Remote Access Guide for PROXIMA 2A

Version 06 April 2023

Revised 26 May 2023

Outline

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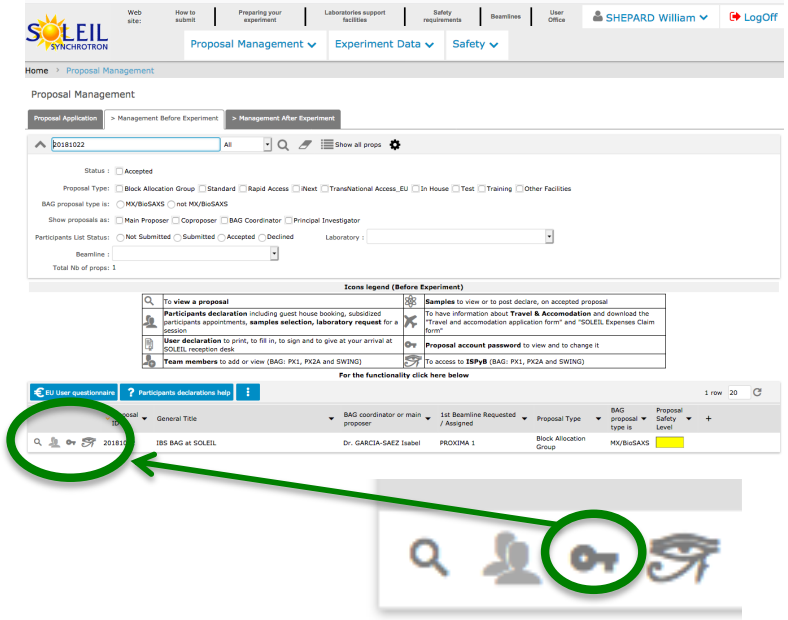
Preparing for REMOTE ACCESS : Sending Dewars

- Please read the tutorial on the PX2-A web site
  - https://www.synchrotron-soleil.fr/fr/lignes-de-lumiere/proxima-2a
- A week before your session, send your Dewar to SOLEIL
  - 2 options:
    - Courrier-delivered (Fedex, DHL, UPS,…)
      - Pre-paid Air Way Bills (SOLEIL, iNext or User)
    - Hand-delivered directly to the SOLEIL gate
      - Please organise a single delivery with the local contact
  - Dewars must arrive:
    - **Monday – Friday, except bank holidays**
    - **At least 1 day before beamtime**
    - **Before 12h00 (mid-day)**
  - Dewars must be properly labelled (especially those hand-delivered):
    - Beamline's Name
    - Local Contact's Name
    - Sender's Name & Telephone number
  - Please include:
    - Hard Disk Drive (≥1 TB)
    - **Return Label or Transporter's Return Air Way Bill**

Note: The PX2-A CATS Dewar holds nine (9) uni-pucks!

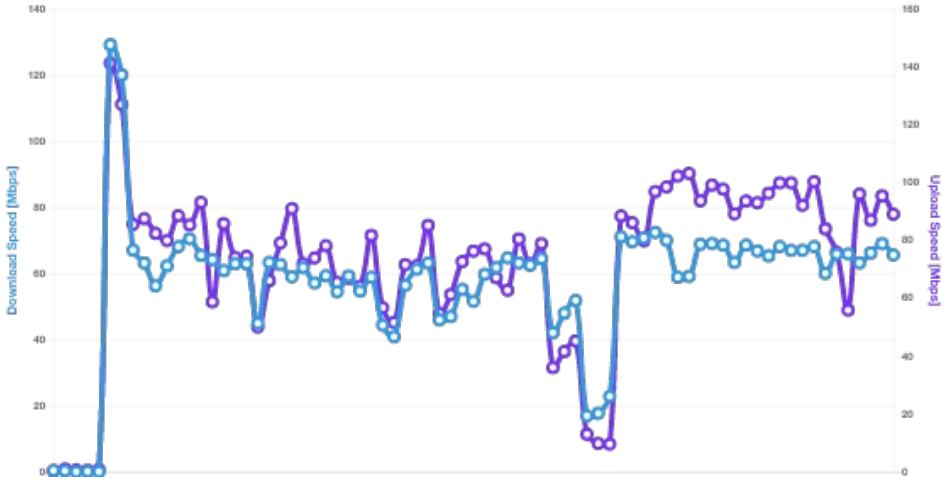
Preparing for REMOTE ACCESS: Account Activation

- Before your remote access session:
  - Obtain your SUNSET **project number and password**
    - E.g. 20190987, wR3nJH9s
  - Declare the remote participants
    - Declare the **Local Contact as the Session Responsable**
  - Test the connection to SOLEIL
    - Remote Access is activated **23 hours before** your session
    - and deactivates **25 hours after** your session
    - Contact the BL staff to set up a Remote Test
  - Send us a telephone number or Skype address
- IMPORTANT, you need:
  - To Install NoMachine
    - Also XQuartz for Mac
  - Decent internet connection
    - e.g. fiber optic, ADSL, 4G or 5G, not a modem
  - QWERTY keyboard
    - Try the command `setxkbmap fr` for AZERTY keyboards
    - Try the command `setxkbmap us` for QWERTY keyboards
  - Mouse with left & right buttons and scroll-wheel
    - To ALIGN, MOUNT and ROTATE samples
  - High resolution display(s) – **This is important!**
    - MXCuBE is optimised for **2560 x 1440**
    - **Otherwise, you will not see the bottom part of the MXCuBE window**



Testing your Internet Connection Speed

- Speedcheck.org
  - Latency
    - Return « ping » of small packets
    - Measure of Responsiveness
  - Download
    - Multiple connections opened
    - Send large file on all connections
  - Upload
    - Multiple connections opened
    - Receive large file on all connections



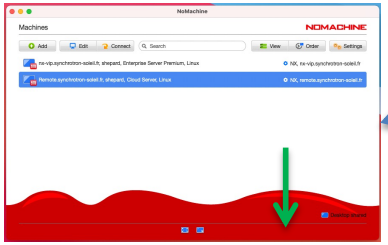
Connection Type	Latency [ms]	Download [Mbps]	Upload [Mbps]	Comments
Phone Hotspot @ PX2-A	120 - 250	0.03 - 0.43	0.33 – 1.00	5 s delays via Google Meet, sluggish but possible
SOLEIL Site @ PX2-A	50-51	120-129	127- 141	SOLEIL Site Network for office PCs, no connection to BL
SOLEIL Wifi @ PX2-A	22-39	144-178	168-192	Via SOLEIL Wifi Network on PX2-A (17/03/2023)
Freebox 4k @ chez Bill, Wifi < 30 cm	25-90	45-65	50-80	NX, MXCuBE, Albula, Webcams, GMeet, Zoom (on 2nd Mac)…
Freebox 4k @ chez Bill, Wifi > 30 m*	35-45	15-55	10-70	Wifi station NOT in line of site, frequent cuts in connection

Updates and Changes

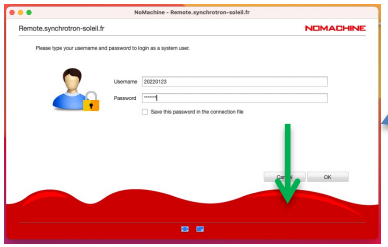
- SOLEIL has a new remote access server:
  - **Host = remote.synchrotron-soleil.fr**
    - **Port = 4000**
    - **Protocol = NX**
  - **nx-vip.synchrotron-soleil.fr** should **NOT** be used
- PROXIMA 2A has a new MXCuBE workstation:
  - **proxima2a-pc4** (pc4)
    - Custom Display ONLY
  - **proxima2a-10** (p10) = old workstation
    - Still available via remote.synchrotron-soleil.fr
    - Physical and Custom Displays available
- NoMachine version 6
  - All workstations have been upgraded the NoMachine version 6
- ALBULA & ADXV
  - ADXV launches automatically with MXCuBE
    - A spot search algorithm (TIOGA) will display blue boxes around spots
  - ALBULA can be launched via command line on **proxima2a-pc4**
    - **albula** or **albula_4.1**

Connect via NoMachine (1): First Steps

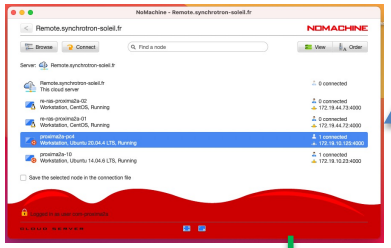
- Start by clicking on the NoMachine icon
  - Within 23 hours before your session



- Click on **`remote.synchrotron-soleil.fr`**

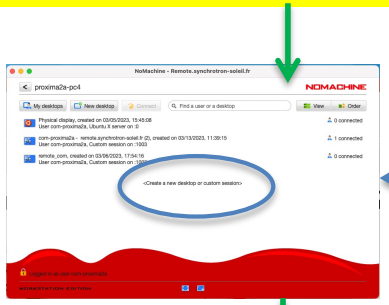


- Enter your project-id and its password
  - For example: **`20230123`** [**`W8d9kJ43`**]

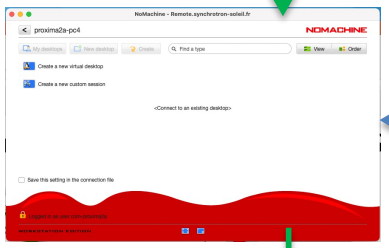


- Click on **`proxima2a-pc4`**
  - This is a new workstation that replaces **`proxima2a-10`**

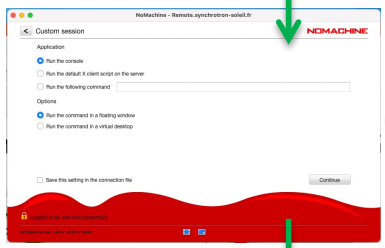
Connect via NoMachine (2): Custom Display



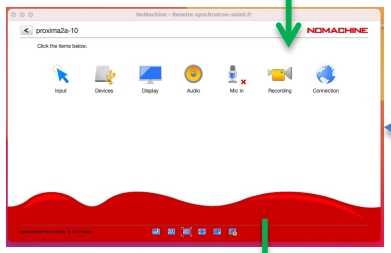
- Click on: **`Create a new desktop or custom session`**



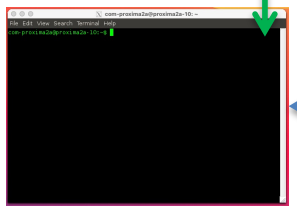
- Click on: **`Create a new custom session`**



- Click on **`Continue`**
  - Activate Run the console
  - Activate Run the command in a floating window

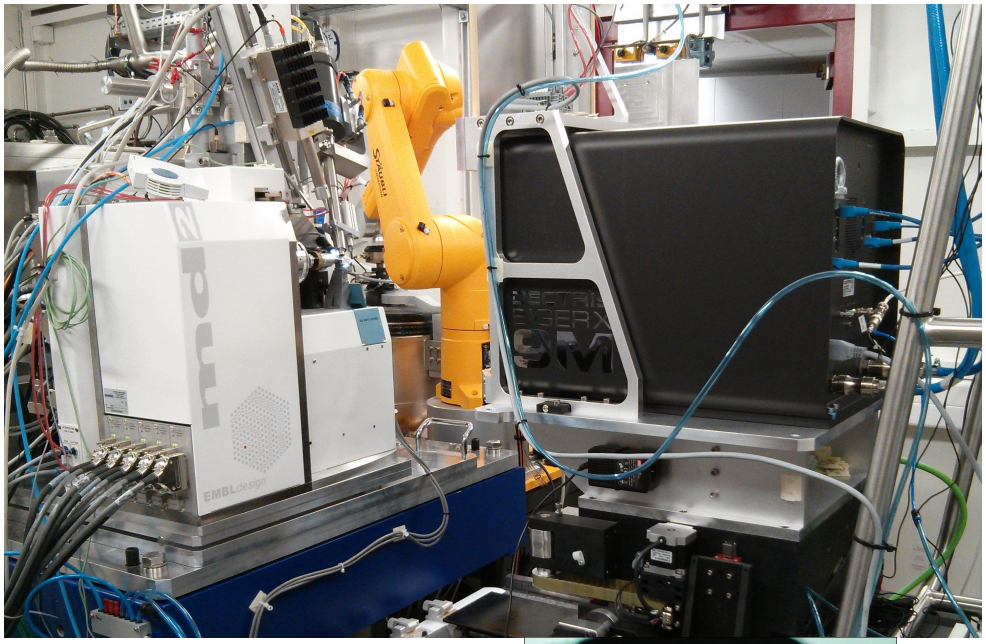


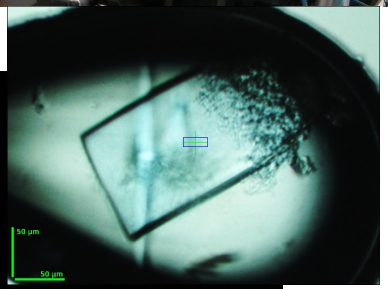
- Machine and Display options window
  - Do not modify the options
  - You will be connected soon…



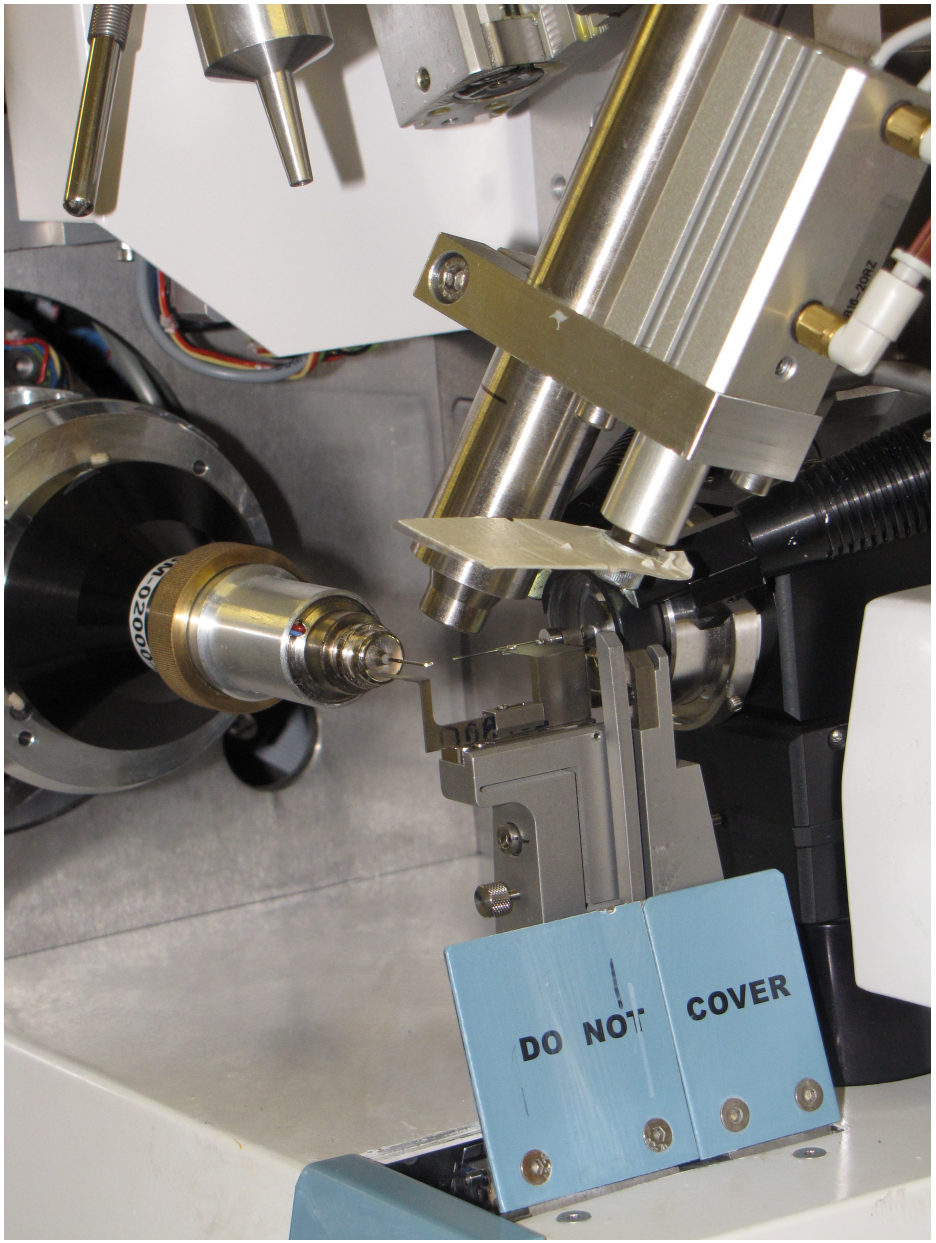
- Success!
  - This last step may take awhile (> 60 seconds)

PX2-A Overview: Sample Environment & Performances





- 10 µm * 5 µm FWHM (H*V)
- Energy range 6 – 18 keV
- X-ray flux ~10^{12} ph/s @ 12.65 keV
- X-ray flux density 2.5x10^{10} ph/s/µm^2
- Stability <1 µm (4-6 hours)

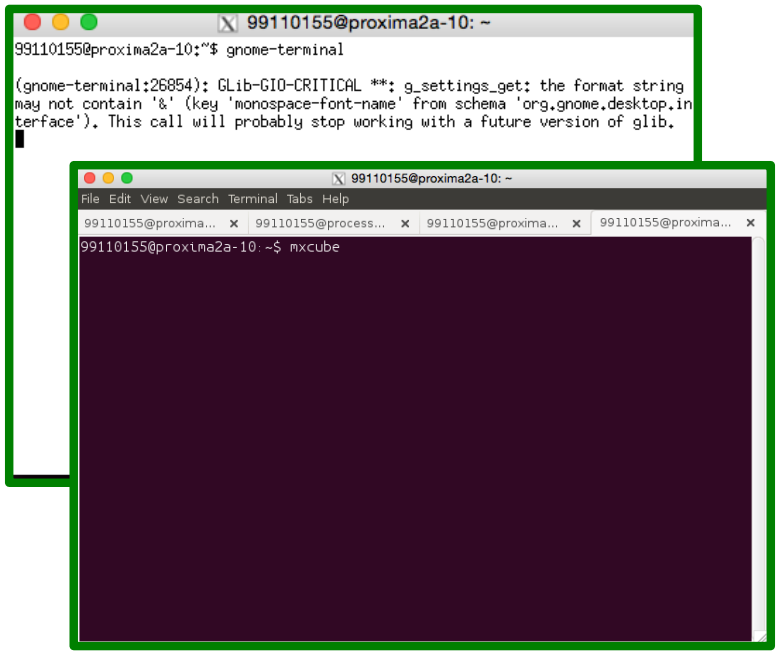


X-Terminals

- NoMachine should display:
  - A NoMachine window with Settings Icons, and
  - A purple gnome-terminal window with a prompt
    - If not, then a white X-terminal should display
    - Type: **`gnome-terminal`**

- If your key board is AZERTY
  - **`setxkbmap fr`** for AZERTY
  - **`setxkbmap us`** for QWERTY

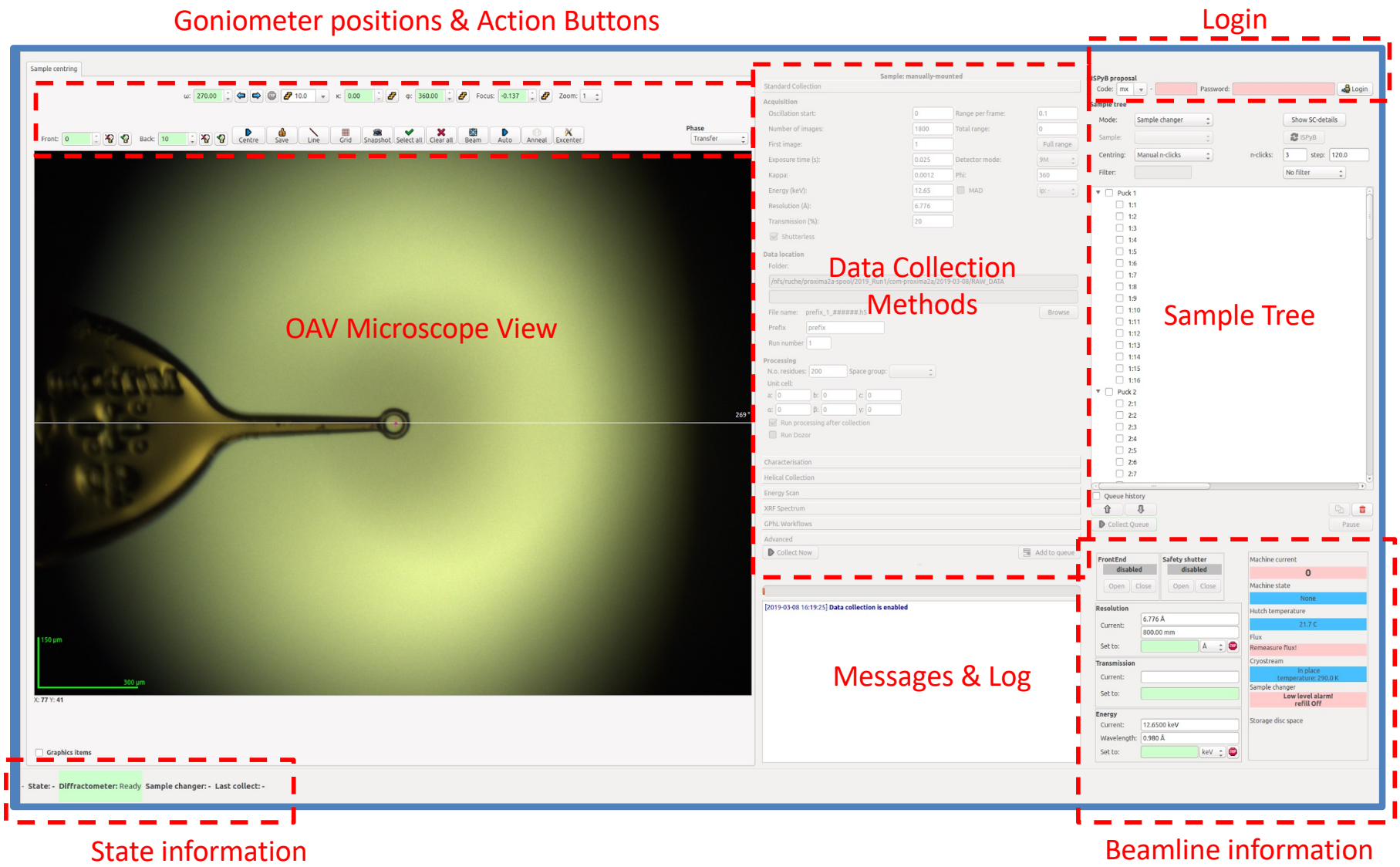
- In the **purple** gnome-terminal , open 4 tabs:
  - **`<shift-ctrl-t>`**
    - Opens a new tab
  - **`mxcube`**
    - Opens an MXCuBE window
  - **`albula`**
    - Opens a window to visualise diffraction images
  - **`firefox -P`**
    - Opens a browser window for web cams
  - **`ssh –X process1`**
    - Connects to the data processing server



- To log out:
  - Type **`exit`** or **`<ctrl-d>`** in the X-terminals
    - This closes the session under NoMachine

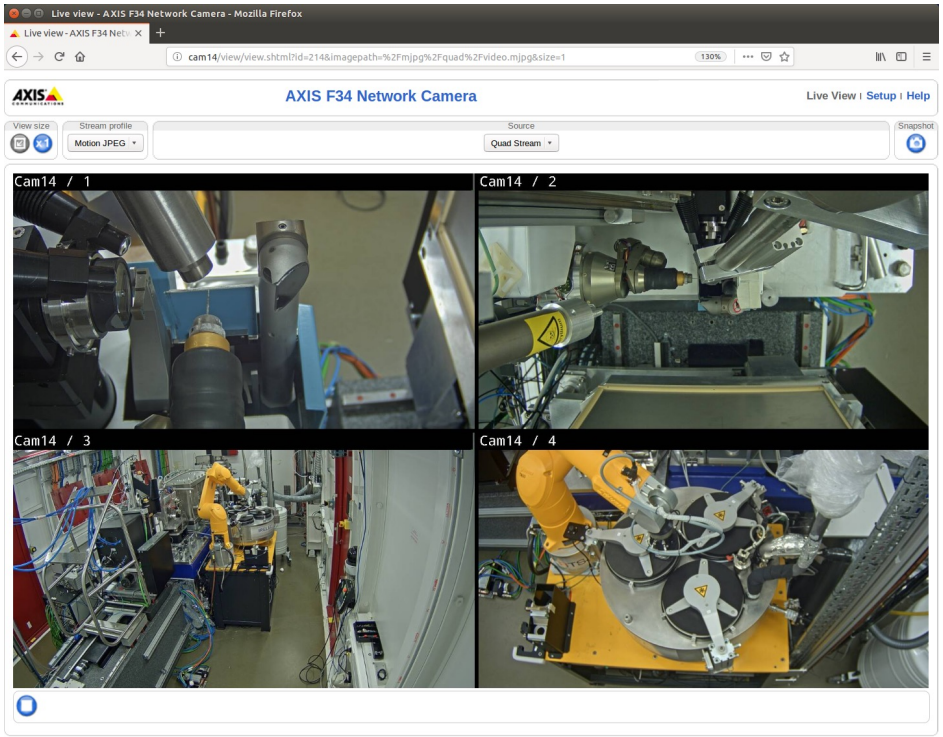
MXCuBE Overview

- Type « **`mxcube`** » in a terminal window
  - Less than 2 minutes to start up
  - Logfile output is displayed in the terminal window
- Login to MXCuBE with your project number and password:
  - For example: **`20230123`** & **`rF67wEr325`**
  - Click **`OK`** when the small dialogue box appears



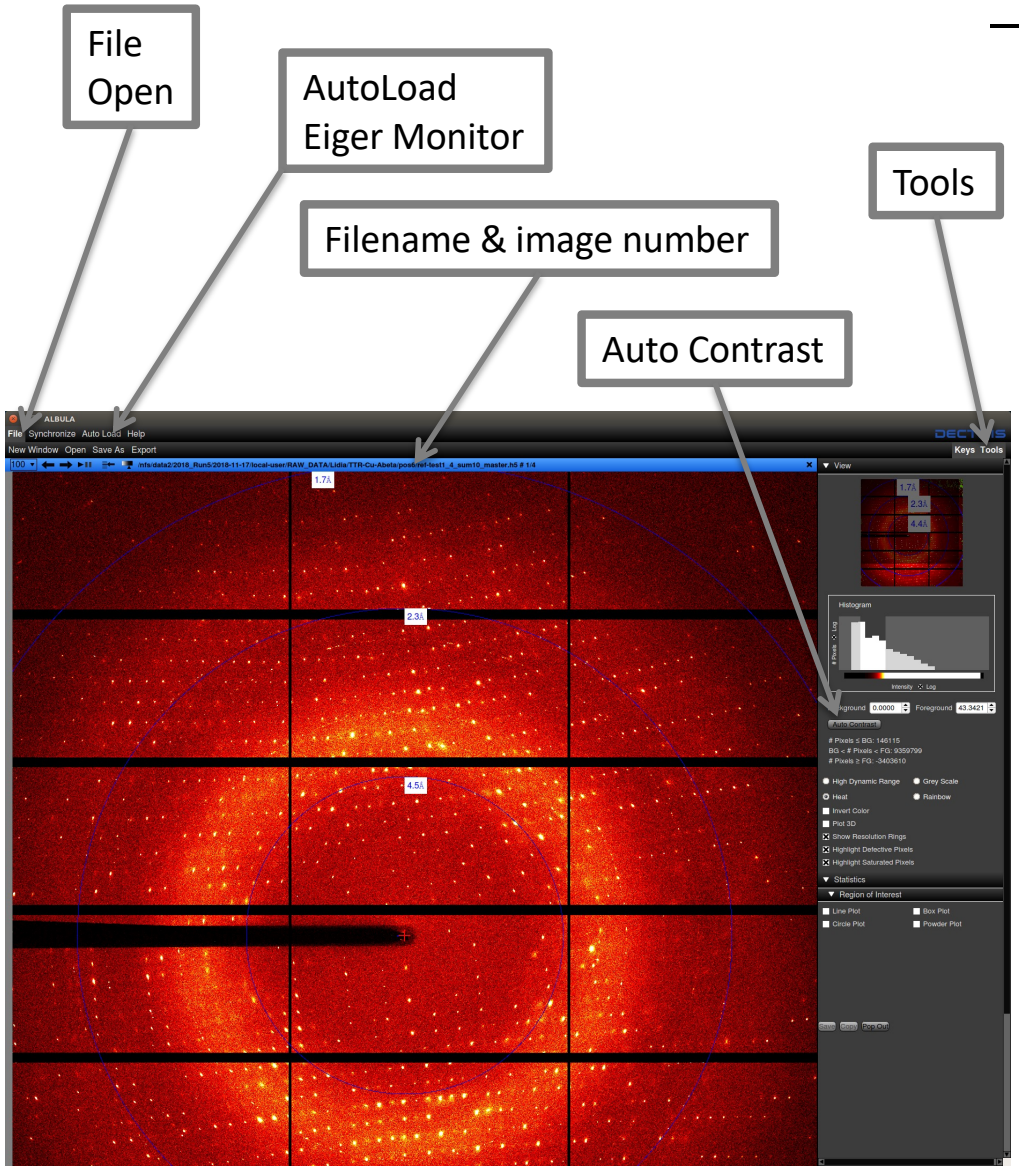
Firefox & Webcams

- Open a tab and type:
  - **`firefox`** or **`firefox -P`**
    - Set AutoDetect Proxy settings
      - Preferences/Network Setting/ AutoDetect Proxy Settings
    - http://cam14/view/view.shtml
      - Four views of sample and beamline
    - http://cam6/view/view.shtml
      - View above hutch door
    - http://cam8/view/view.shtml
      - Overhead view of CATS Dewar
    - http://cam13/view/view.shtml
      - Motorized view of CATS, MD2 & EIGER
    - http://cam1/view/view.shtml
      - Motorized view of sample pin



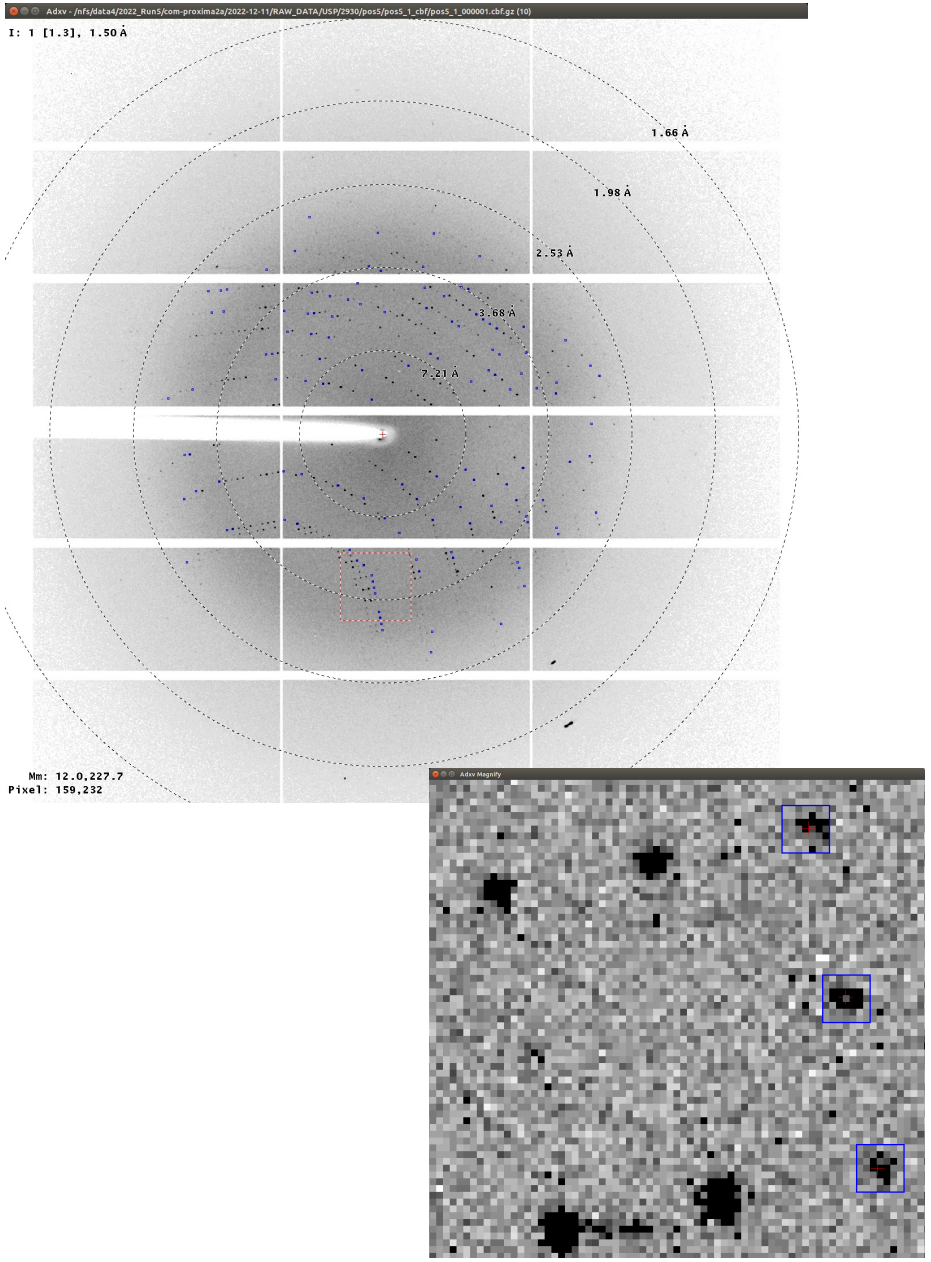
Cam14 views

ALBULA



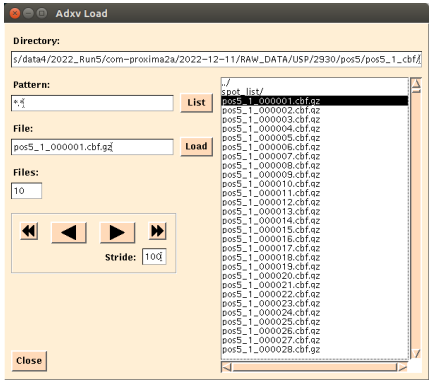
- Open a tab and type:
  - **`albula`**
    - Visualises diffraction images
    - Click **Tools**
      - to change colour map, add resolution rings, etc…
    - Click **Autoload/Eiger_Monitor**
      - To visualise the last image collected
      - Click on the DOWN ARROW to verify
        - » Host: 172.19.10.26
        - » Port: 80
        - » Min Pause (s): 1
    - Click **File/Open**
      - Select a master file
        - » **`*_master.h5`**
      - Wedges of summed images
        - » **`*_sum10_master.h5`**
    - Click on **Auto Contrast**
      - To adjust the contrast
    - Known Bugs
      - Refresh the resolution rings with the scroll wheel
      - Differences between **pc4** and **p10**:
        - » AutoLoad does not work on **p10**
        - » Only SUM10 images on **p10**
        - » When remote, the **pc4** physical display needs to be logged in as project_number

ADXV



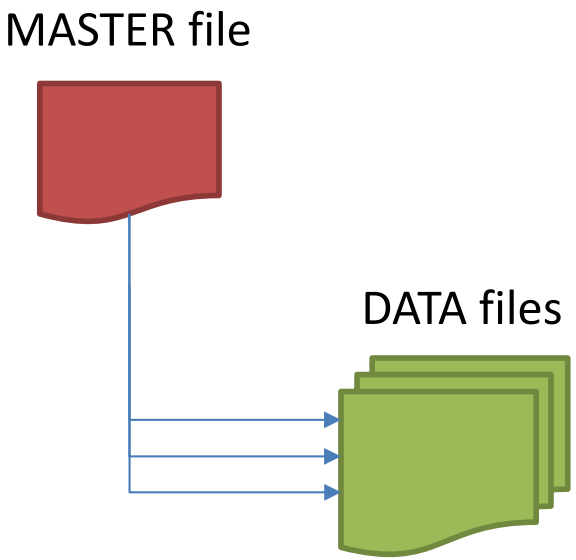
- ADXV_FOLLOW
  - Displays diffraction images automatically during collections
  - Launched with MXCuBE
  - If not, in an X-terminal window type:
    - **`adxv_follow`**
    - or **`adxv`** to display single images
  - TIOGA
    - Fast spot finding algorithm
    - Appears as blue squares
      - **It may become "out-of-sync"**

- ADXV Commands
  - Loads **`*.cbf.gz`** files
  - Video
  - Files = Sums N images
  - Stride = Skips N images
  - Type "**`h`**" to auto-adjust contrast

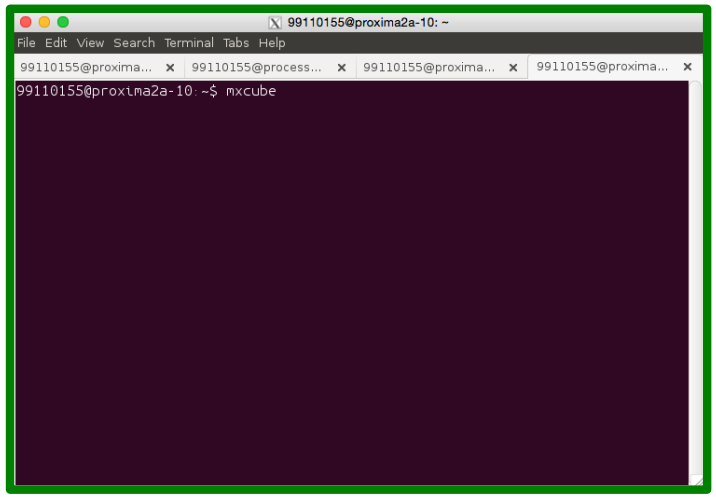


EIGER HDF5 File Architecture

- HDF5 files are “structured containers” made up of two types of files:
  - ONE **MASTER** file
  - MANY **DATA** files
- MASTER file
  - **`*_master.h5`**
  - Meta data
    - X-ray wavelength
    - Distance
    - Beamcenter
    - Goniometer angles
    - Pointers to DATA files
    - etc…
- DATA files
  - **`*_data.h5`**
  - Blocks of images per file
    - 1 to 1000s
- DO NOT CHANGE HDF5 FILE NAMES!!!
  - Keep master and data files in same directory
- Editing scripts
  - **`fix_negative_transformation.py`**
    - Fixes a geometrical parameter required by DIALS & XIA2



Data processing on “Process1”



- Open an X-terminal, type:
  - **`ssh –X process1`**
  - 288-core server
  - Dedicated to processing
- Some basic commands:
  - **`goimg`**
    - Go the latest data collection directory
    - **`/nfs/data2/2023_Run2/20220789/2023-03-17/RAW_DATA/MyProj/process`**
  - **`goxdsme`**
    - Go to the latest directory and launch XDSME on latest data collected
    - **`/nfs/data2/2023_Run2/20220789/2023-03-17/RAW_DATA/MyProj/process/xdsme_MyXtal_1`**
  - **`goxdsme --brute`**
    - Process for difficult indexing cases
  - **`goxdsme --weak`**
    - Process for weakly diffracting data
  - **`xdsme –help`**
    - More information…

Data processing with XDSME

- For **quick** processing in the X-terminal type:
  - **`goimg`**
    - To go to the « process » directory of the **most recently** collected data
  - **`goxdsme`**
    - To process the **most recently** collected data

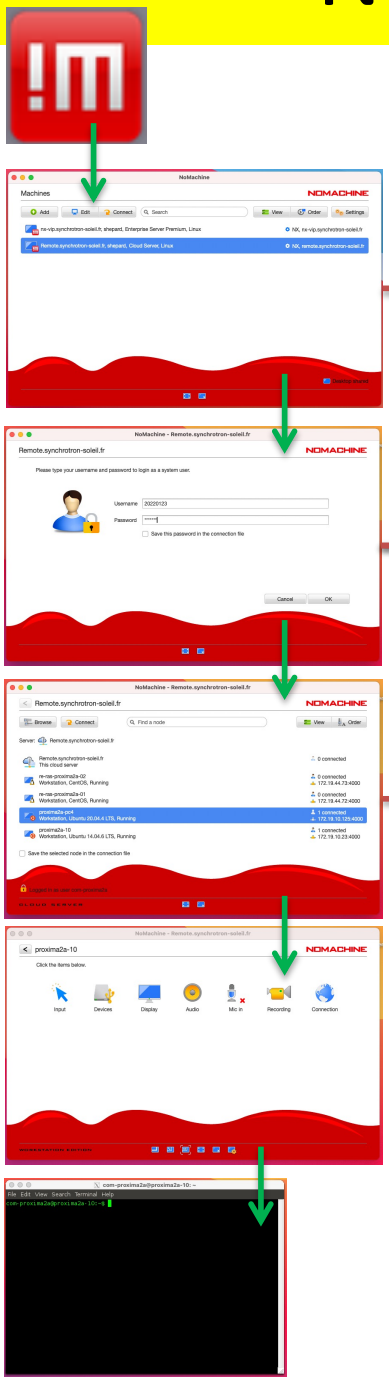
- For processing older data :
  - Go to the directory of the **most recently** collected data
    - **`goimg`**
  - Change to the desired « process » directory, for example:
    - **`cd ../../../puck4356/pin15/process`**
  - Process the specific master file with **xdsme** (not goxdsme):
    - **`xdsme ../pin15_2_master.h5`**

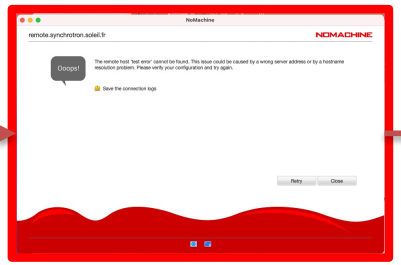
- Common XDSME options:
  - **`xdsme --brute ../pin15_2_master.h5`**
    - Tries hard to index…
  - **`xdsme --weak ../pin15_2_master.h5`**
    - For cases with weak diffraction
  - **`xdsme –r 3.5 ../pin15_2_master.h5`**
    - Limits the resolution to 3.5 Å
  - **`xdsme –s P2 –c “102 124 87 90 97 90” ../pin15_2_master.h5`**
    - Inputs space group and unit cell
  - **`xdsme –F 301 –L 3300 ../pin15_2_master.h5`**
    - Processes from images 301 (first) to 3300 (last)
  - **`xdsme –h`**
    - Prints out “help” and more options

Help, Hints, FAQs & Bugs

- Some DON'Ts
  - DON'T use VPN at the same time as No Machine
    - Disconnect your VPN software (Junos Pulse, etc…)
- Some DOs
  - DO use GNOME-TERMINAL
    - Use the command: **gnome-terminal**
  - DO create your own FIREFOX profile
    - Use the "-P" option: **`firefox –P`**
- Keyboard Settings
  - Use the command **`setxkbmap fr`** for AZERTY
  - Use the command **`setxkbmap us`** for QWERTY
- NoMachine Errors
  - Ooops! Negociation failed…
    - Your user_id does not have permission to connect to the NX server
    - DO NOT USE: **`nx-vip.synchrotron-soleil.fr`**
    - INSTEAD USE: **`remote.synchrotron-soleil.fr`**
  - Ooops! The remote host "name" can not be found…
    - Check the host name, port number and protocol are correct
  - Authentication failed…
    - Check the project_id and password are correct
  - Ooops! Could not connect to server. Error 60 Timed out
    - The project_id may not have permission to connect
    - Verify the current time is within 23 hours before and 25 hours after the session time
- HINTS
  - If the Data Collection widgets are GREYED OUT
    - Check that you are logged in to MXCuBE
    - Click on the Sample Line in the Sample Tree
  - To highlight which sample is mounted
    - Use the "ISpyB" button to refresh the Sample Tree
  - If you can NOT find your HDF5 images
    - Check the project_number in the pathname
    - Check that "downloader" is running under your user_id
      - Type in an X-terminal: **`downloader status`**
      - If it is NOT RUNNING : **`downloader start`**
      - If it is RUNNING under another user_id
        - » Call the Local Contact
  - Robot collisions
    - Check the position of the robot arm via the webcams
    - Try the **SAFE** button in MXCuBE
    - If not, the call the BL or EHOs (ext 9797)
  - If the microscope image is dark (deactivated)
    - Check that the "camera" device server is running
      - Type in an X-terminal: **`camera restart`**
- Telephone numbers
  - Beamline telephone numbers:
    - +33-1-6935-8181 (wireless)
    - +33-1-6935-8180 (landline)
  - Experimental Hall Operators (EHOs)
    - +33-1-6935-9797 (after 11 pm)

NoMachine Connection Errors

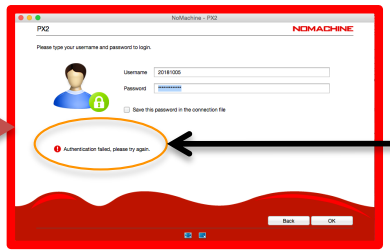




"Oops! The remote host can not be found":

1) Click EDIT
2) Check the host, port and protocol
   - Look for typographical errors

```
Host = remote.synchrotron-soleil.fr
Port = 4000
Protocol = NX
```



1) The username/password is wrong, or
2) REMOTE ACCES has **not** been activated for the project number.
   - Please wait until 23 hours before the session
   - If not then contact the LC

"Oops! Could not connect to the server"

1) Try switching off any VPN?
2) Maybe the NX node is saturated?
   - Please contact the LC

?

"Oops! The session negociation failed."

1) Maybe too early to connect?
2) Maybe the NX node is saturated?
   - Please contact the LC

?