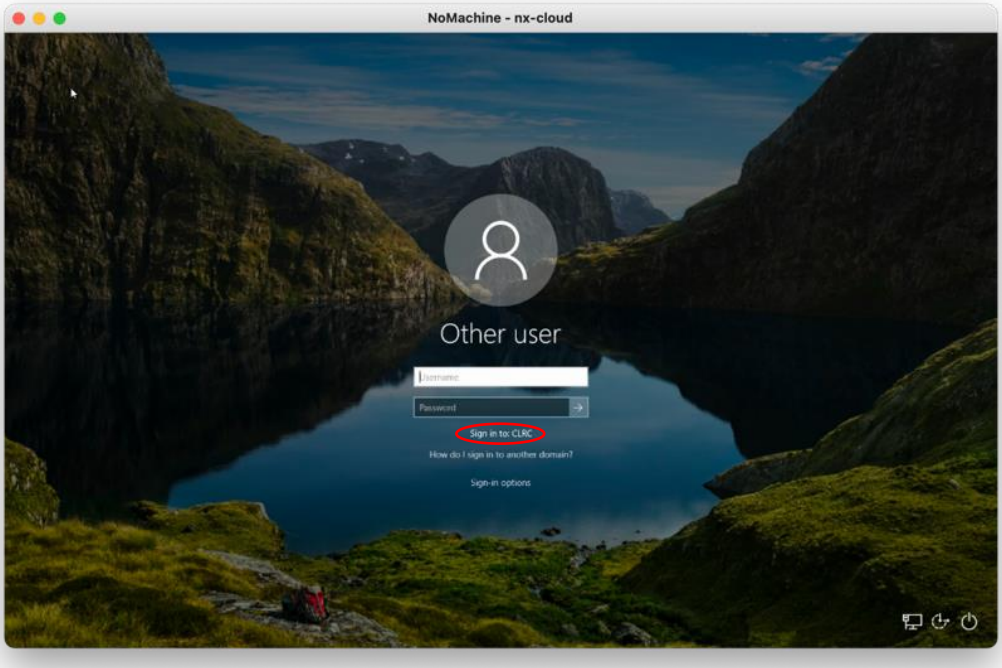


☐ Press the special sequences button in the bottom left of the screen (1) then select 'Ctrl+Alt+Del' from the list to send this to the remote machine

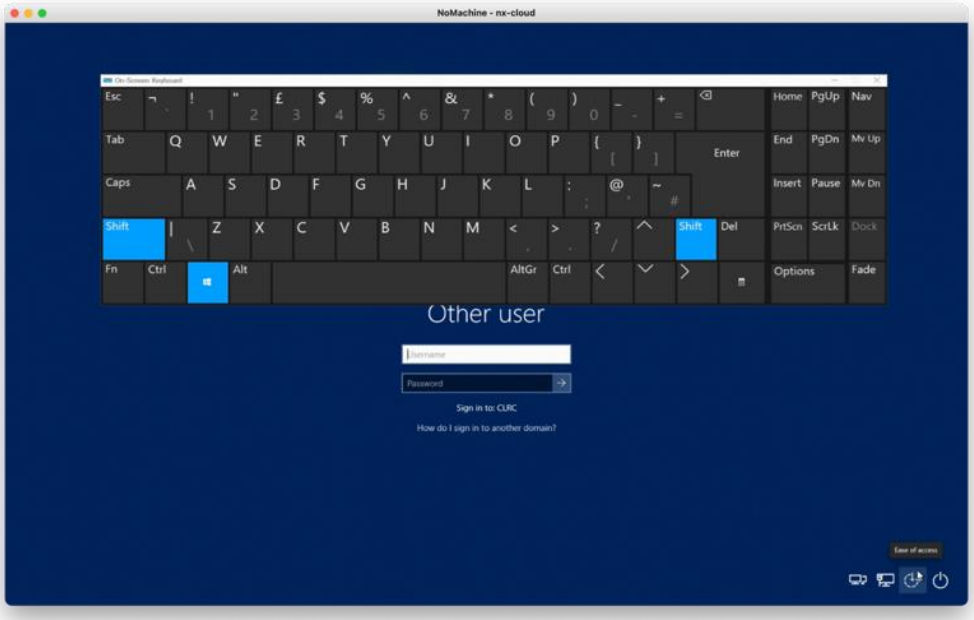
☐ Return to the login screen on the remote machine by pressing the back arrow on the top left (3)

☐ Enter your FedID and password

If ‘Sign in to: CLRC’ is displayed as highlighted, then enter only your FedID
If this is not displayed, then enter the prefix ‘clrc\’, then your FedID (i.e. ‘clrc\rtg01234’)
Some users may be required to enter your FedID in its long form (i.e. ‘rtg01234@fed.cclrc.ac.uk’)



A keyboard can be accessed via the ‘Ease of Access’ button should you have a different keyboard layout to the remote machine. This can also be accessed once logged in via:
Start > Settings > Ease of Access > Keyboard



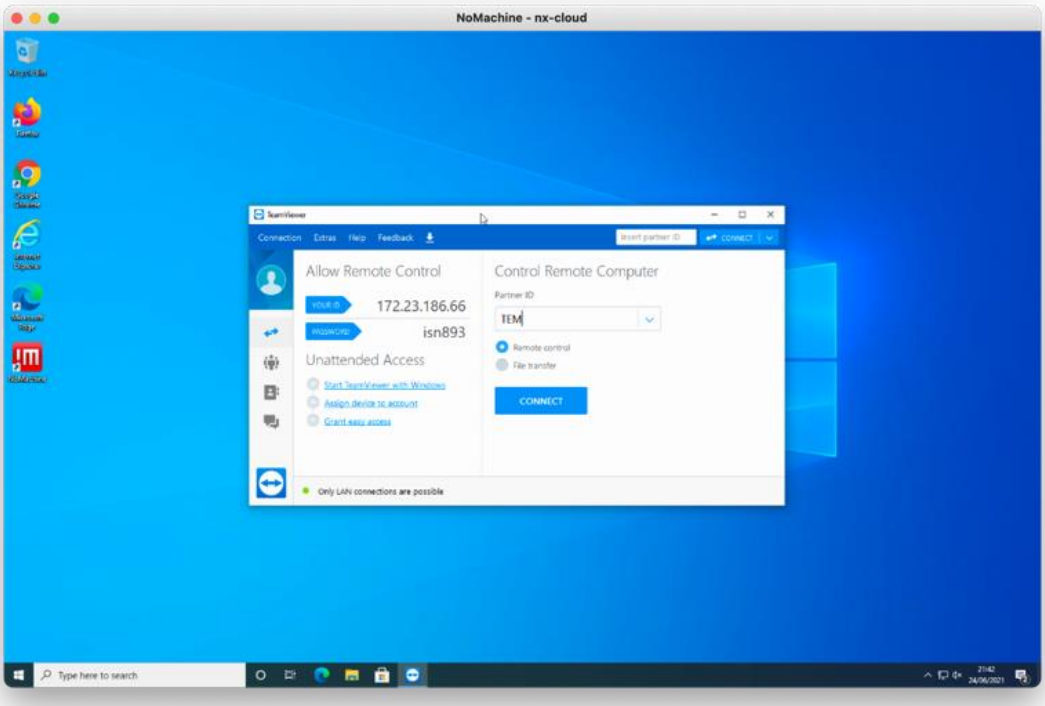
1.4 Connect to the microscope using TeamViewer

You are now connected to a windows virtual support PC via NoMachine. This machine has TeamViewer installed.

From the windows virtual support PC, you can now connect to your microscope using TeamViewer.

☐ Start TeamViewer, enter 'TEM' as the Partner ID and press Connect

☐ Enter the TeamViewer password. Check the table below for each instrument's password.



Instrument	TeamViewer user	TeamViewer password
Krios I (m02)	TEM	diamondkrios1
Krios II (m03)	TEM	diamondkrios2
Krios III (m06)	TEM	diamondkrios3
Krios IV (m07)	TEM	diamondkrios4

You will now be connected to the TEM user interface at the microscope on monitor 1. You may use TeamViewer to switch to monitor 2 where EPU or TOMO will be started.

☐ To switch between the TEM PC and EPU/TOMO monitors press the button

☐ Set TeamViewer to 'Best Fit' under the 'View' tab

To closely inspect on-screen elements and data you may find ‘Scaling: Original 1:1’ and ‘Quality: Optimize quality’ useful.

☐ It is not normally necessary to adjust the TeamViewer Screen resolution. Optimal settings for your display can normally be found using the NoMachine display configuration.

1.5 Configure the NoMachine display

☐ Press Ctrl+Alt+0 (Win) or Ctrl+Option+0 (Apple) on your keyboard to access NX options

Note: *You may also access the NX options by hovering your mouse in the top right corner of the screen and pressing the 'page turn' graphic however you must be careful not to accidentally press the red 'x' of the TEM user interface or EPU/TOMO.*

☐ Configure your display settings:

Display > Scale to window

Display > Change settings > Best Quality

Display > Change settings > Set resolution appropriate to your system

To closely inspect on-screen elements and data, you may find selecting 'Enable viewport mode' to view the remote desktop at 1:1 scaling helpful.

Please do not use 'Resize remote display'.

The following settings work well on a 13-inch screen with a resolution of 2560 x 1600 pixels.
Selecting "Disable client side image post-processing" can improve image quality.

NoMachine - nx-cloud (Microscope)
Display settings
NOMACHINE
Change the settings below or click the '<' back button to close the menu.
Display
Quality
Best speed
Best quality
Resolution
1280x768
1680x1050
1920x1080
2560x1600
3280x2048
Use custom resolution
W
H
Monitor
Ask the desktop resolution upon connecting
Options
Modify the advanced display settings
Modify
Display 1920x1080, codec H.264 QS/VDA, audio Opus 22kHZ stereo
ENTERPRISE DESKTOP

Change the settings below or click the '<' back button to close the menu.
Disable network-adaptive display quality
Disable multi-pass display encoding
Disable frame buffering on decoding
Disable client side image post-processing
Disable client side hardware decoding
Request a specific frame rate
60 FPS

2 Setting up your data collection

2.1 Setting up your data collection session

eBIC actively maintain User Guides for EPU and TOMO5 that are designed to complement your training. You may find them helpful to follow for guidance in setting up your data collection session.

Set up your data collection and work with your local contact to start the collection and data transfer.

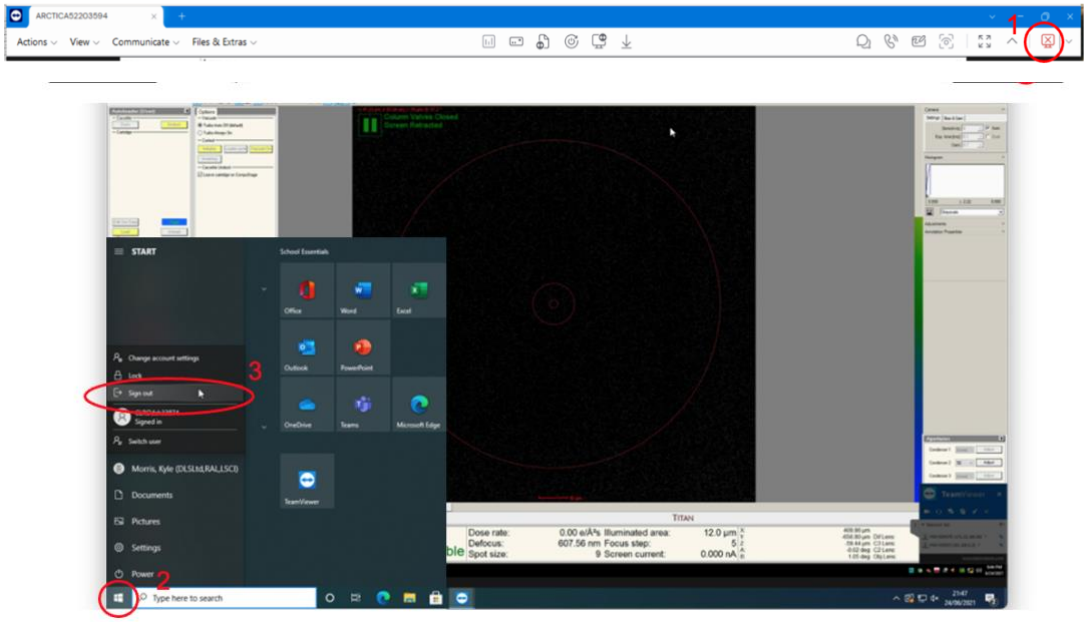
2.2 At the end of your session

☐ Close Teamviewer:

- Click on the cross (1)

☐ Sign out of the remote support PC

- Click on (2 and 3)



☐ Disconnect from NoMachine:

- Press Ctrl+Alt+0 (Win) or Ctrl+Option+0 (Apple) on your keyboard to access NX options
- Click on (3) 'Connection'
- Click on (4) 'Disconnect' to disconnect from the NoMachine nx-cloud session

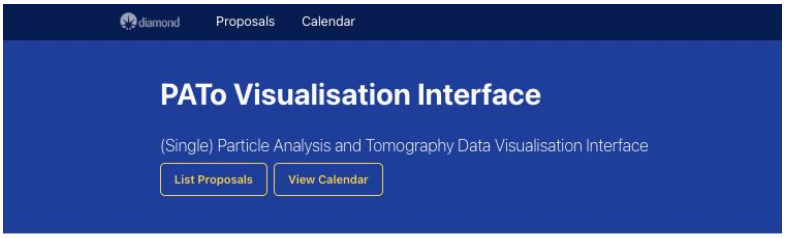
3 Monitor your session and view analysis via PATo

This assumes you have set your data output to the correct folder ***(i.e.,*** *Z:\[your session ID, i.e., biXXXXXX])*
If you have not set your data output folder to the correct session in the Z drive, data will not be automatically transferred and processed via PATo. In this case, speak to your LC

3.1 Accessing PATo

☐ Navigate to ebic-pato.diamond.ac.uk and log in with your fedID and password.

You should then see the following or similar:

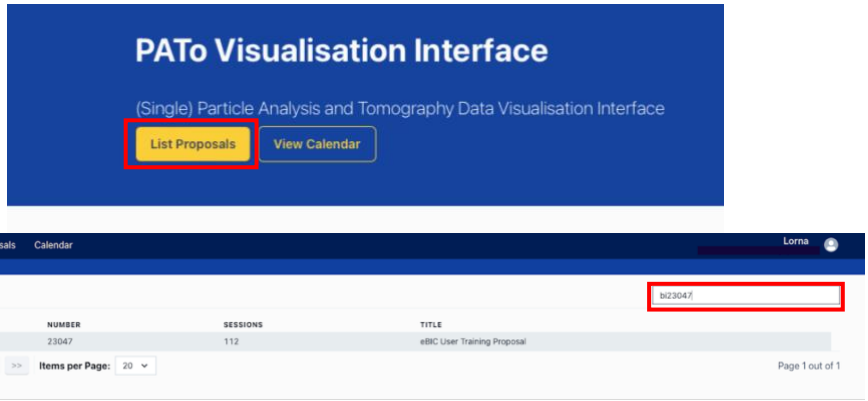


If this does not display inform your local contact specifying your browser (Chrome, Safari, etc.) and operating system. You may want to try logging into an NX session and opening a browser from there.

3.2 Finding your session in PATo

☐ Locate your visit, this may be displayed on the home screen but if not:

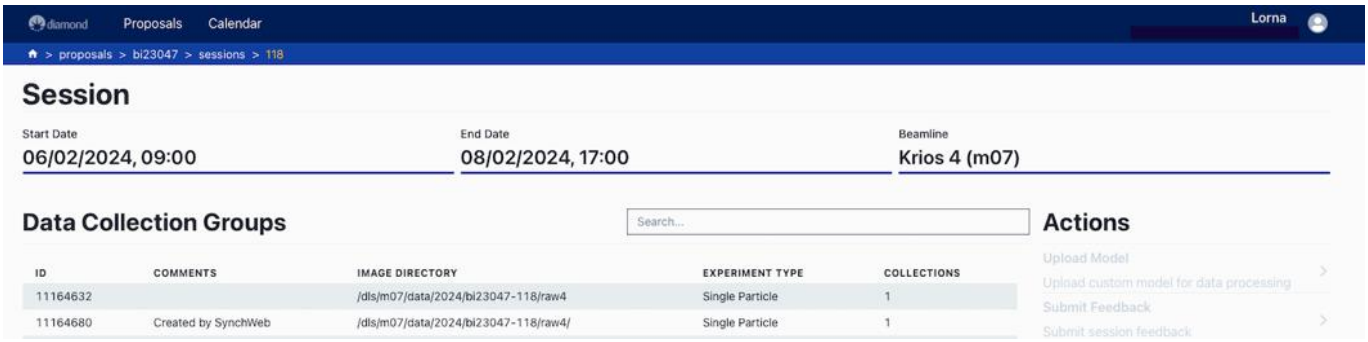
- Navigate to the proposal list via the “List Proposals” button and search for your proposal number into the search bar on the right (i.e., biXXXXX without the visit id).



3.3 Monitor your on-the-fly data analysis via PATo

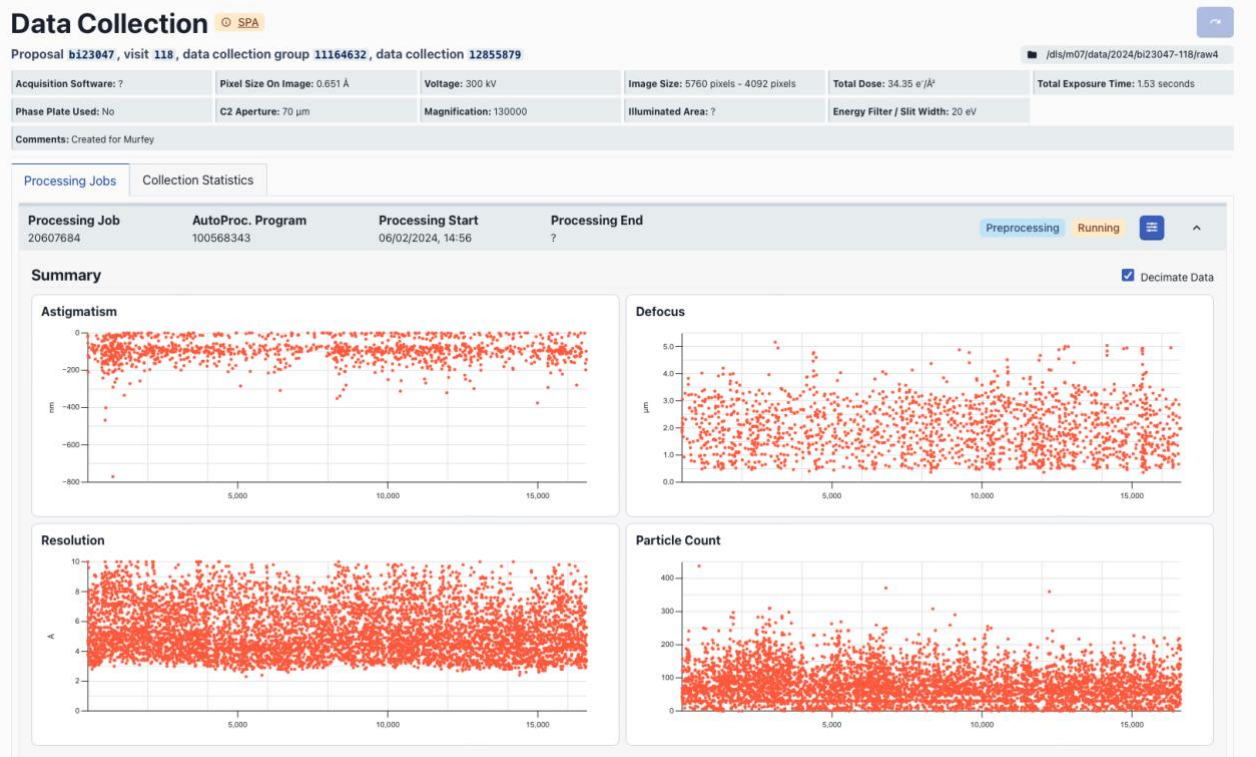
The on-the-fly data analysis pipeline is being actively developed at eBIC. The reporting interface will show increasing amounts of information and analysis as this development progresses. In the meantime, the following sections will help you learn how to inspect your data analysis results.

☐ Once you have navigated to your proposal you will be presented with a list of all visits in that proposal. Select the relevant visit from the list and you should see a screen similar to the following displaying all data collections for that visit:



Data collection sessions should appear within 15 minutes of the start of acquisition. If this doesn't happen speak to your LC.

☐ Select a data collection to see processing results, you should be presented with a screen like the following:



From here you can monitor various collection statistics and keep an eye on how on-the-fly processing is going

For EPU, our on-the-fly processing will carry out motion correction, CTF estimation, 2D classification and selection, initial model generation and 3D classification.

For TOMO, PATo will carry out motion correction, CTF estimation, tilt stack generation and subsequent alignment and reconstruction and finally denoising.

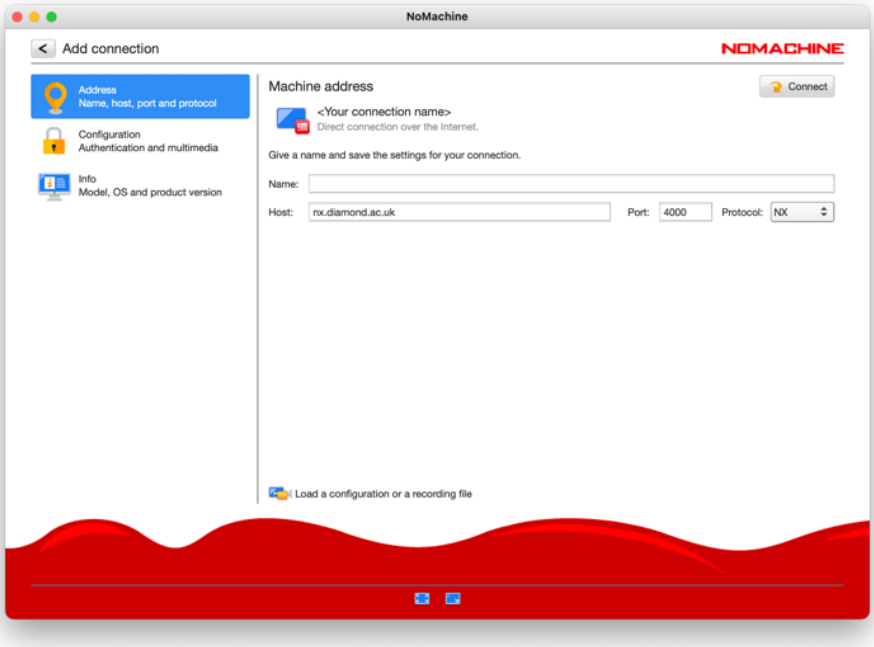
4 Monitor your session and view analysis via NoMachine

4.1 Connect to a Linux machine via NX

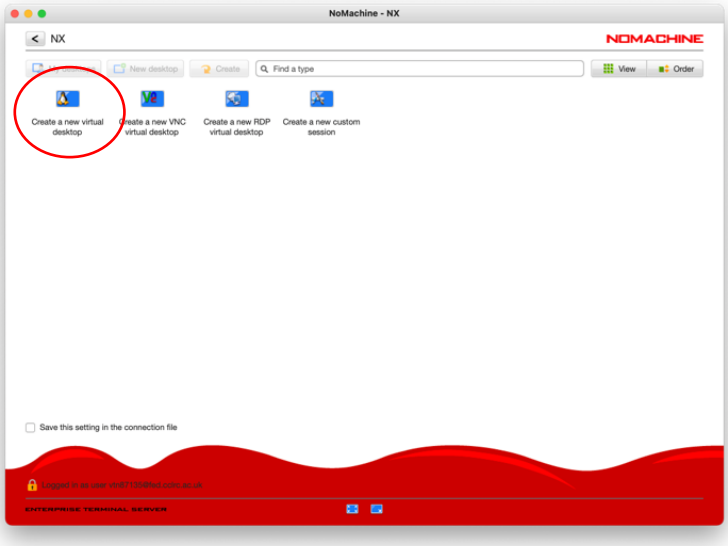
For the duration of your session, you may also log in to a remote Linux machine to inspect your on-the-fly data analysis results and monitor the progression of your data collection.

☐ Follow **section 1.1** to create a new NX connection but enter the following host name:

'nx.diamond.ac.uk'



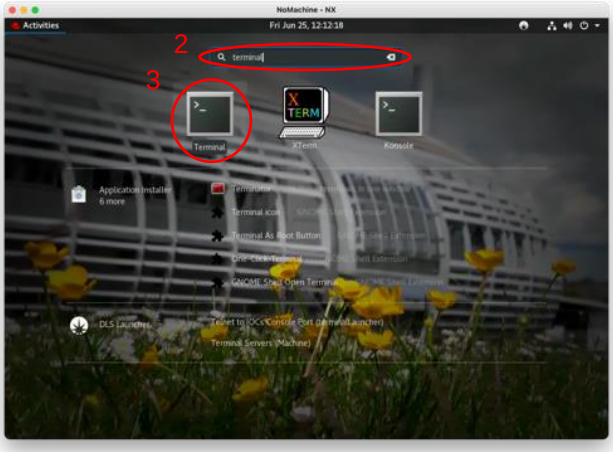
☐ Double-click on 'Create a new virtual desktop'

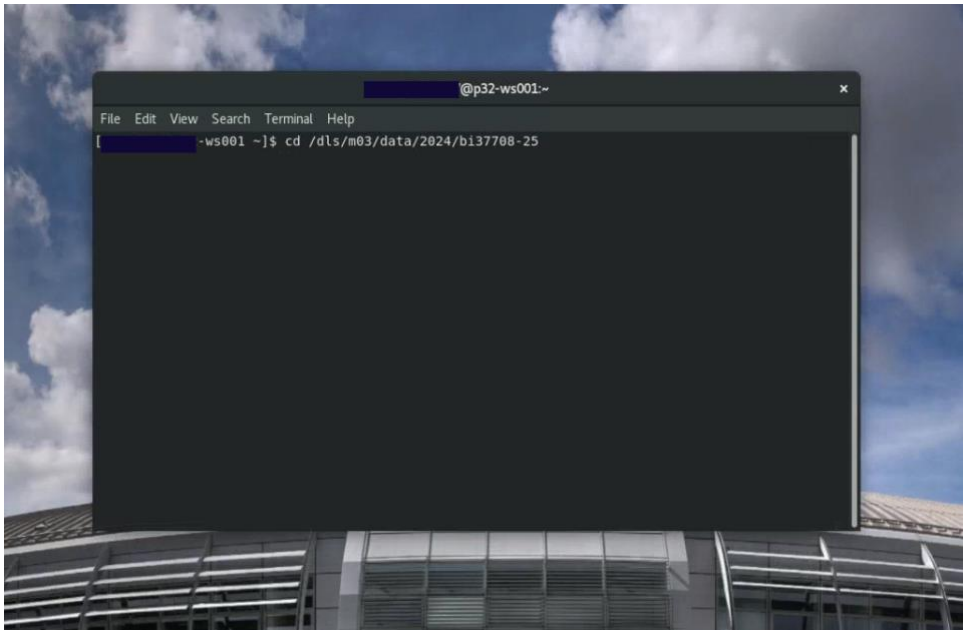


☐ Follow section 1.5 to configure the display for your computer

☐ Click on (1) the applications menu, (2) search for ‘Terminal’ and (3) launch a terminal

1





4.2 EPU: Check data is being written to your visit directory

Atlas, processing and raw directories are located in your visit directory, a typical structure is shown below:

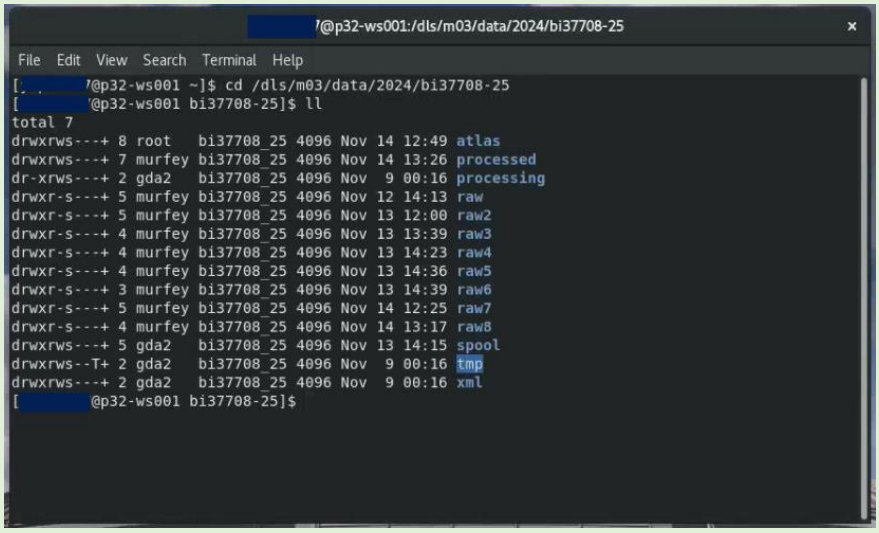
./*atlas | Images that make up the grid overview
./*processed | Images processed by our on-the-fly processing software
./raw | Movie frames and metadata for each data acquisition session

All directories are protected from accidental modification, but you can still execute commands to inspect the data. The following present several different ways you can monitor your incoming data.

☐ Use the terminal to navigate to your visit directory

```
$ cd /dls/{beamline}/data/{year}/{visit number}
      e.g. /dls/m03/data/2024/bi37708-25
```

A typical structure session directory structure containing an atlas directory, processing directory and a 'raw' directory for each data acquisition session that has been set up:



4.2.1 Check data is still being collected and transferred via a terminal

```
# To count the movies in the raw directory
$ find ./raw/GridSquare*/Data -name '*fractions.tiff' | wc -l

# To list the recent movies in the raw directory
$ find ./raw/GridSquare*/Data -name '*fractions.tiff' -printf '%TF %TR 1 %p\n' | sort -n | cat -n | tail

# To monitor the number of movies in the raw directory at a 5 sec interval
$ watch -n 5 'find ./raw/GridSquare*/Data -name '*fractions.tiff' -print0 -printf '\n' | wc -l'

# To monitor several useful parameters at a 0.5 sec interval
$ export command='find ./raw/GridSquare*/Data -name '*fractions.tiff' -printf '%T@ %Tc %p\n' | sort -n'

$ watch -n 5 'export mic=$(eval $command | tail -n 1) && echo Latest micrograph: && echo $mic && echo ''
&& echo Total micrographs collected: && eval $command | wc -l'
```

4.2.2 View the most recent unaligned movie frame average in imod

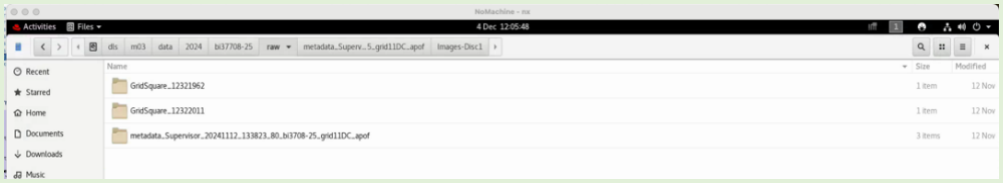
```
# Load the imod module (you only need to do this once per session)
$ module load imod

# Return the name and path of the most recent unaligned movie frame average
$ ls -ltr ./{EPU_session_directory}/Images-Disc1/GridSquare*/Data/*.mrc | tail -n 1

# Open the most recent unaligned movie frame average
# You may copy and paste the path from the previous command output
$ 3dmod ./{file_path}/{filename}
```

A 3dmod control window and micrograph will load. Please remember to close this window after you have finished checking your micrograph. Please keep in mind that this micrograph will NOT be motion corrected.

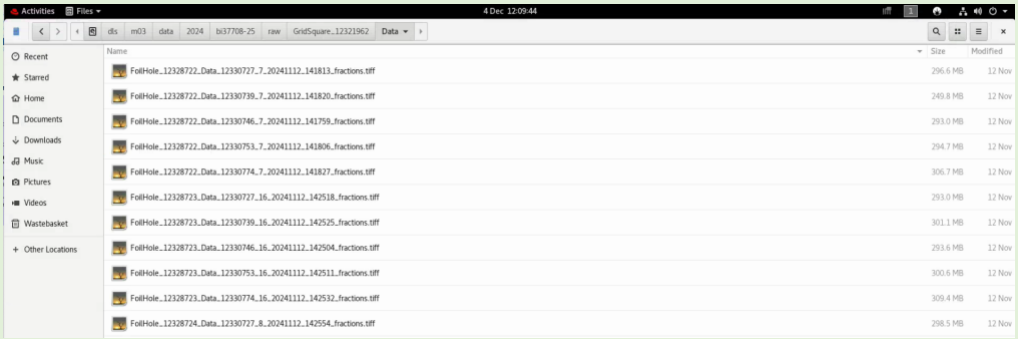
4.2.3 View the list of files being written by EPU/TOMO in a file browser

```
# Use the Linux file browser, Nautilus, to open the raw directory
$ nautilus ./{session_directory}/raw/
```

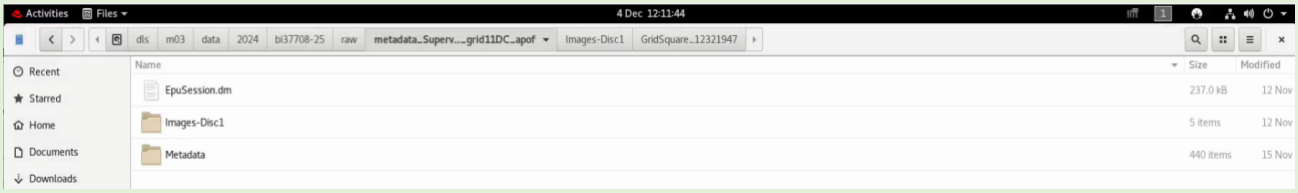
The **raw directory** contains all of the movie frames (organised by GridSquare) and metadata for each data acquisition session.



The **raw movies** can be found in the /[session_directory]/raw/GridSquare*/Data directory



The **metadata** can be found in the /[session_directory]/raw/metadata_[session_name]* directory



4.2.4 Monitor your data collection session

☐ **Verify that new micrographs are being collected during your session**

☐ **In particular, follow section 4.2.1 and ensure that new files appear in the list and that they have a recent time stamp.**

Please note that EPU will pause collecting images (for all sessions) when LN_2 is being refilled, or if you use a K3 camera, when GIF ZLP is being adjusted. However, this should not last longer that 15-20 minutes. Additional time might be required for EPU to move to a new target and acquire an image.

Therefore, if after 30 minutes no new files appear from the command in **section 4.2.1**, please, contact your Local Contact (LC) directly during normal working hours (Monday-Friday 9am to 5pm) or Experimental Hall Coordinators (EHC) outside normal working hours (EHC contact phone number 01235 77 8787).

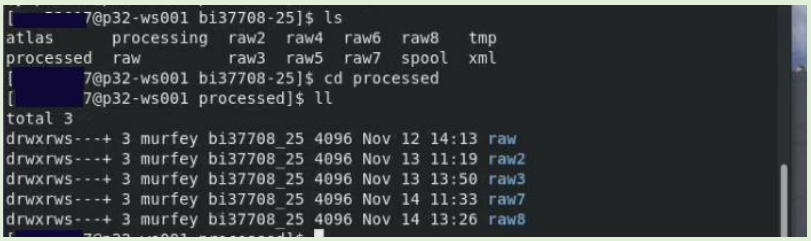
4.3 EPU: Inspect the on-the-fly data analysis results

Having navigated to your visit directory by following **section 4.1**, you can then use the terminal to inspect the progress of the on-the-fly analysis.

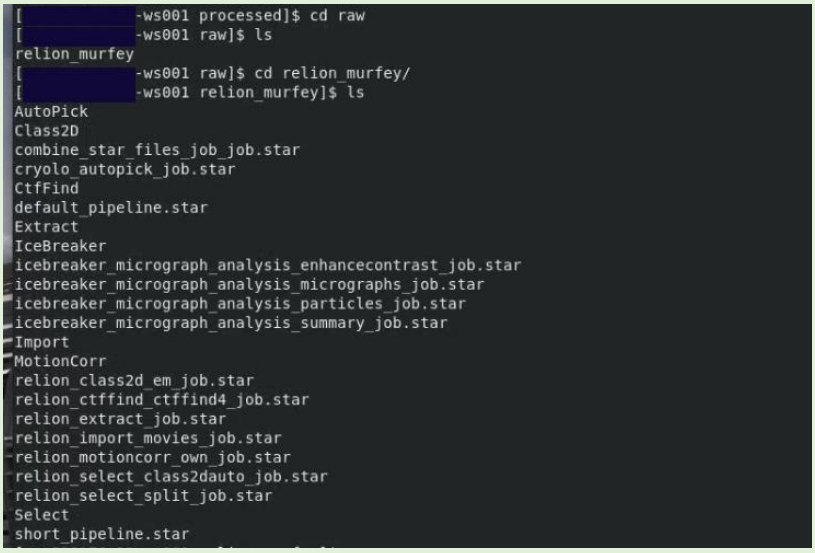
Diamond provides several EM analysis software packages, which can be listed and loaded using the module system.

$ module avail EM/

The on-the-fly data analysis results for each data collection session will be contained in the ./processed folder of your visit directory.



You can view the processing results for each data collection session in the terminal by navigating to the relevant raw directory and subsequent 'relion_murfey' directory:



☐ Load Relion to inspect the on-the-fly data analysis results

```
# Load the Relion module
$ module load EM/relion

# Change directory into the desired analysis job
$ cd ./processed/relion

# Load Relion in read only mode
$ relion --readonly
```

You may then use the Relion GUI to inspect the on-the-fly analysis results in the usual way. Please note, other programs such as Chimera and EMAN are available in the module system for exploring your data.

4.4 TOMO5: Check data is being written to your visit directory

Atlas, processing and raw directories are located in your visit directory, a typical structure is shown below:

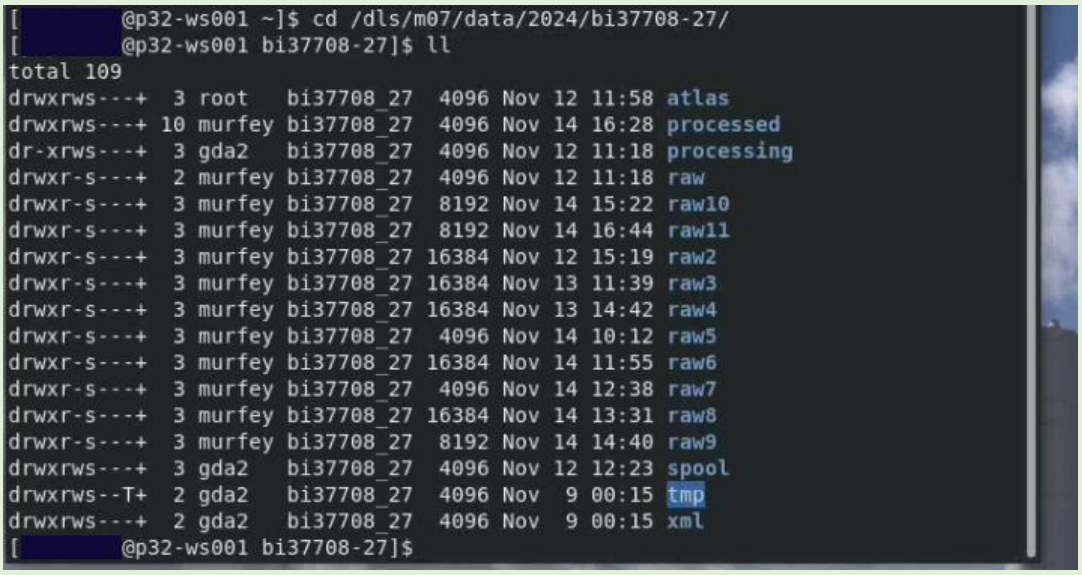
```
./*atlas       | Images that make up the grid overview
./*processed | Images processed by our on-the-fly processing software
./raw          | Movie frames and metadata for each data acquisition session
```

All directories are protected from accidental modification, but you can still execute commands to inspect the data. The following present several different ways you can monitor your incoming data.

☐ Use the terminal to navigate to your visit directory

```
$ cd /dls/{beamline}/data/{year}/{visit number}
      e.g. /dls/m07/data/2024/bi37708-27
```

A typical structure session directory structure containing an atlas directory, processing directory and a 'raw' directory for each data acquisition session that has been set up:




```
# To list the recent tilted movie frames in the raw directory
$ ls -ltr ./raw/*.mrc | tail

# To count the tilted movie frames in the raw directory
$ ls -ltr ./raw/*.mrc | wc -l

# To return the name and path of the most recent tilted movie frames
$ ls -ltr ./raw/*.mrc | tail -n 1

# To monitor the number of tilted movies in the raw directory at a 1 sec interval
$ watch -n 1 'ls -ltr ./raw/*.mrc | wc -l'
```

If you do not see the latest tomogram file being updated for longer than 20 minutes then you should reach out to your Local Contact (LC) during normal working hours (Monday-Friday 9am to 5pm) or Experimental Hall Coordinators (EHC) outside normal working hours (EHC contact phone number 01235 77 8787).

5 Download your data following your session

If your session was **fewer than 40 days ago**, your data will still be on the Diamond file system. Use Globus Online to transfer datasets over 20GB, or FTP, SFTP or rsync for under 20GB.
If your visit was **more than 40 days ago** it has probably been removed from the beamline storage systems. Use TopCAT to access your data from the archive. For Diamond Light Source data restore help, learn more here.

For more information please visit https://www.diamond.ac.uk/Users/Experiment-at-Diamond/IT-User-Guide/Not-at-DLS/Retrieve-data.html