

I16 Remote User Manual

Remote Experiments Autumn 2020

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:

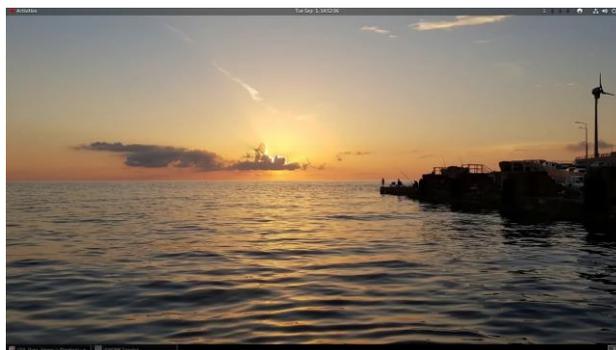
- Open NoMachine
- Create "New" connection:
 - Protocol – NX
 - Host – **nx-user.diamond.ac.uk**, Port: **4000**
 - Password, no proxy
- Open new connection:
 - Enter username and password – **your FedID**, as used in the user account system (UAS) for proposals.
 - Create a new virtual desktop

You are connected and have a virtual desktop to Diamond's 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/2020/mm####-1</code>	Data directory (mm####-1 = your experiment ID)	Read only
<code>/dls_sw/i16/scripts/2020/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.



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 shows the I16 Data Viewer interface. On the left, a terminal window displays the following output:

```
-----Gauss Fit:-----  
Peak Height = 1.8112(0)e+05  
Peak Centre = 4.2161 (0)  
FWHM = 0.01377 (0)  
Background = 46189 (0)  
Area = 2579.1 (0)  
CHI^2 = 7.8419603E+09  
CHI^2 per free par = 8.08E+07  
  
-----pVoigt Fit:-----  
Peak Height = 2.1166(0)e+05  
Peak Centre = 4.2161 (0)  
FWHM = 0.01129 (0)  
Lorz Frac = 1.18184 (1)  
Background = 35640 (0)  
Area = 3949.39 (0)  
CHI^2 = 5.2545619E+08  
CHI^2 per free par = 5.47E+06
```

The main window displays a plot of intensity versus ppp_offset for scan #820912. The plot shows a sharp peak at approximately 4.22. The y-axis ranges from 5e+04 to 2.5e+05. The x-axis ranges from 4.18 to 4.26. The plot is titled "#820912".

Below the plot, the following parameters are displayed:

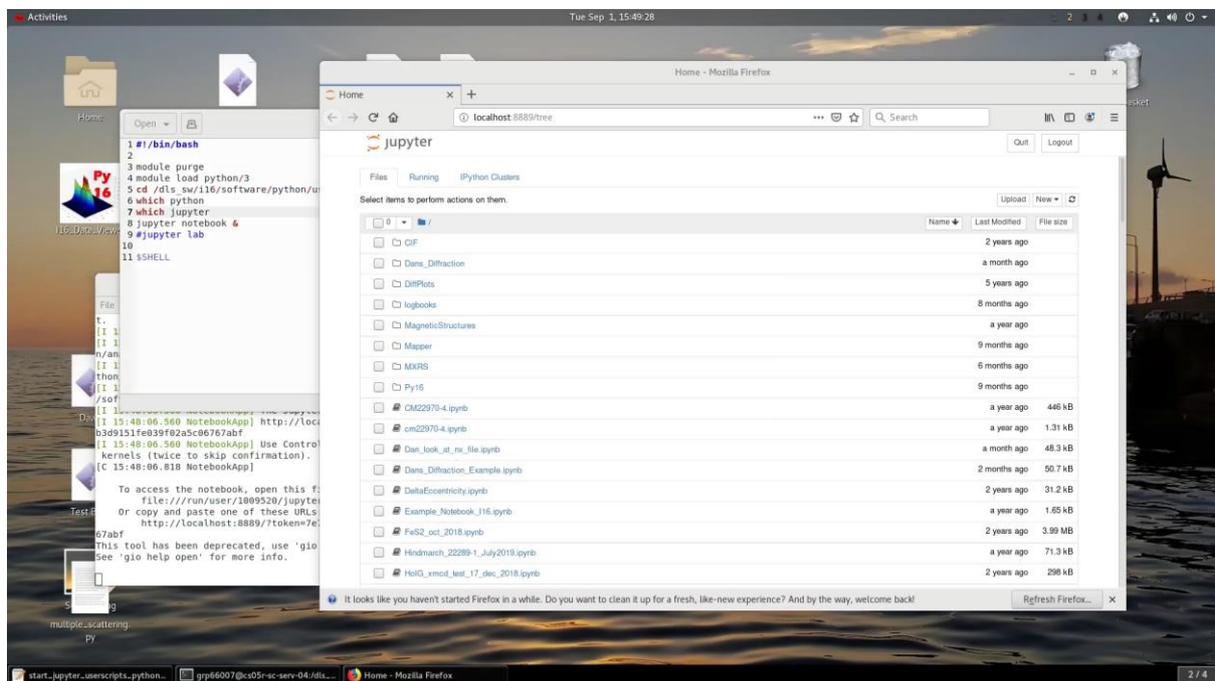
```
Command : scannc ppF1lm1 [0.0, 0.001] 101 pph2 BeamOK t 1  
Scan No: 820912  
Npoints : 101  
HKL : (0,0,0)  
Energy : 2.99keV  
Temp : 300K  
Atten : 0 (100%)  
Minimirsors : in (0.45 deg)  
Detector offset: 0  
thp: -38.0279 thp: -75.263 pol: 90  
eta: -0.0 mu: 0.0  
delta: 0.0 gamma: 0.0  
chi: 90.0 phi: -0.0  
psi: 666 (0.8165,-0  
sx: -0.5301 sy: 0.4881 sz: 7.7307  
sper: 0.4881 spara: -0.5301  
Sample Slits: 0.50x0.50 mm  
Detector Slits: 2.00x2.00 mm  
Ran on : Fri Mar 6 07:46:27 2020  
Time Taken : 0 hours, 6 mins, 25.19999999995
```

The bottom of the interface includes a 'Last scans window' and a 'Check Log' section.

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).



The screenshot shows a Jupyter Notebook in a Firefox browser window. The notebook is titled "I16 Experiment cm26473-1/ca2rumno4". The main content area contains an "Experiment Logbook for I16" section with the following fields:

- Date: Tue Mar 3 12:53:41 2020
- Data directory: /dls/i16/data/2020/cm26473-1/ca2rumno4
- Scripts: /dls_sw/i16/scripts/2020/cm26473-1/ca2rumno4
- Users: who?
- Local Contact:
- Sample: what?
- Beamline setup: which?

Below the logbook is a code cell with the following Python code:

```
In [12]: %autosave 60
%matplotlib notebook
import sys, os
import numpy as np
import matplotlib.pyplot as plt

sys.path.append('/dls_sw/i16/software/python/userscripts/i16user/Dans_Diffraction')
sys.path.append('/dls_sw/i16/software/python/Py16')
sys.path.append('/dls_sw/i16/software/python')
sys.path.append('/dls_sw/i16/software/python/userscripts/steve')
sys.path.append('/dls_sw/i16/software/python/DMS_Code')

import Py16progs as dp
import Dans_Diffraction as dif
```

Useful Commands

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

Jupyter Logbook

Experiment logbooks, written as Jupyter notebooks, are automatically generated (if turned on and updated) from GDA and can be accessed from:

```
/dls_sw/i16/software/python/userscripts/i16user/logbooks/2020/mm####-1.ipynb
```

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
```

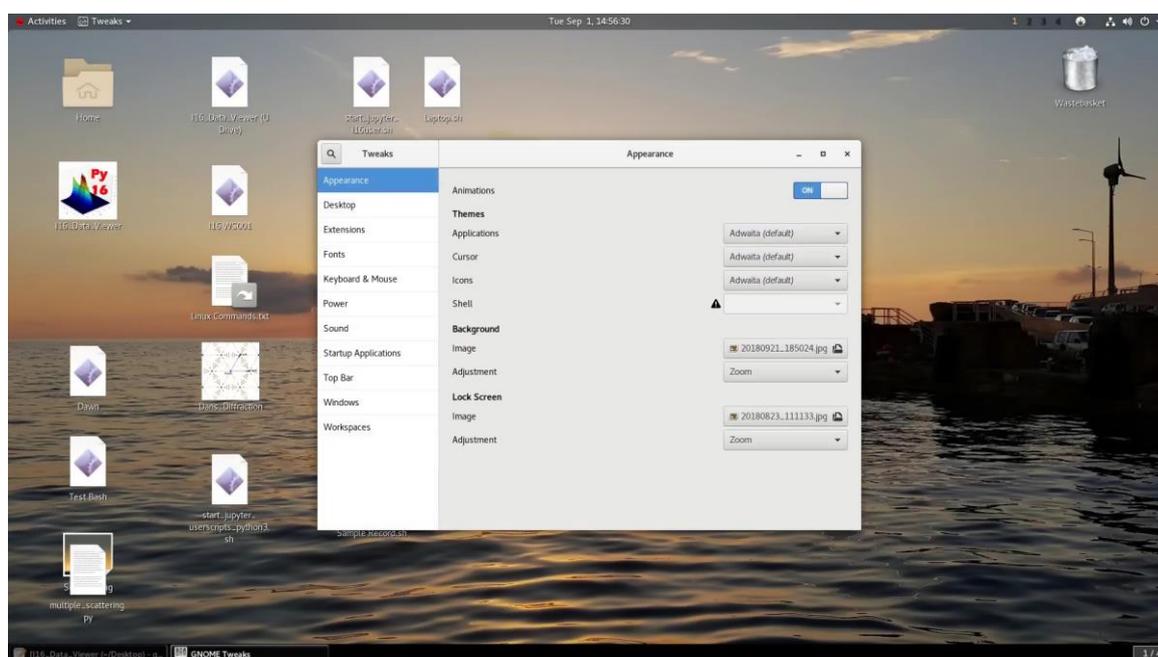
```
ln -s /dls_sw/i16/software/python/userscripts/i16user/logbooks/$currentyear \
~/i16/logbooks$currentyear
```

```
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



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>