

I16 Remote Access Manual

Remote Access to Data and Software for I16 Users

The following explains how to access data and watch data collection during your experiment.

NoMachine and nx-user

The simplest way to access data remotely is by connecting to Diamond's remote NX server. To connect you must have NoMachine installed, available from:

<https://www.nomachine.com/>

Once installed, create a connection using the steps below or see [here](#) for more info:

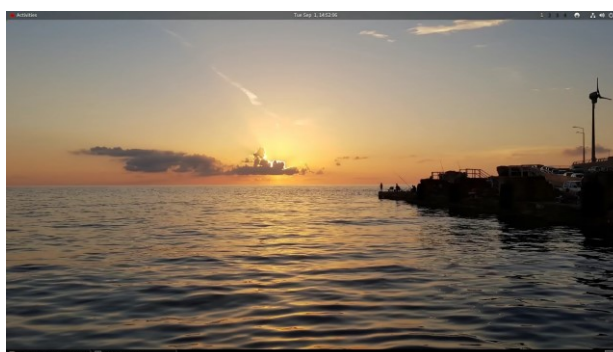
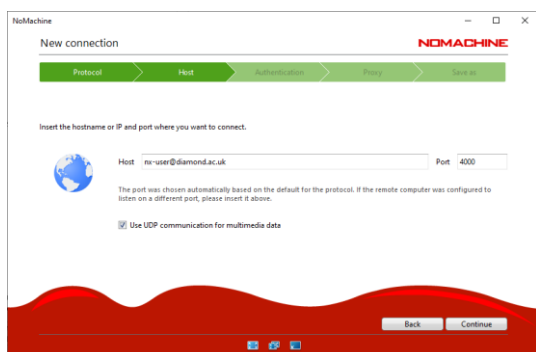
- Open NoMachine
- Create "New" connection (or Add+):
 - Protocol – NX
 - Host – **nx-user.diamond.ac.uk**, Port: **4000**
 - Password, no proxy
- Open new connection:
 - Enter username and password – **your FedID/ email address**, as used in the user account system (UAS) for proposals.
 - Create a new virtual desktop
 - To create shortcuts in your home directory and on the desktop, run the following bash script: `/dls_sw/i16/scripts/Users/i16_rhel7_user_setup.sh`

You are connected and have a virtual desktop to Diamonds RedHat Linux distribution. The desktop is your own and any files saved in personal directories are only accessible by yourself. Settings and layouts will be saved for the next time you log in (see the last page for useful settings to change).

You have access to your own personal home directory and to the I16 software, scripts and data directories:

<code>/dls/i16/data/2023/mm####-1</code>	Data directory (mm####-1 = your experiment ID)	Read only
<code>/dls_sw/i16/scripts/2023/mm####-1</code>	Scripts directory	Read/ write
<code>/dls_sw/i16/software/python/userscripts/i16user</code>	Software directory	Read/ write

To change settings including resolution, or to close the connection, you can access the settings menu by **hovering your mouse at the top right** of the screen/ window.



Activating Software in Diamond Linux

The Diamond RedHat Linux distribution does not allow root privilege so installation of software is not possible. Software and environments can be activated via the module load system. The following Terminal commands are useful:

Terminal Command	Description
module load ...	Load a piece of software called ...
module load python/3	Activate python 3 environment with Anaconda
module avail ...	Search module system for software
pip install --user ...	Install python packages to user directory (no root required)

I16 Data Viewer

The I16 Data Viewer is a simple way to look at the latest data and perform various analysis including fits and new regions of interest. Start the software by running Py16GUI.py from the terminal:

- Open a Terminal (Activities>Terminal)
- Use the following commands:

```
➤ module load python/3
➤ ipython -i --matplotlib tk /dls_sw/i16/software/python/Py16/Py16GUI.py
```

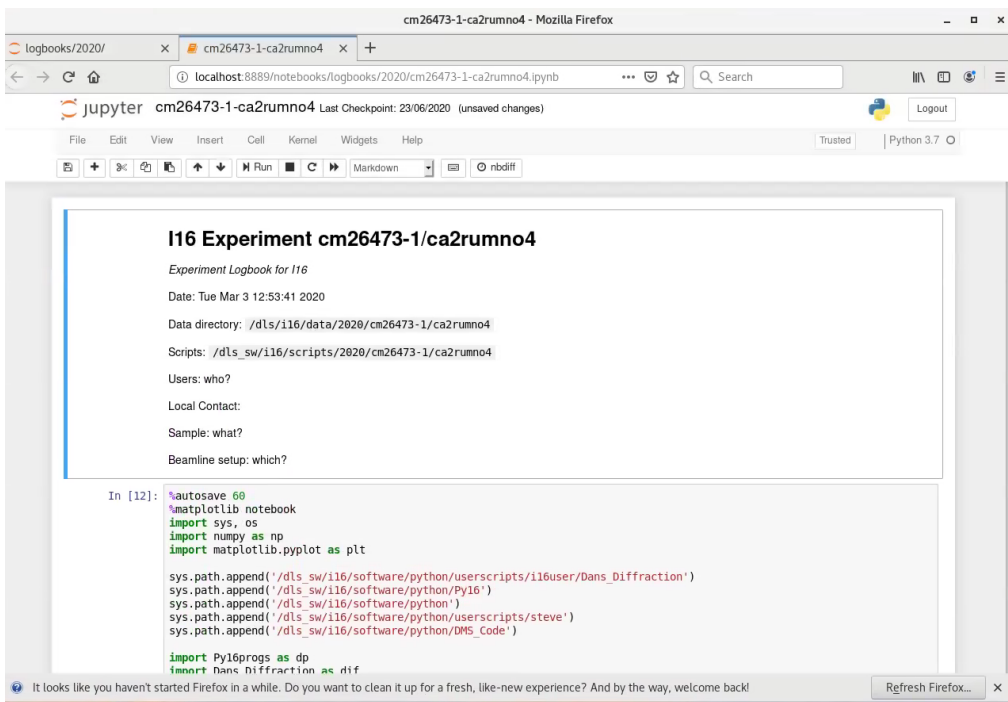
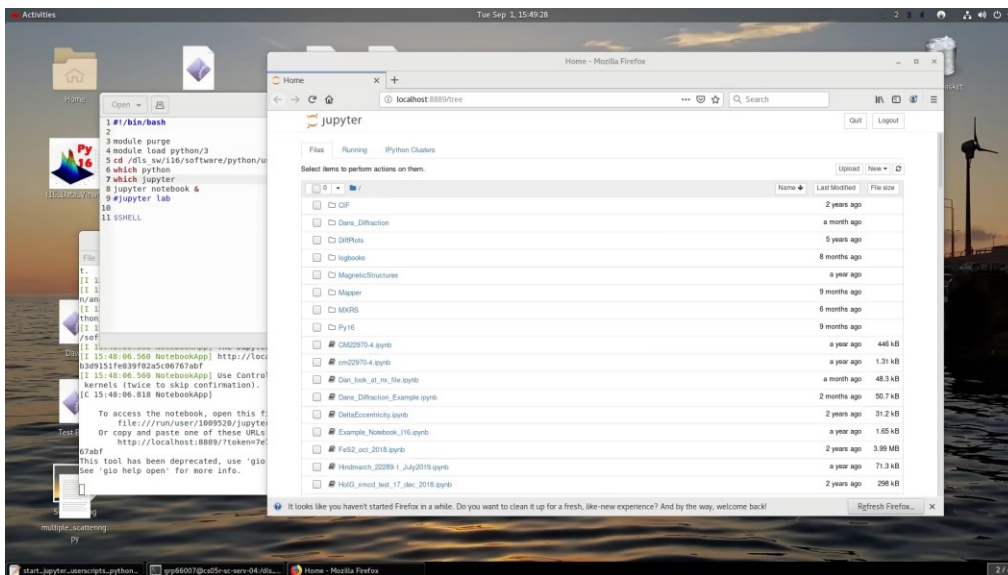
- Once the interface has opened, set your Data folder (/dls/i16/data/2020/mm####-1)
- Press “Last” to see the latest scan.
- Press “Update Pilatus Plot” to see the detector images for the currently selected scan.
- Press “Last scans window” (bottom left) to open a list of the previous scans.
- Press “Peak Analysis” (Top right) to open multi-plotting and multi-fitting options.
- Further information can be found here: <https://github.com/DanPorter/Py16>

The screenshot displays the I16 Data Viewer application. On the left, a terminal window shows the output of a scan analysis, including parameters like Peak Height, FWHM, Background, Area, and χ^2 per free par. The main window features a plot of intensity (APD/100000) versus ppp_offset, showing a prominent peak at approximately 4.22. The plot is labeled with scan number #820912. To the right of the plot, a list of parameters is displayed, including Scan No, Command, Npoints, HKL, Energy, Temp, Atten, Minimirrors, Detector offset, and various slit and detector parameters. At the bottom, there are several control buttons and a status bar indicating the current scan and time taken.

Jupyter Notebook

Jupyter is a great environment for analysing data and writing experiment logbooks, start a server and open in FireFox using the following commands:

- Open a Terminal (Activities>Terminal)
- Use the following commands:
 - `module load python/3`
 - `cd /dls_sw/i16/software/python/userscripts/i16user`
 - `jupyter notebook &`
- Note Jupyter opens in the current directory and can't move upwards, so if you want to create a logbook in your home directory, open jupyter there (it can't be accessed by anyone else).



Useful Jupyter Commands

Ctrl+Enter	Run Cell (don't continue)
Shift+Enter	Run Cell (Continue to next line)
H	Show shortcuts
P	Issue Command

Symbolic Links (shortcuts) to I16 Directories

Set up symbolic links from your home directory to the I16 data directory.

#!/bin/bash

Create symbolic links to I16 folders in ~/i16

Make directory

```
mkdir -p ~/i16
```

```
currentyear=$(date +"%Y")
```

create links

```
ln -s /dls/i16/data/$currentyear ~/i16/data$currentyear
```

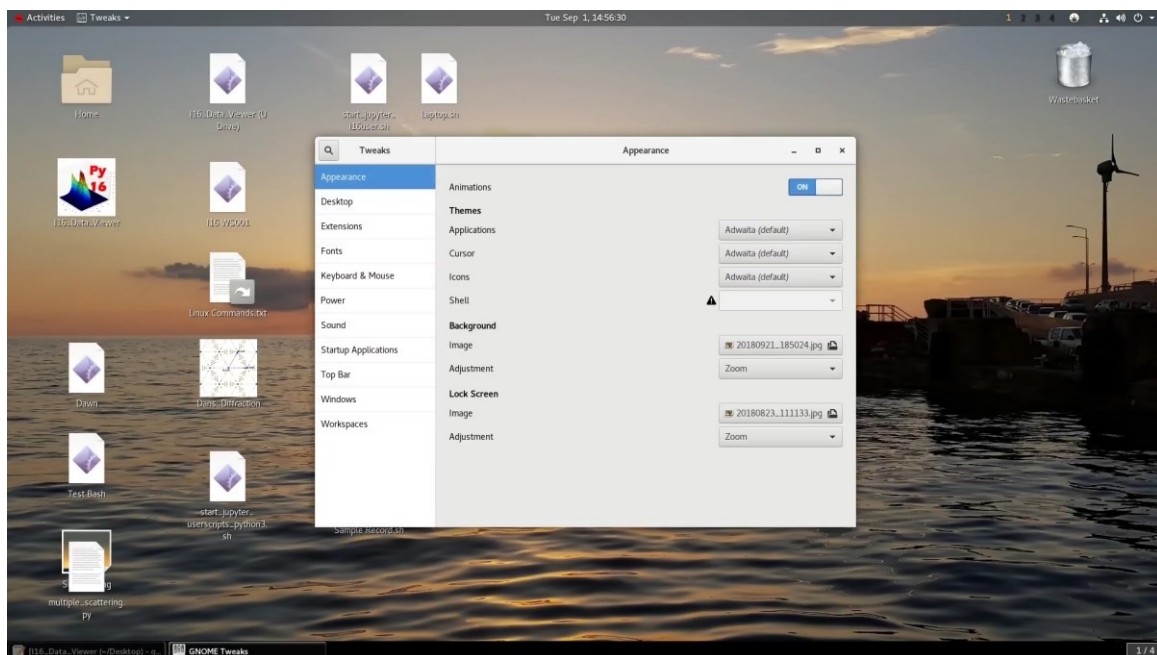
```
ln -s /dls_sw/i16/software/python/userscripts/i16user/logbooks/$currentyear \
~/i16/logbooks$currentyear
```

```
ln -s /dls_sw/i16/software/python/userscripts/i16user ~/i16/i16user
```

Linux Customisation

You have some ability to customise how linux looks and operates – including adding the desktop and other useful features from “Tweaks”:

- Click on Activities, search for and run “Tweaks”
- Switch Desktop>Show Icons to ON
- Switch Extensions>Workspace grid and Workspace buttons to ON.
 - Configure Extensions>Workspace grid using the settings menu

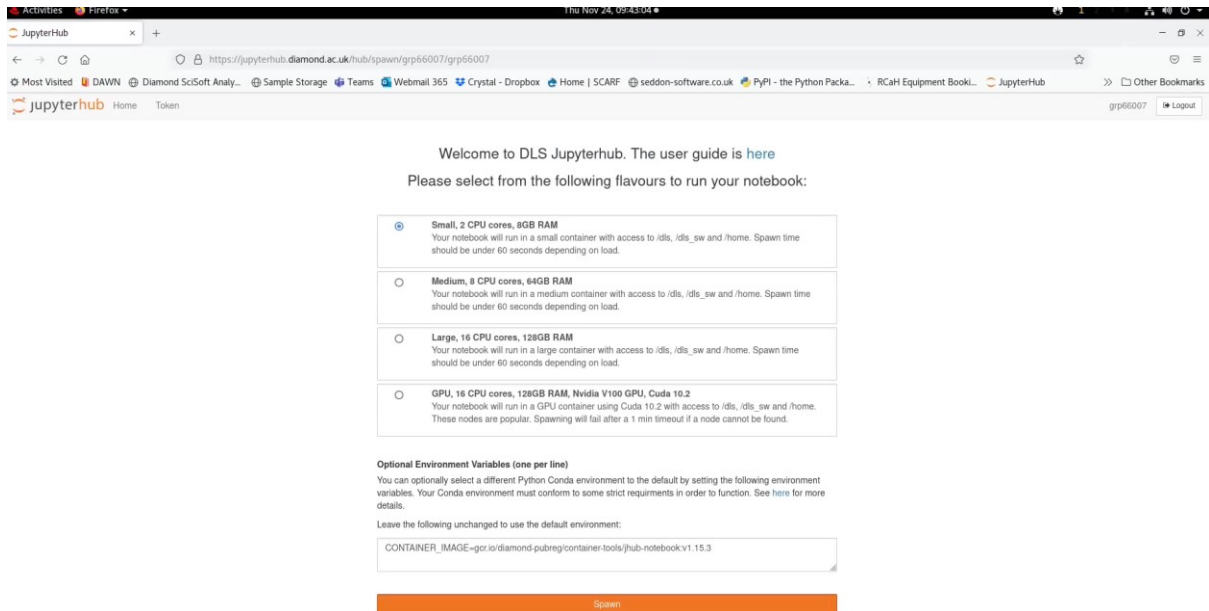


JupyterHub

Another way to access Jupyter is using JupyterHub – a server based Jupyter Notebook with access to more significant computing resources. Access is via the website:

<https://jupyterhub.diamond.ac.uk>

Note: JupyterHub is still in development and only available inside the Diamond Firewall (from nx-user). User access and support is not guaranteed.

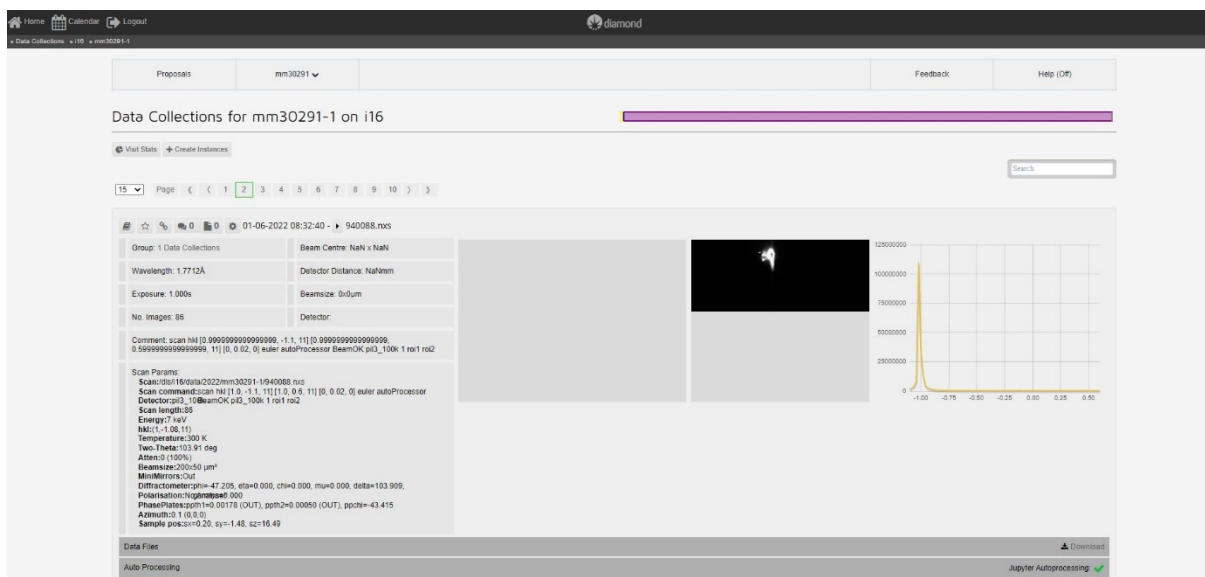


ISpyB

It is possible monitor your experiment offsite at the ISpyB website:

<https://ispyb.diamond.ac.uk>

Your FedID & Password are required to access the service. Metadata and simple plots of completed scans are shown, as well as completed auto-processed jupyter notebooks.



MaRS

Calculations of the Magnetic Resonant Scattering of crystals are possible using the MaRS calculator, available inside the Diamond Firewall (from the nx-user) at the website:

<https://mars.diamond.ac.uk/>

Incident Beam Properties

Energy: keV Polarization:

Crystal Properties

Warning:: the space group symbol is not yet used in the calculations, even ions related by translational symmetry will need to be manually entered and the Fourier Components constrained applying the correct phase factor.

Space Group*

Not yet in use! Space group full name symbols, space separated e.g. I 41/a 2/c 2/d

Lattice Parameters

a b c
 α 90 β 90 γ 90

Crystal Orientation

	h	k	l
Specular	$h0^*$	$k0^*$	$l0^*$
	<input type="text"/>	<input type="text"/>	<input type="text"/>
Reference	h azimuthal reference*	k azimuthal reference*	l azimuthal reference*
	<input type="text"/>	<input type="text"/>	<input type="text"/>

Magnetically active ions

Remote Data Access

Accessing your data remotely is possible in a number of ways. Here are a couple of links to useful methods on the Diamond user website. FTP is probably easiest for individual files, but to download the entire dataset its better to use the Globus system. These systems are only available within 40 days of the experiment, after this you must use the archive retrieval tool (iCAT).

FTP: <https://www.diamond.ac.uk/Users/Experiment-at-Diamond/IT-User-Guide/Not-at-DLS/Retrieve-data/in40days/ftp.html>

- FTP address: fedecks.diamond.ac.uk, port 21
- Login: Your FedID and password
- Data directory: /dls/i16/data/2020/mm#####-# (your experiment number)

Globus: <https://www.diamond.ac.uk/Users/Experiment-at-Diamond/IT-User-Guide/Not-at-DLS/Retrieve-data/in40days/Globus.html>

- <http://www.globus.org/>
- Login: Create Globus account or use your institution's.
- Endpoint: diamondftp#transit.diamond.ac.uk
- Data directory: /dls/i16/data/2020/mm#####-# (your experiment number)

Other systems: <https://www.diamond.ac.uk/Users/Experiment-at-Diamond/IT-User-Guide/Not-at-DLS/Retrieve-data.html>