

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

Revision: 2.0

Revision date: 04 April 2024

Revision summary: 1) Change of on-the-fly processing platform from SynchWeb to PATo  
2) Updated instructions for data download via Globus, FTP, SFTP and rsync

Comments to: Lorna Malone

Acknowledgements: We would like to acknowledge all eBIC staff both past and present for their invaluable efforts and contributions towards the writing of this documentation, in particular Kyle Morris, Yuriy Chaban, Daniel Hatton and Stephen Riggs.

## Introduction

This document is intended as a guide for trained eBIC users to assist them in accessing eBIC systems using NoMachine (NX), initiating and monitoring 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](mailto: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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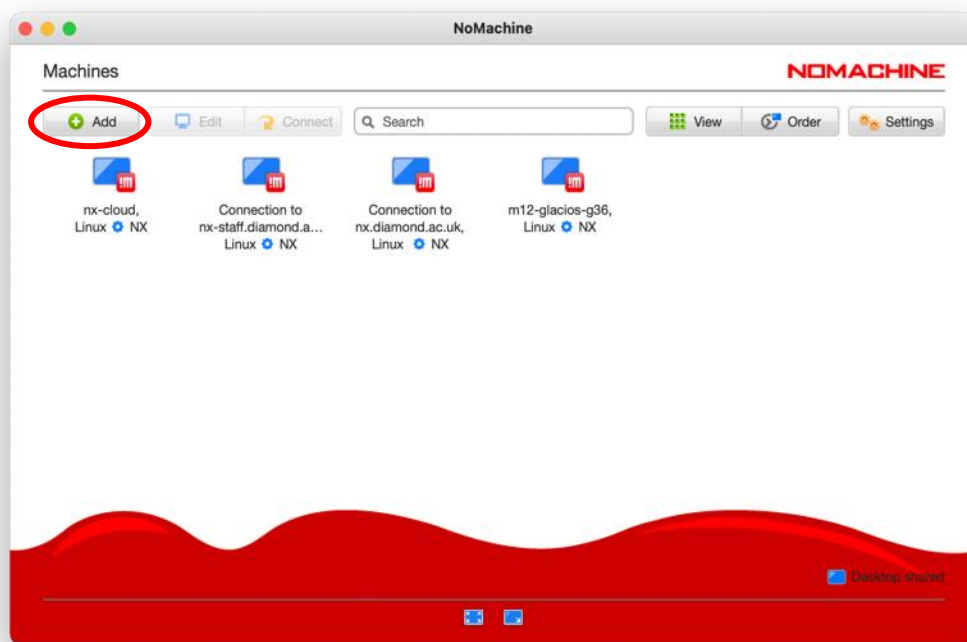
## 1 Access eBIC microscopes using NoMachine

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.

### 1.1 New nx-cloud connection

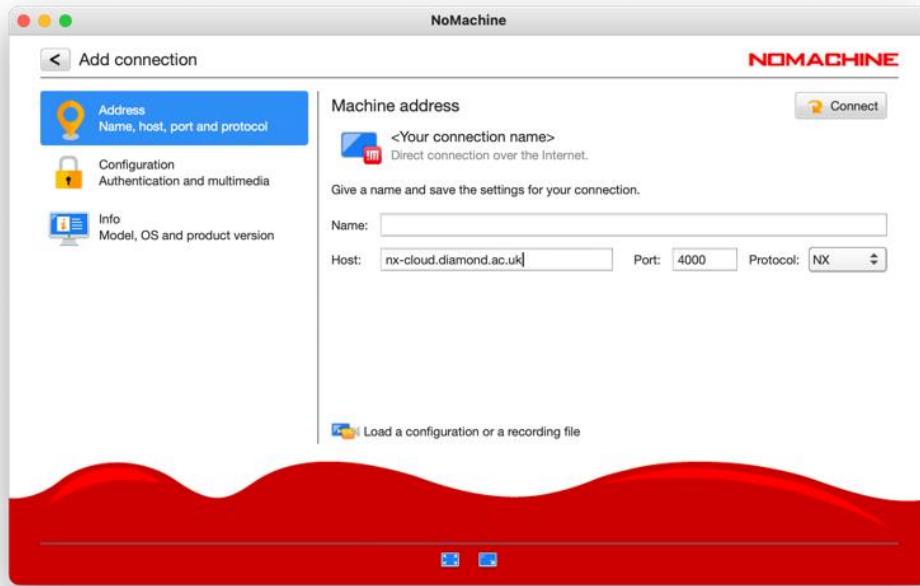
- Click 'Add' to create a new connection for using nx-cloud



- 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'

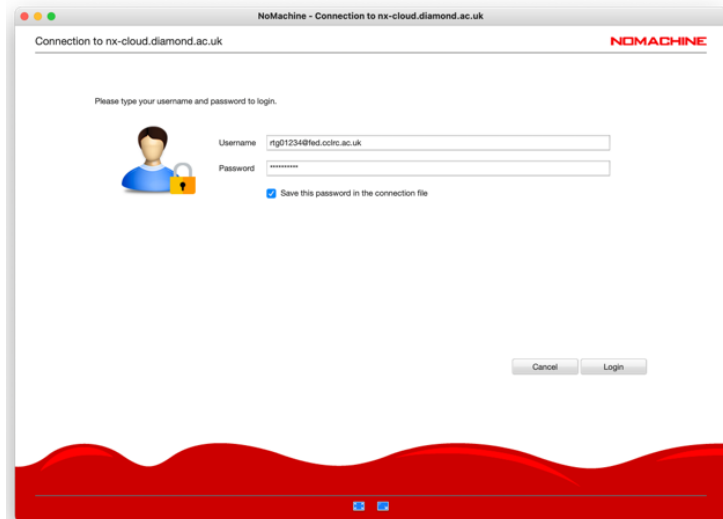


Enter your FedID and password

**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'

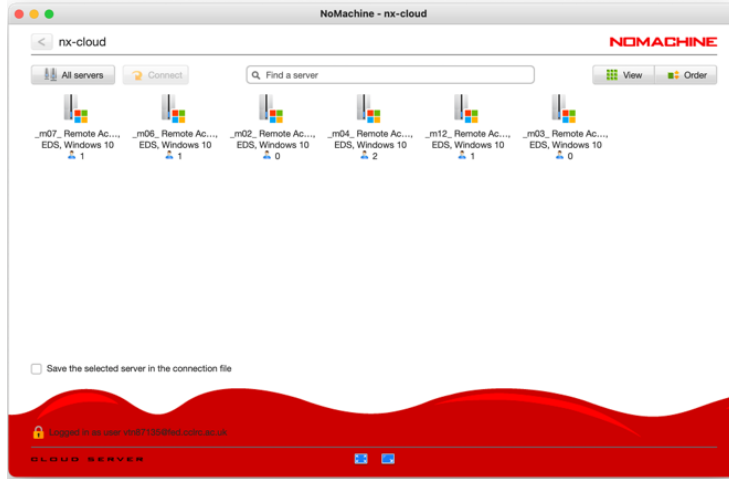


### **Troubleshooting authentication errors:**

Note that your account will be locked after 5 failed attempts, it will then unlock after 30 minutes. 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.

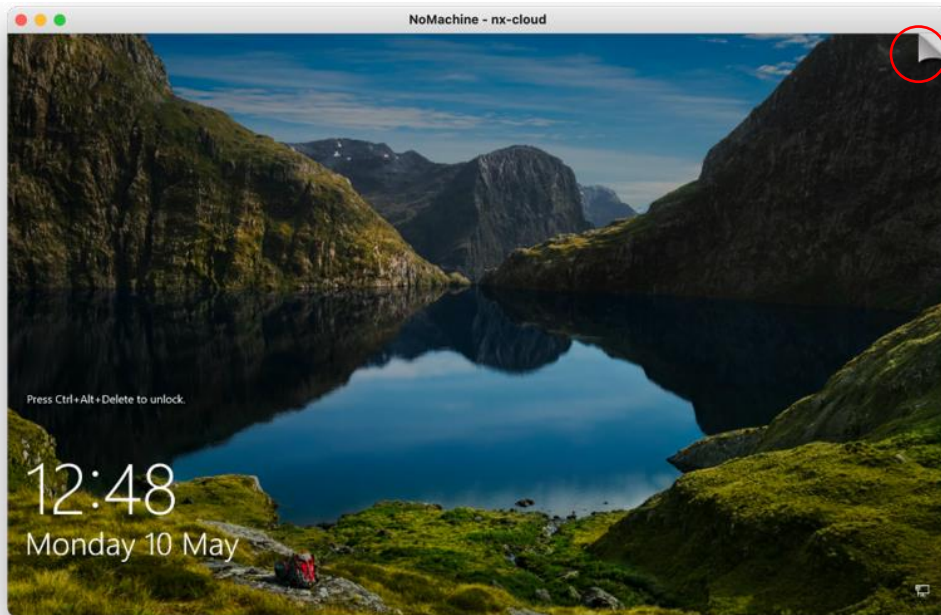


Waiting for the desktop user to authorize your connection

### 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.



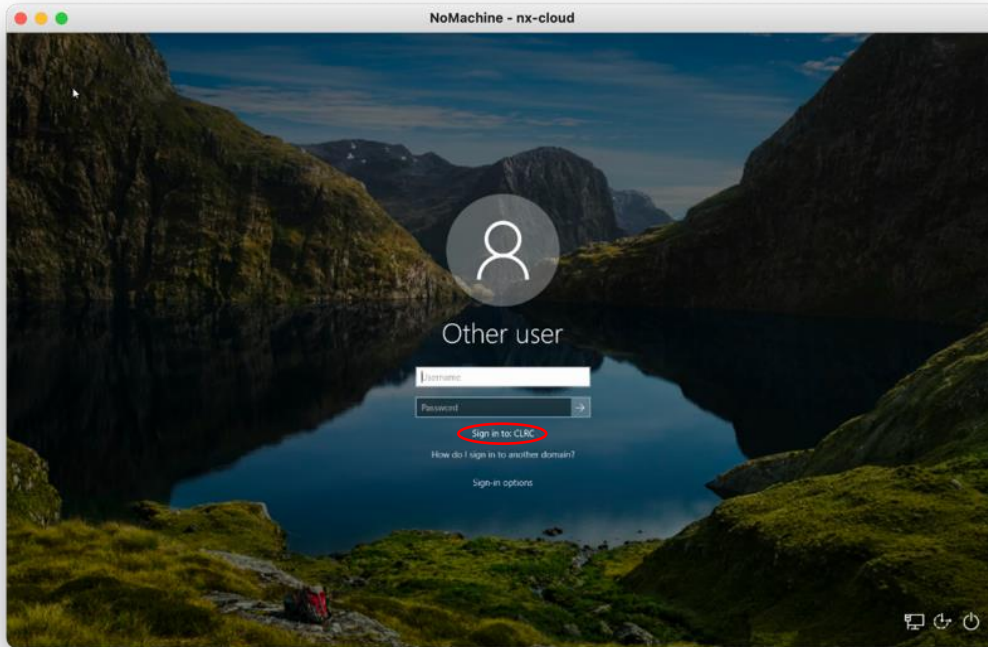
- Press the special sequences button in the bottom left of the screen (1) then select 'Ctrl+Alt+Del' from the list to send this to the remote machine



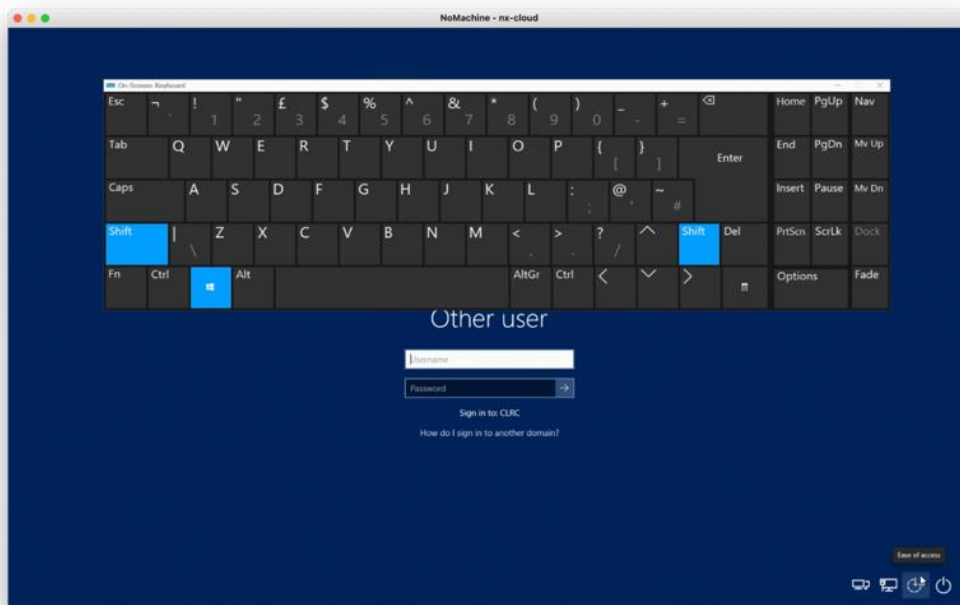
- Return to the login screen on the remote machine by pressing the back arrow on the top left (3)

- 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

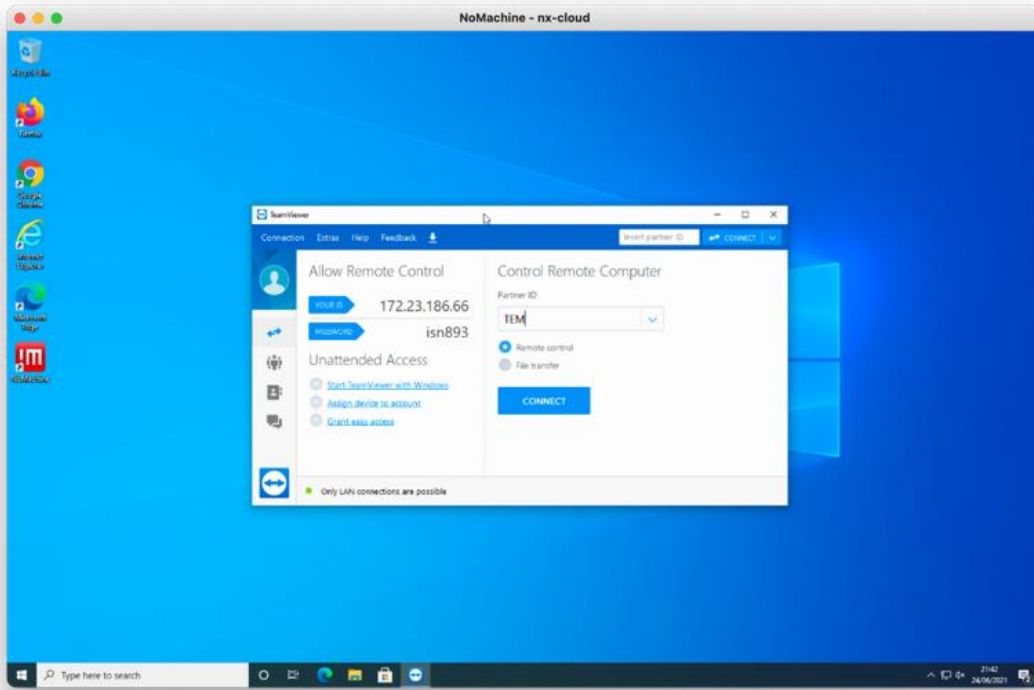




## 1.4 Connect to the microscope using TeamViewer




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.

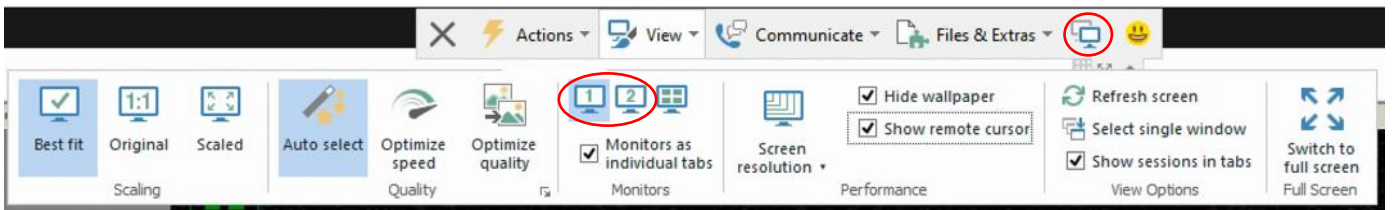
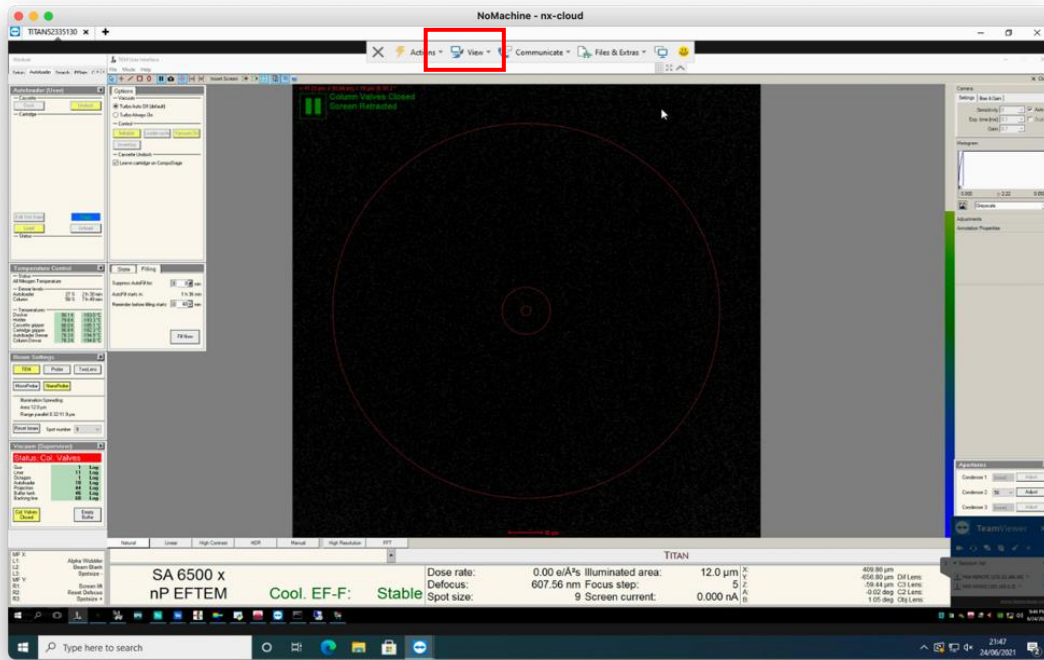
- Start TeamViewer, enter 'TEM' as the Partner ID and press Connect
- Enter the TeamViewer password. Check the table below for each instrument's password.



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 'View' at the top of the teamviewer screen and select the 'Monitor:1/2' buttons (   ) or use 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.

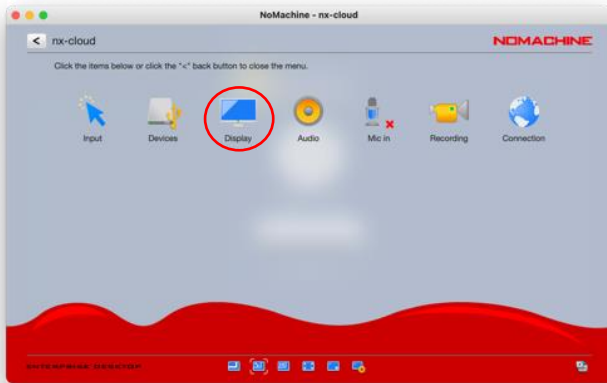
- Configure your display settings:

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.



## 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

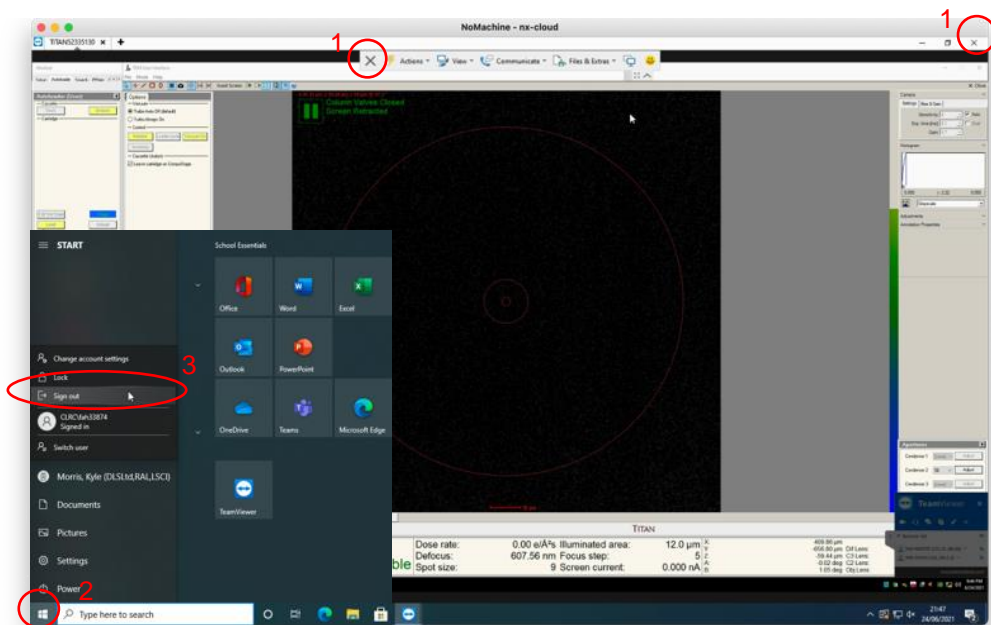
Close Teamviewer:

- Click on the cross (1)

**(Take care that you do not accidentally close the 'TEM User Interface')**

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



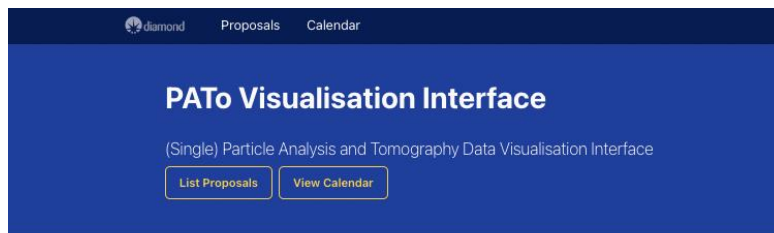
### 3 Monitor your session and view analysis via PATo

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 to initiate data transfer via scripts and you will need to set up on-the-fly processing manually (see section xxxx)

#### 3.1 Accessing PATo

Navigate to [ebic-pato.diamond.ac.uk](http://ebic-pato.diamond.ac.uk) and log in with your fedID and password.

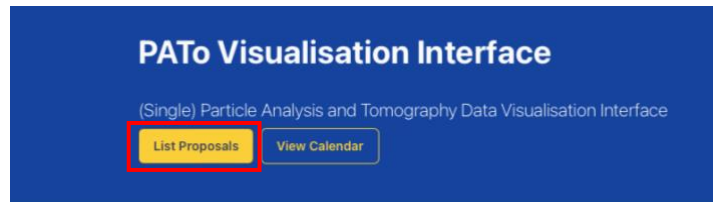
You should then see the following or similar:



*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

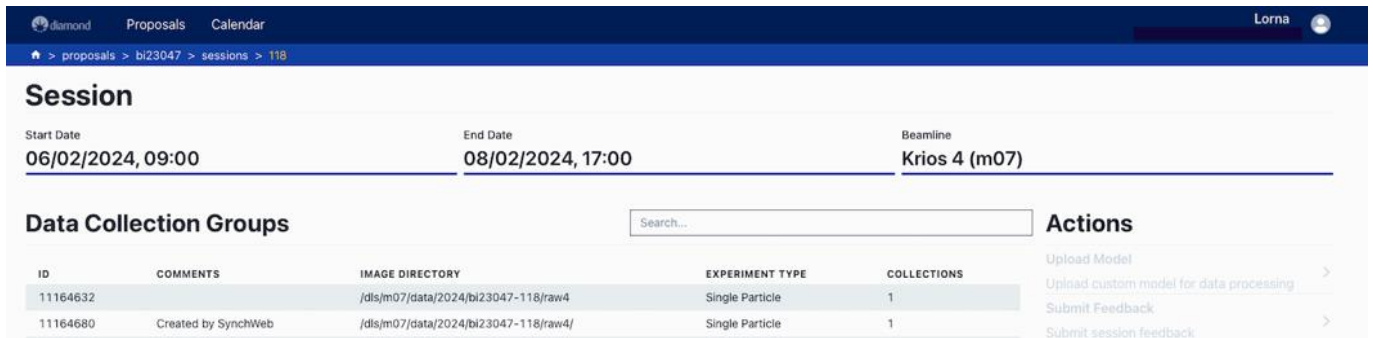
- Locate your visit, this may be displayed on the home screen but if not:
- Navigate to the proposal list via the “List Proposals” button and search for your proposal number into the search bar on the right (*i.e.*, biXXXXX without the visit id).



### 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.

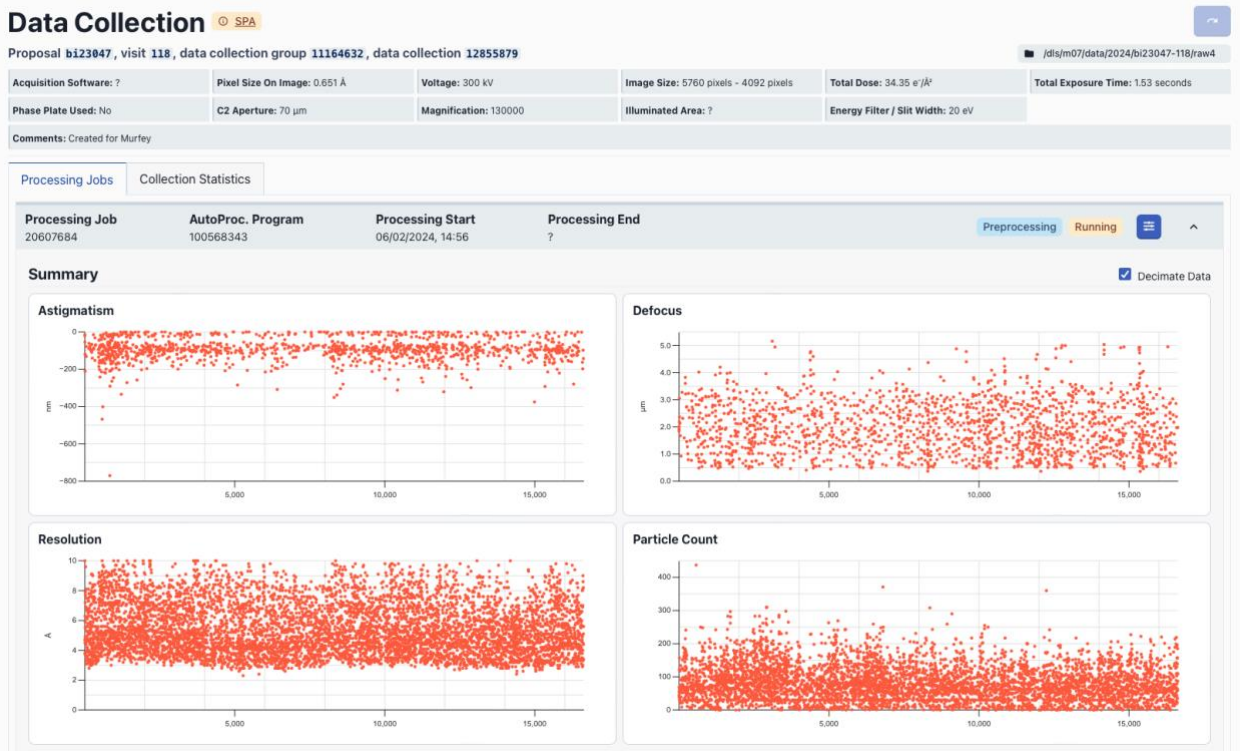
Once you have navigated to your proposal you will be presented with a list of all visits in that proposal. Select the relevant visit from the list and you should see a screen similar to the following displaying all data collections for that visit:



ID	COMMENTS	IMAGE DIRECTORY	EXPERIMENT TYPE	COLLECTIONS
11164632		/dls/m07/data/2024/bi23047-118/raw4	Single Particle	1
11164680	Created by SynchWeb	/dls/m07/data/2024/bi23047-118/raw4/	Single Particle	1

*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:



**Data Collection** SPA

Proposal **bi23047**, visit **118**, data collection group **11164632**, data collection **12855879**

Acquisition Software: ? Pixel Size On Image: 0.651 Å Voltage: 300 kV Image Size: 5760 pixels - 4092 pixels Total Dose: 34.35 e<sup>-</sup>/Å<sup>2</sup> Total Exposure Time: 1.53 seconds

Phase Plate Used: No C2 Aperture: 70 µm Magnification: 130000 Illuminated Area: ? Energy Filter / Slit Width: 20 eV

Comments: Created for Murfey

Processing Jobs | Collection Statistics

Processing Job	AutoProc. Program	Processing Start	Processing End
20607684	100568343	06/02/2024, 14:56	?

Summary

Decimate Data

**Astigmatism** (µm vs. frames)

**Defocus** (µm vs. frames)

**Resolution** (Å vs. frames)

**Particle Count** (count vs. frames)

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.

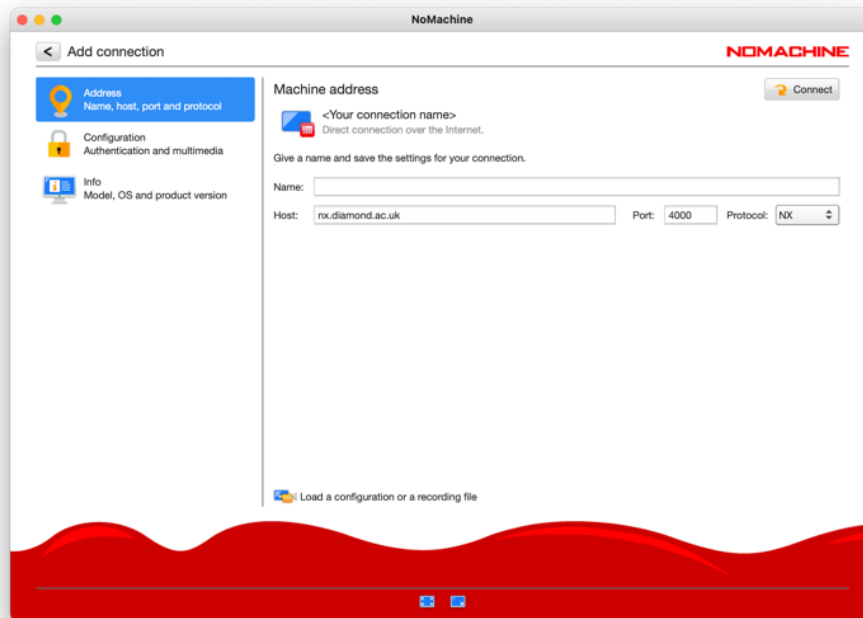
For TOMO, PATo will carry out motion correction, CTF estimation, tilt stack generation and subsequent alignment and reconstruction and finally denoising.

## 4 Monitor your session and view analysis via NoMachine

### 4.1 Connect to a Linux machine via NX

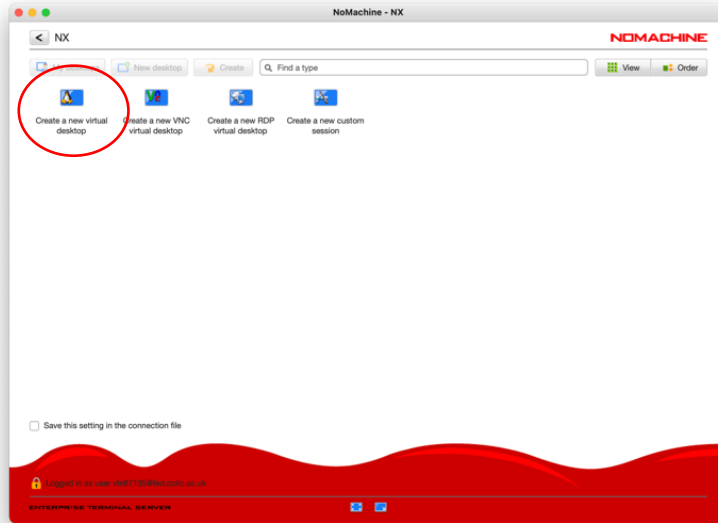
For the duration of your session, you may also log in to a remote Linux machine to inspect your on-the-fly data analysis results and monitor the progression of your data collection.

- Follow section 1.1 to create a new NX connection but enter the following host name:  
'nx.diamond.ac.uk'

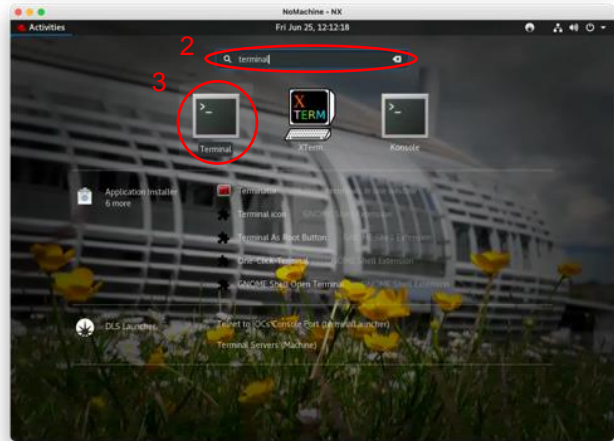


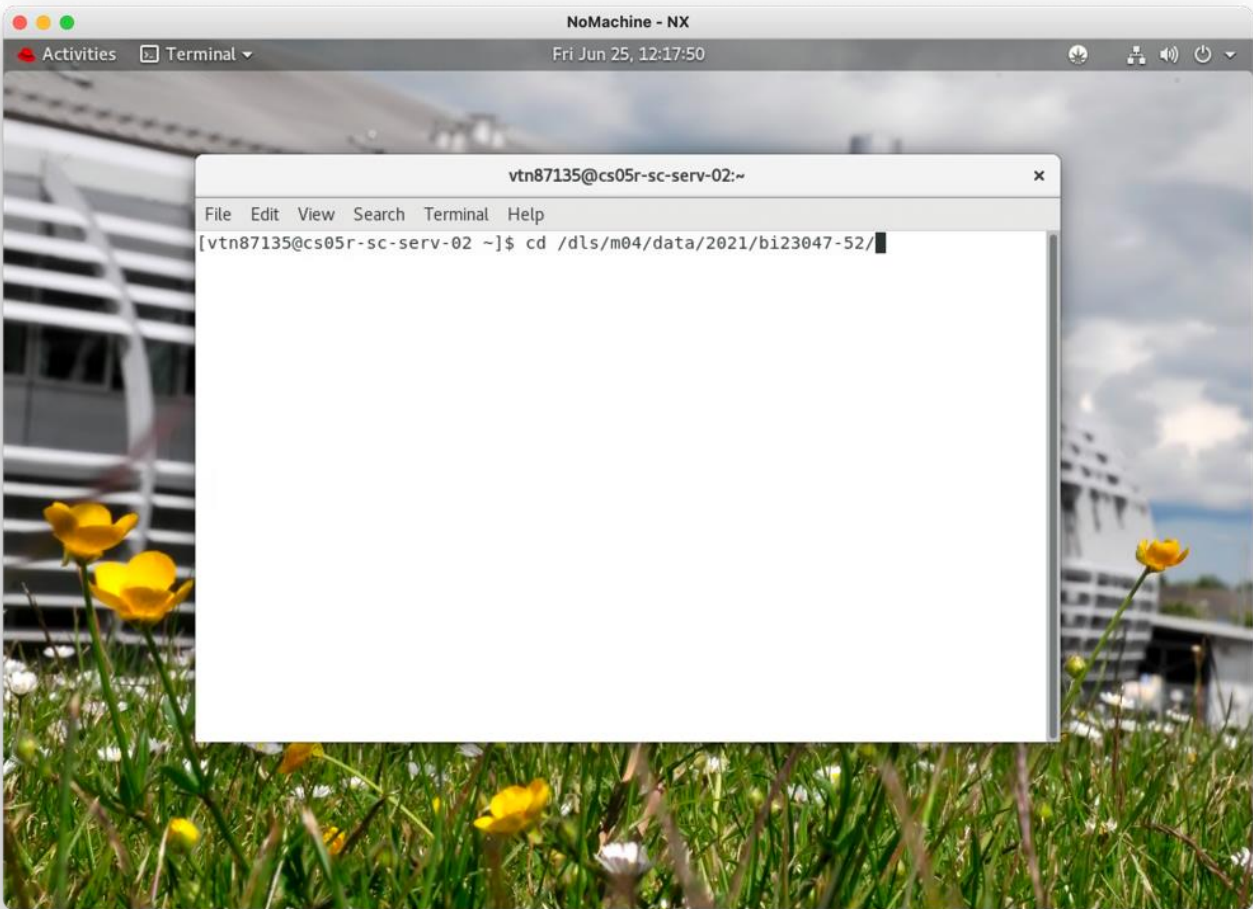
- Double-click on 'Create a new virtual desktop'





- 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





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

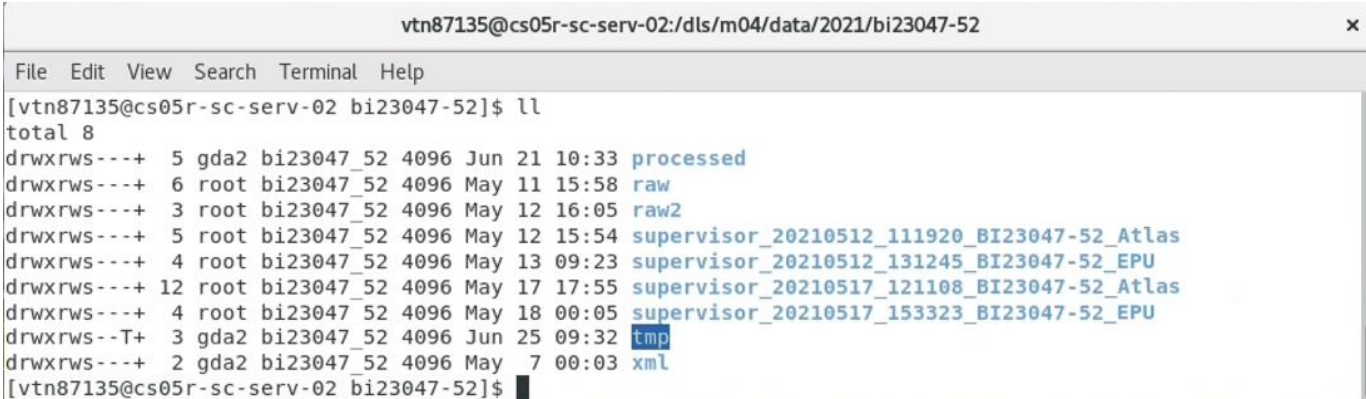
Atlas, EPU and raw directories are located in your visit directory, a typical structure is shown below:

./*_Atlas	Images that make up the grid overview
./*_EPU	Images collected during EPU setup and acquisition
./raw	Movie frames, organised in the same directory structure as in the EPU directory

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/m04/data/2021/bi23047-52/
```



```
vtn87135@cs05r-sc-serv-02:/dls/m04/data/2021/bi23047-52 x  
File Edit View Search Terminal Help  
[vtn87135@cs05r-sc-serv-02 bi23047-52]$ ll  
total 8  
drwxrws---+ 5 gda2 bi23047_52 4096 Jun 21 10:33 processed  
drwxrws---+ 6 root bi23047_52 4096 May 11 15:58 raw  
drwxrws---+ 3 root bi23047_52 4096 May 12 16:05 raw2  
drwxrws---+ 5 root bi23047_52 4096 May 12 15:54 supervisor_20210512_111920_BI23047-52_Atlas  
drwxrws---+ 4 root bi23047_52 4096 May 13 09:23 supervisor_20210512_131245_BI23047-52_EPU  
drwxrws---+ 12 root bi23047_52 4096 May 17 17:55 supervisor_20210517_121108_BI23047-52_Atlas  
drwxrws---+ 4 root bi23047_52 4096 May 18 00:05 supervisor_20210517_153323_BI23047-52_EPU  
drwxrws--T+ 3 gda2 bi23047_52 4096 Jun 25 09:32 tmp  
drwxrws---+ 2 gda2 bi23047_52 4096 May 7 00:03 xml  
[vtn87135@cs05r-sc-serv-02 bi23047-52]$
```

### 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

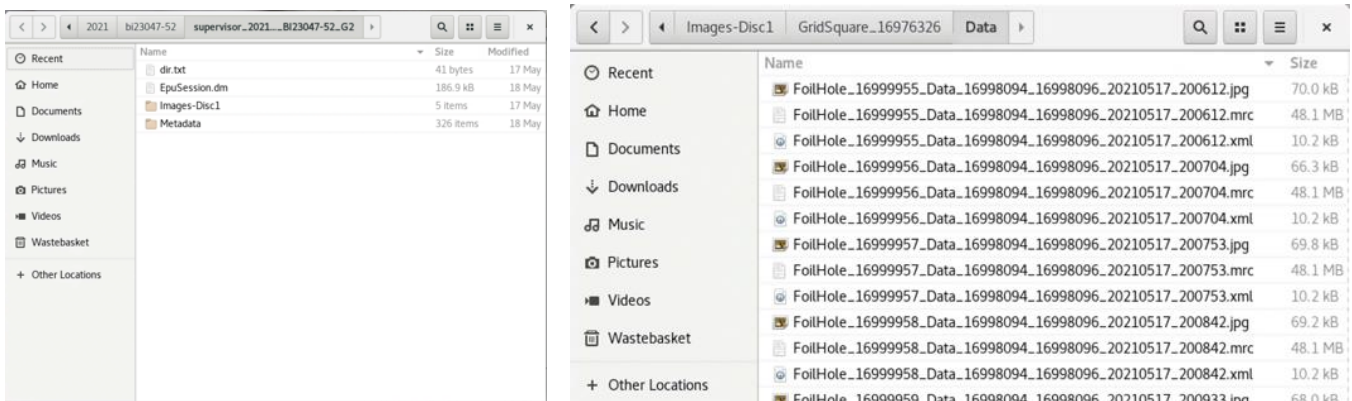
# Return the name and path of the most recent unaligned movie frame average
$ ls -ltr ./{EPU_session_directory}/Images-Disc1/GridSquare*/Data/*.mrc | tail -n 1

# 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 in a file browser

```
# Use the Linux file browser, Nautilus, to open the EPU directory
$ nautilus ./{EPU_session_directory}/Images-Disc1/
```



#### 4.2.4 View the compressed \*.jpgs of the unaligned movie frame averages

```
# Use the Linux image browser, eye of gnome, to browse the movie frame averages
$ eog ./{EPU_session_directory}/Images-Disc1/GridSquare*/Data/*.jpg
```

#### 4.2.5 Monitor your data collection session

- Verify that new micrographs are being collected during your session
- In particular, follow 4.2.1 and ensure that new files appear in the list and that they have a recent time stamp.

**Document Title:**

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

**Comments to:**

Lorna Malone

**Version:**

2.0

**Date:**

04 April 2024



Please note that EPU will pause collecting images (for all sessions) when LN2 is being refilled, or if you use a K3 camera, when GIF ZLP is being adjusted. However, this should not last longer than 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).

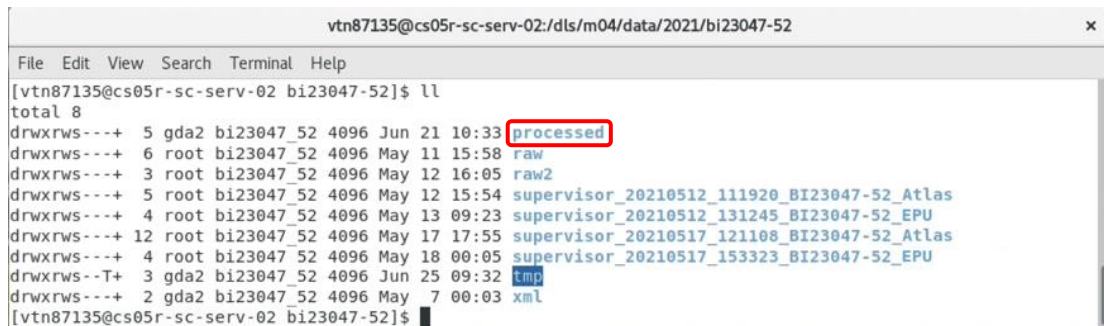
### 4.3 EPU: Inspect the on-the-fly data analysis results

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.

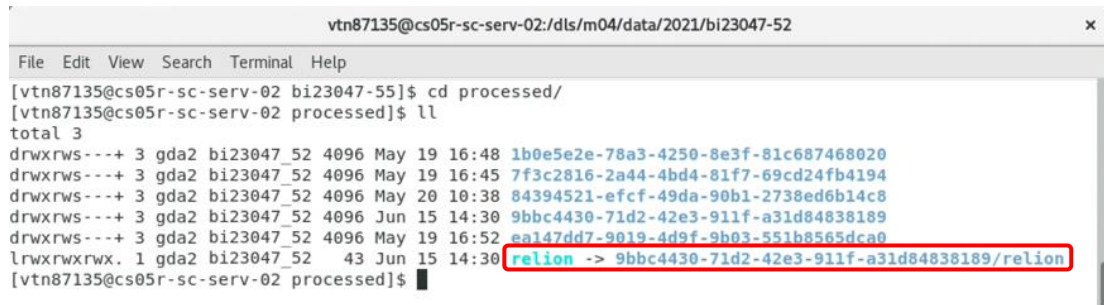
```
$ module avail EM/
```

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



```
vtn87135@cs05r-sc-serv-02:/dls/m04/data/2021/bi23047-52
File Edit View Search Terminal Help
[vtn87135@cs05r-sc-serv-02 bi23047-52]$ ll
total 8
drwxrws---+ 5 gda2 bi23047_52 4096 Jun 21 10:33 processed
drwxrws---+ 6 root bi23047_52 4096 May 11 15:58 raw
drwxrws---+ 3 root bi23047_52 4096 May 12 16:05 raw2
drwxrws---+ 5 root bi23047_52 4096 May 12 15:54 supervisor_20210512_111920_BI23047-52_Atlas
drwxrws---+ 4 root bi23047_52 4096 May 13 09:23 supervisor_20210512_131245_BI23047-52_EPU
drwxrws---+ 12 root bi23047_52 4096 May 17 17:55 supervisor_20210517_121108_BI23047-52_Atlas
drwxrws---+ 4 root bi23047_52 4096 May 18 00:05 supervisor_20210517_153323_BI23047-52_EPU
drwxrws--T+ 3 gda2 bi23047_52 4096 Jun 25 09:32 tmp
drwxrws---+ 2 gda2 bi23047_52 4096 May 7 00:03 xml
[vtn87135@cs05r-sc-serv-02 bi23047-52]$
```

Analysis jobs are given a unique identifier and a symbolic link (relic) is created pointing to the most recent analysis job:



```
vtn87135@cs05r-sc-serv-02:/dls/m04/data/2021/bi23047-52
File Edit View Search Terminal Help
[vtn87135@cs05r-sc-serv-02 bi23047-55]$ cd processed/
[vtn87135@cs05r-sc-serv-02 processed]$ ll
total 3
drwxrws---+ 3 gda2 bi23047_52 4096 May 19 16:48 1b0e5e2e-78a3-4250-8e3f-81c687468020
drwxrws---+ 3 gda2 bi23047_52 4096 May 19 16:45 7f3c2816-2a44-4bd4-81f7-69cd24fb4194
drwxrws---+ 3 gda2 bi23047_52 4096 May 20 10:38 84394521-efcf-49da-90b1-2738ed6b14c8
drwxrws---+ 3 gda2 bi23047_52 4096 Jun 15 14:30 9bbc4430-71d2-42e3-911f-a31d84838189
drwxrws---+ 3 gda2 bi23047_52 4096 May 19 16:52 ea147dd7-9019-4d9f-9b03-551b8565dca0
lrwxrwxrwx. 1 gda2 bi23047_52 43 Jun 15 14:30 relic -> 9bbc4430-71d2-42e3-911f-a31d84838189/relic
[vtn87135@cs05r-sc-serv-02 processed]$
```

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

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

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

# Load Relion in read only mode
$ relic --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

Having navigated to your visit directory by following section 4.1, you can then use the terminal to inspect the progress of the data collection. A typical TOMO5 directory structure is shown below. Follow a similar procedure to 4.2 and list the latest tomogram that was written to disk. Check the time stamp as it should be updated frequently.

```
vtn87135@cs05r-sc-serv-02:/dls/m04/data/2021/bi23047-52
File Edit View Search Terminal Help
[vtn87135@cs05r-sc-serv-02 bi23047_5]$ ll
total 523
dr-xrws---+ 2 gda2      bi23047_5  4096 Jun 18 00:03 processing
drwxrws---+ 2 root     bi23047_5 524288 Jun 23 09:41 raw
drwxrws---+ 2 gda2     bi23047_5  4096 Jun 18 00:03 spool
drwxrwxr-x+ 6 m06detector bi23047_5  4096 Jun 21 13:46 Supervisor_20210621_BI23047-5_atlas
drwxrwxr-x+ 3 m06detector bi23047_5  8192 Jun 23 10:46 Supervisor_20210621_BI23047-5_tomo
drwxrws--T+ 2 gda2     bi23047_5  4096 Jun 18 00:03 tmp
drwxrws---+ 2 gda2     bi23047_5  4096 Jun 18 00:03 xml
[vtn87135@cs05r-sc-serv-02 bi23047_5]$
```

```
# 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).

**Document Title:**

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

**Comments to:**

Lorna Malone

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## 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>