

Accessing HB2A data

HB2A Instrument Team
High Flux Isotope Reactor
November 2019

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

Quick Guide Contents

- Downloading your Autoreduced Data from ONCat
- Accessing the Analysis Cluster
- Manual Data Reduction, Plotting and Saving with Mantid
 - Finding your data on the Analysis cluster
 - Plot diffraction pattern
 - Plotting Individual Detectors (e.g. Order Parameter Plots)
 - Saving your manually reduced data

Quick Links

- All data is autoreduced and can be downloaded through ONCat: <https://oncat.ornl.gov/#/>
- Scan run numbers, title, etc are also viewable through ONCat.

- Manual viewing, plotting, reduction and saving of your data with Mantid can be done at <https://analysis.sns.gov/>

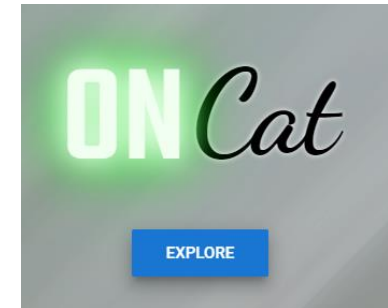
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How To View Scan Details and Download Autoreduced Data

- Every completed scan is autoreduced and accessible through ONCat

<https://oncat.ornl.gov/#/>



Steps to access your data from ONCat

1) Login to the system using your unique 3-character code and password

ON*Cat*

Username

Password

LOGIN

[CONTACT](#)

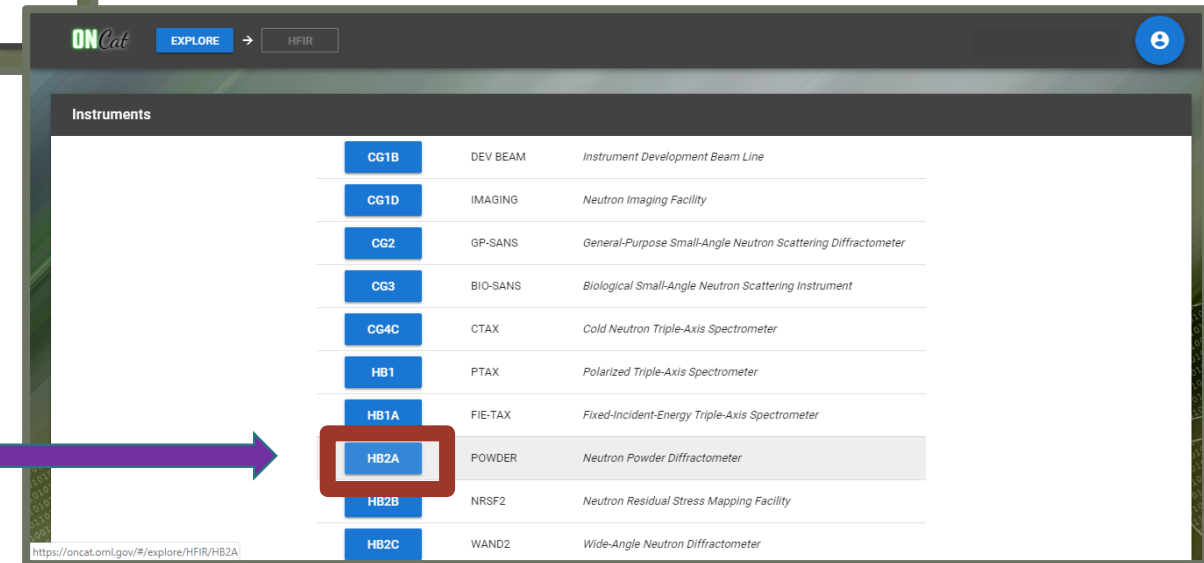
OAK RIDGE
National Laboratory

U.S. DEPARTMENT OF ENERGY | Office of Science

Notice to Users: Use of this system constitutes consent to security monitoring and testing. All activity is logged with your host name and IP address.



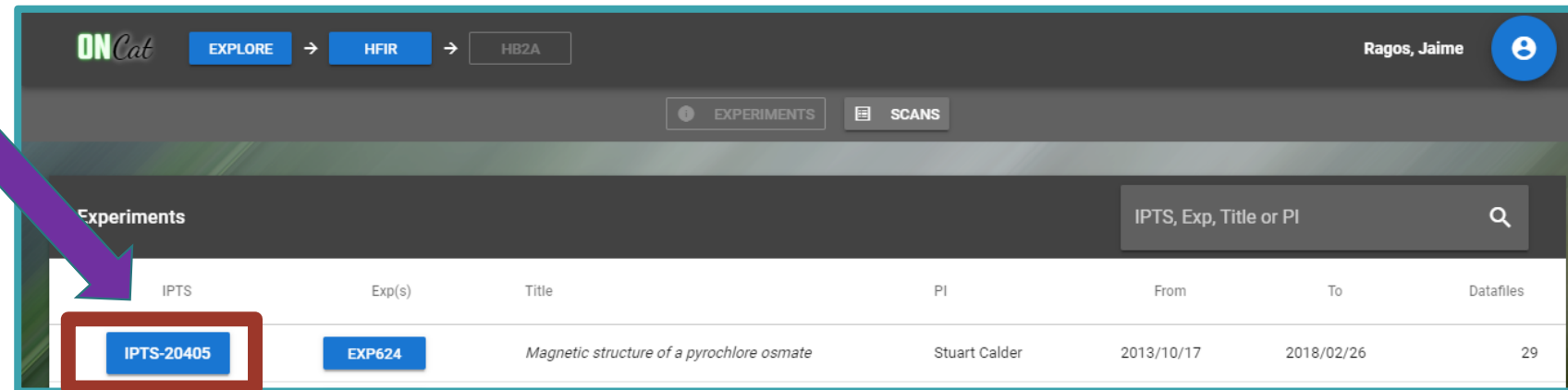
2) Click on HFIR



3) Click on HB2A

4) There will be a list of all experiments ran on HB-2A. Click on the IPTS you want to access.

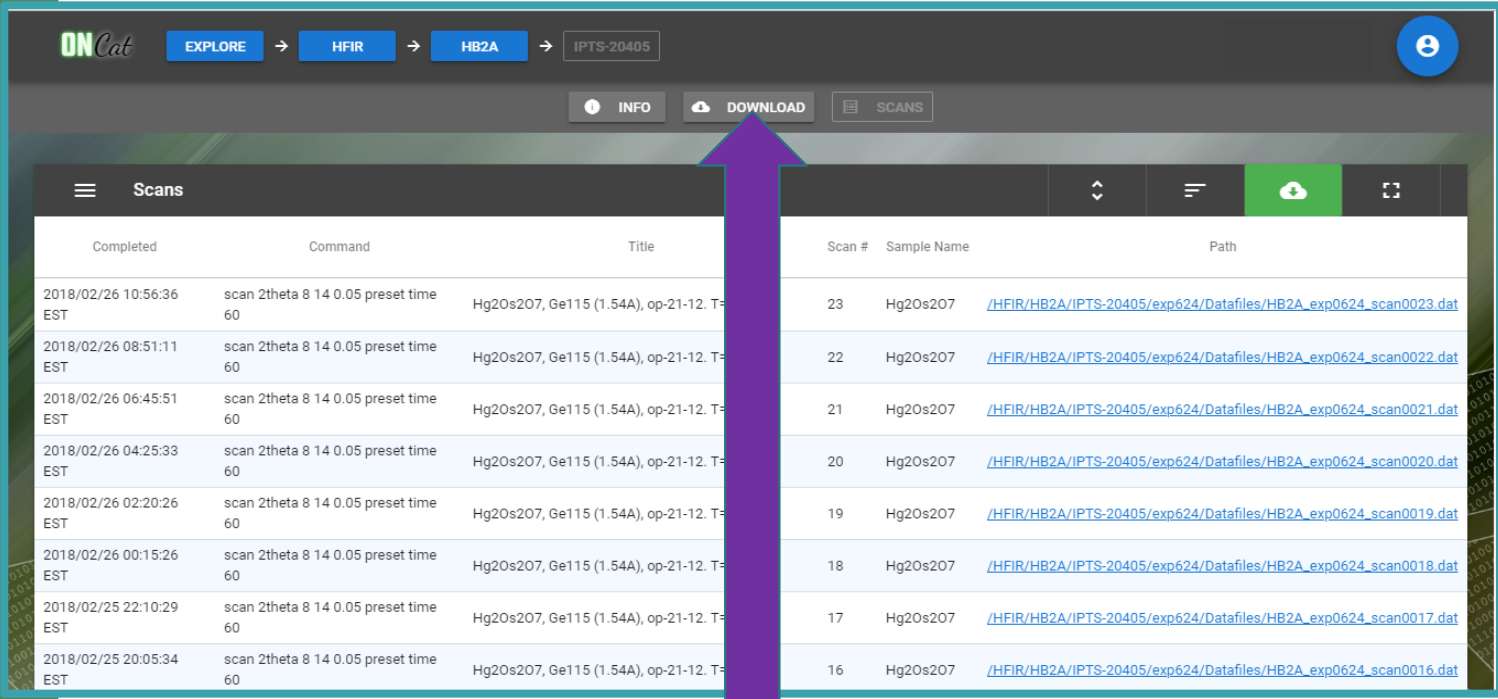
NOTE: you can also select the experiment number, but downloading this folder will NOT include autoreduced data, so this is not recommended.



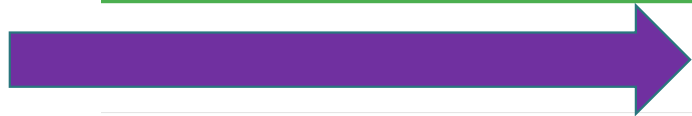
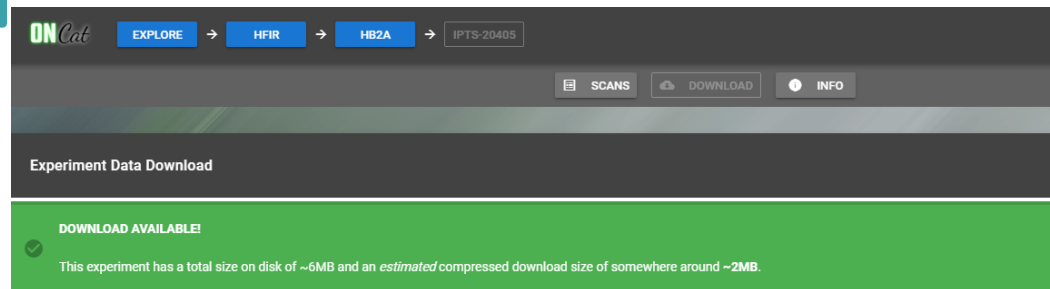
A Listing of All the Scans Performed is shown

The screenshot shows the ON Cat interface with a 'Scans' table. The table has columns for 'Completed', 'Command', 'Title', 'Scan #', 'Sample Name', and 'Path'. Four callout boxes highlight specific columns: an orange box for 'Command', a green box for 'Title', a pink box for 'Scan #', and a purple box for 'Path'. The 'Completed' column shows dates and times in EST. The 'Command' column contains 'scan 2theta 8 14 0.05 preset time 60'. The 'Title' column contains 'Hg20s207, Ge115 (1.54A), op-21-12. T=110 K' or 'T=25 K'. The 'Scan #' column contains numbers 16 through 23. The 'Sample Name' column contains 'Hg20s207'. The 'Path' column contains file paths like '/HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0023.dat'.

Completed	Command	Title	Scan #	Sample Name	Path
2018/02/26 10:56:36 EST	scan 2theta 8 14 0.05 preset time 60	Hg20s207, Ge115 (1.54A), op-21-12. T=110 K	23	Hg20s207	/HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0023.dat
2018/02/26 08:51:11 EST	scan 2theta 8 14 0.05 preset time 60	Hg20s207, Ge115 (1.54A), op-21-12. T=110 K	22	Hg20s207	/HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0022.dat
2018/02/26 06:45:51 EST	scan 2theta 8 14 0.05 preset time 60	Hg20s207, Ge115 (1.54A), op-21-12. T=110 K	21	Hg20s207	/HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0021.dat
2018/02/26 04:25:33 EST	scan 2theta 8 14 0.05 preset time 60	Hg20s207, Ge115 (1.54A), op-21-12. T=25 K	20	Hg20s207	/HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0020.dat
2018/02/26 02:20:26 EST	scan 2theta 8 14 0.05 preset time 60	Hg20s207, Ge115 (1.54A), op-21-12. T=25 K	19	Hg20s207	/HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0019.dat
2018/02/26 00:15:26 EST	scan 2theta 8 14 0.05 preset time 60	Hg20s207, Ge115 (1.54A), op-21-12. T=25 K	18	Hg20s207	/HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0018.dat
2018/02/25 22:10:29 EST	scan 2theta 8 14 0.05 preset time 60	Hg20s207, Ge115 (1.54A), op-21-12. T=25 K	17	Hg20s207	/HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0017.dat
2018/02/25 20:05:34 EST	scan 2theta 8 14 0.05 preset time 60	Hg20s207, Ge115 (1.54A), op-21-12. T=25 K	16	Hg20s207	/HFIR/HB2A/IPTS-20405/exp624/Datafiles/HB2A_exp0624_scan0016.dat



5) Click Download, then “Start Download” on next screen to get your data.
 Autoreduced data is in:
 IPTS-XXXX/shared/autoreduce/



File System Report

Directory Path	File Count	Size on Disk
/HFIR/HB2A/IPTS-20405	0	0 Bytes
/HFIR/HB2A/IPTS-20405/exp624	7	3MB
/HFIR/HB2A/IPTS-20405/exp624/calibration	0	0 Bytes
/HFIR/HB2A/IPTS-20405/exp624/Configs	23	529KB

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Manually View and Save Your Data

- All scans are autoreduced into a format ready for viewing and refinement.
- **But** if you need to manually view, plot, reduce, save your data then the following steps show how to do this using Mantid through analysis.sns.gov

Remote Analysis Service

Remote Desktop Capabilities

As a Neutron Sciences user, you can view, analyze and download your data from anywhere you go. You will be on a machine just like one you use in our Instrument Hall or Target Building. You can work with your data and use the Data Analysis tools provided. To get started using our webclient click the "Launch Session" button below. For more information about different ways to access your data, please see the "Connection Options" section below.

Launch Session

Launch Session

Mantid Workbench

File View Interfaces Help

Workspaces

Load Delete Group Sort Save

Workspaces

LaB6_standard_Ge113

Messages

Using scort file: /WFIR/HB2A/IPTS-0/exp680/Data/files/HB2A_exp680_Ge_115_2M_vcorr.txt
HB2AReduce successful, Duration 0.97 seconds
RenameWorkspace started
RenameWorkspace successful, Duration 0.00 seconds

Algorithms

Execute HB2AReduce

Arithmetic
CorrectionFunctions
Crystal
DataHandling
Diagnostics
Diffraction
Events

Algorithms Plots

HB2AReduce input dialog

Performs data reduction for HB-2A POWDER at HFIR

Filename [Browse]
IPTS 18985
Exp 680
ScanNumbers 23
Vanadium [Browse]

Normalise
ExcludeDetectors
DefX
 IndividualDetectors
 BinData
BinWidth 0.05
Scale 2000
OutputWorkspace aaa

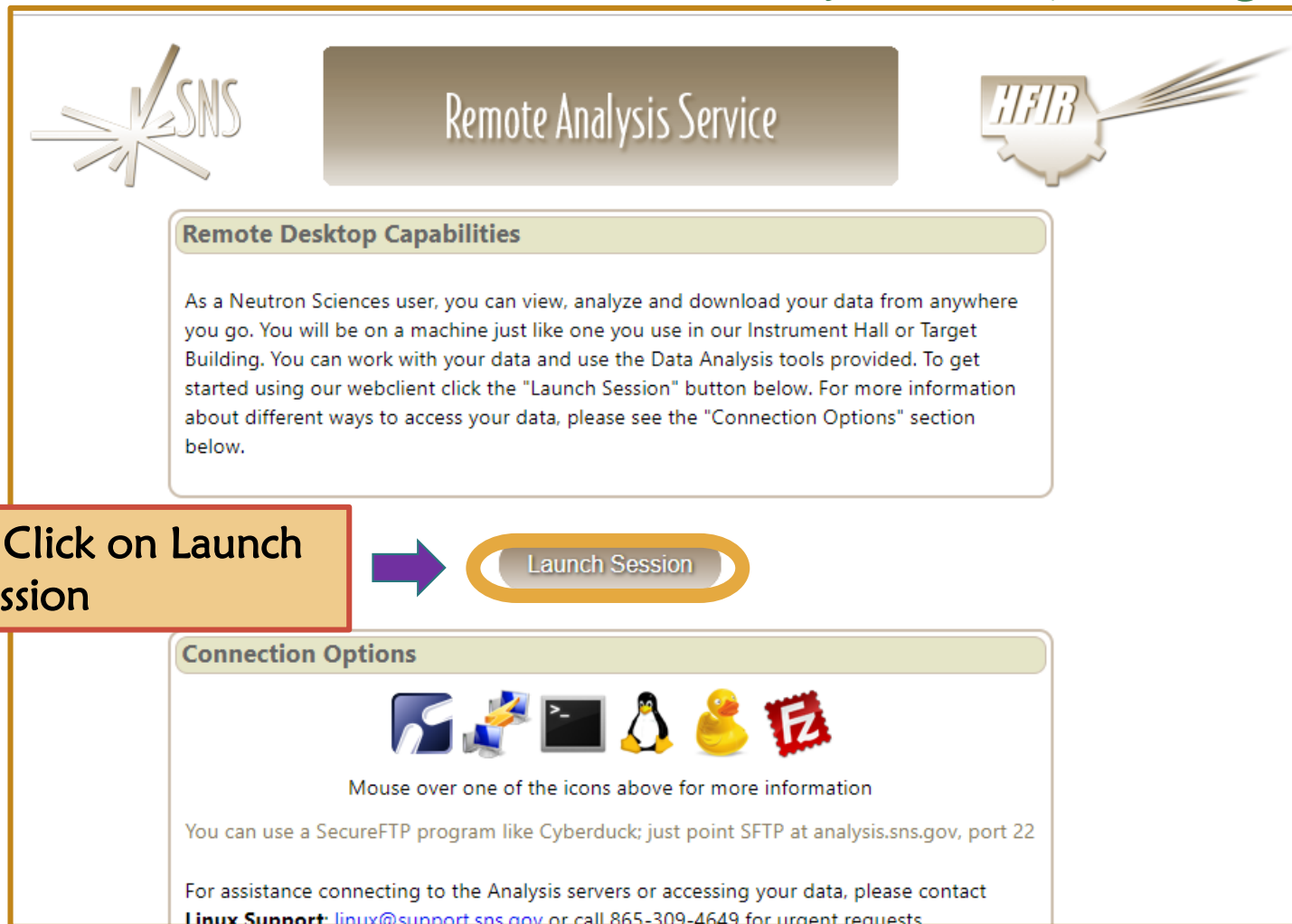
Keep Open Run Close

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Accessing the analysis service

Go to <https://analysis.sns.gov>



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1) Click on Launch Session → **Launch Session**

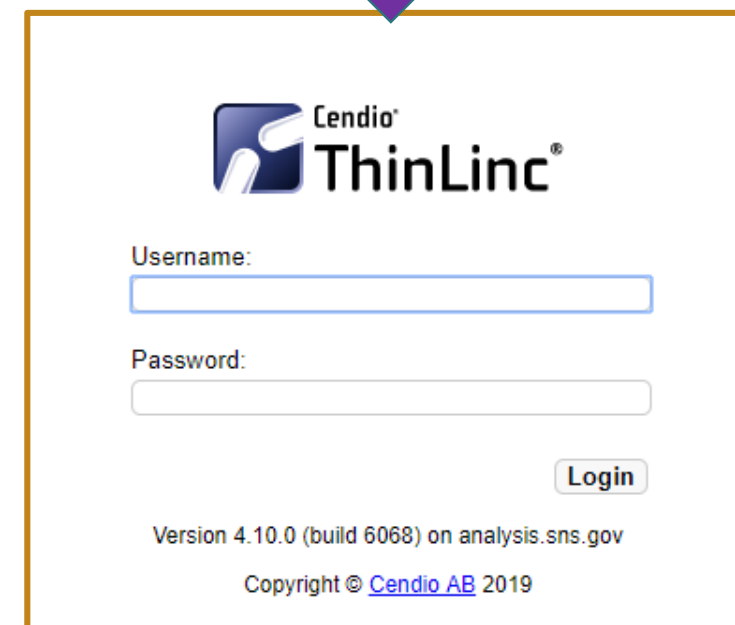
Connection Options

Mouse over one of the icons above for more information

You can use a SecureFTP program like Cyberduck; just point SFTP at analysis.sns.gov, port 22

For assistance connecting to the Analysis servers or accessing your data, please contact
Linux Support: linux@support.sns.gov or call 865-309-4649 for urgent requests.

2) You should be redirected to this site where you will need to login with your unique 3-character code and password or your guest username and password

Cendio ThinLinc®

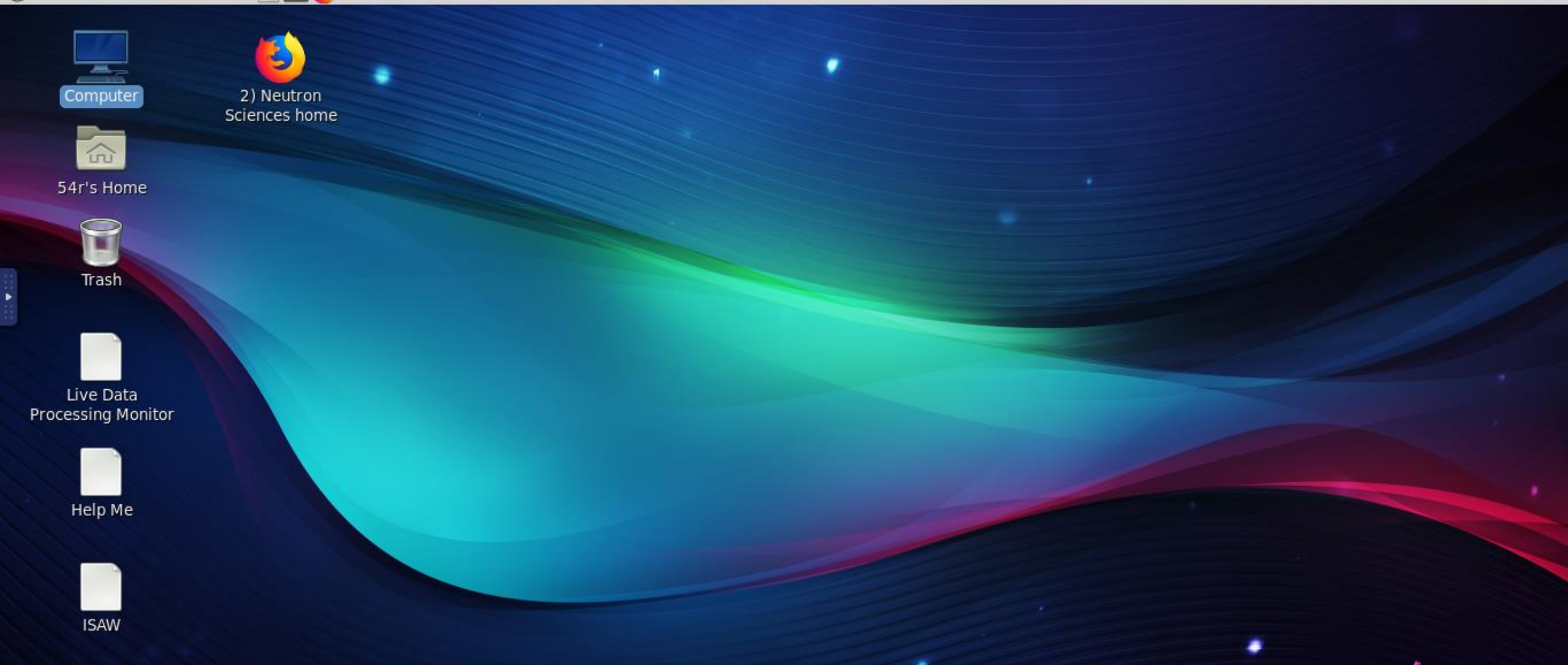
Username:

Password:

Login

Version 4.10.0 (build 6068) on analysis.sns.gov

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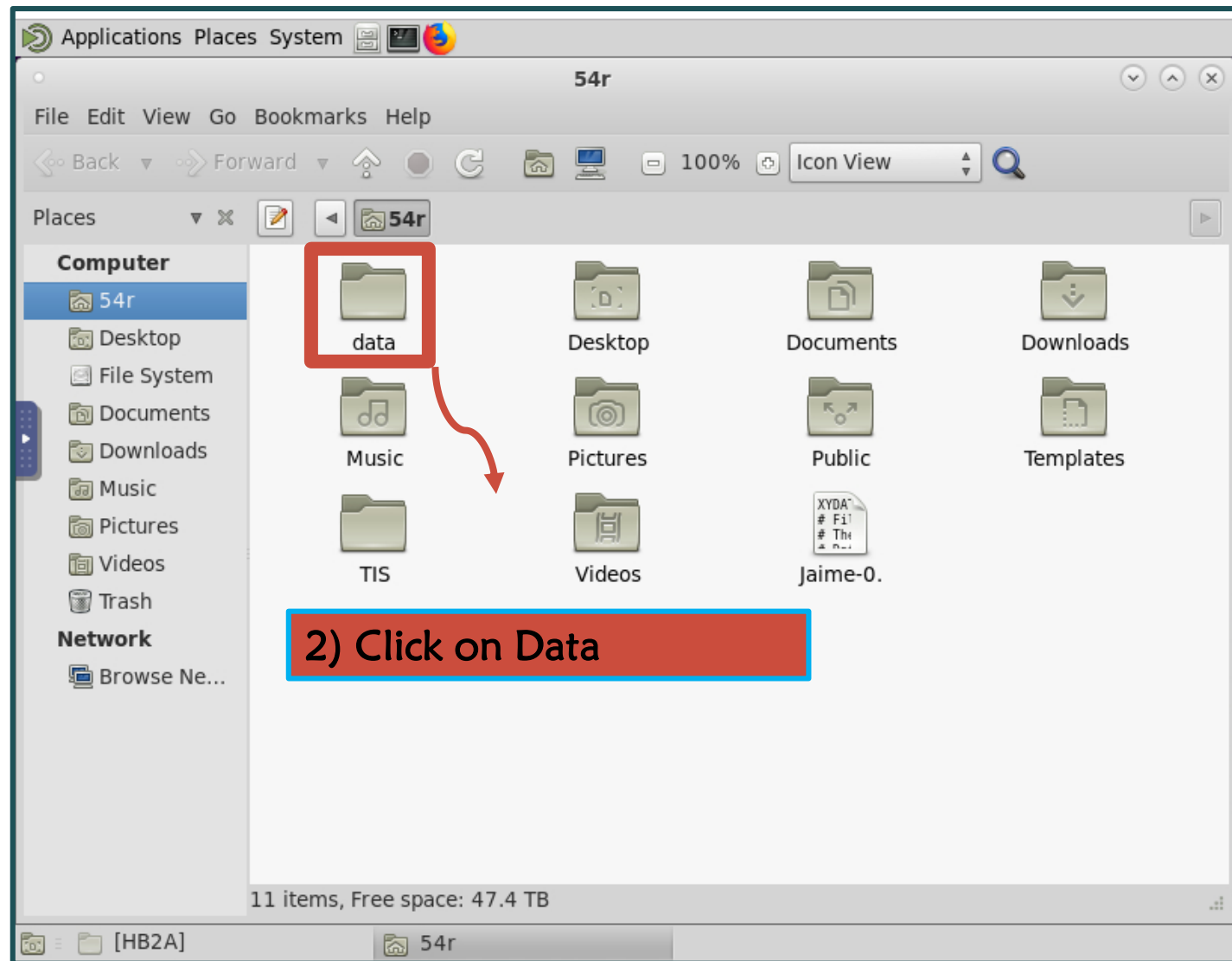
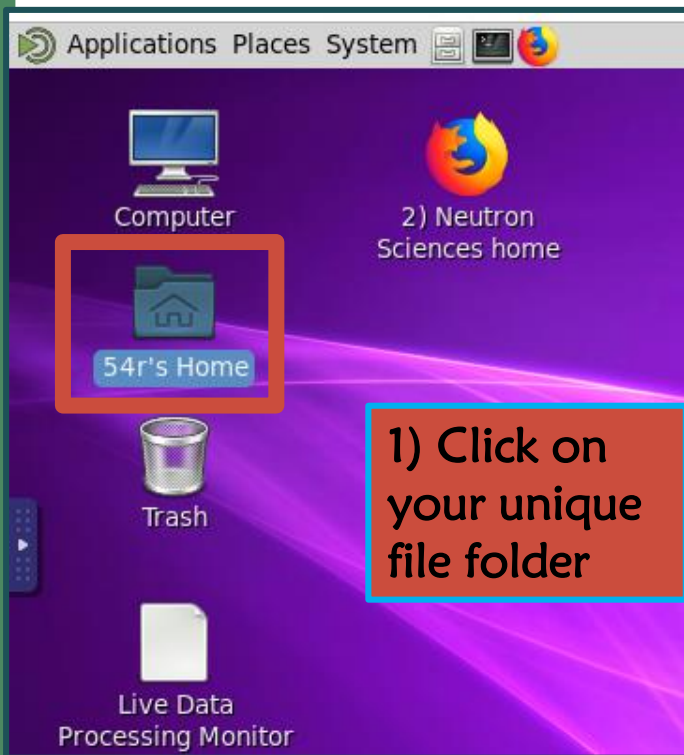
3) After logging in a second time you should have a remote desktop open

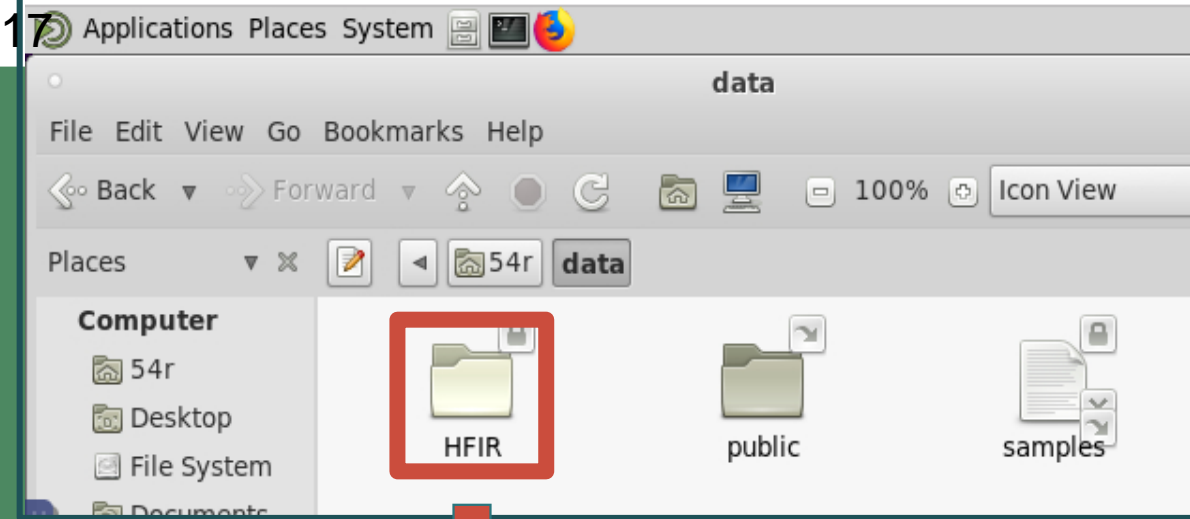
***Note:** After any long period of inactivity you will be asked to login again

Quick Guide Contents

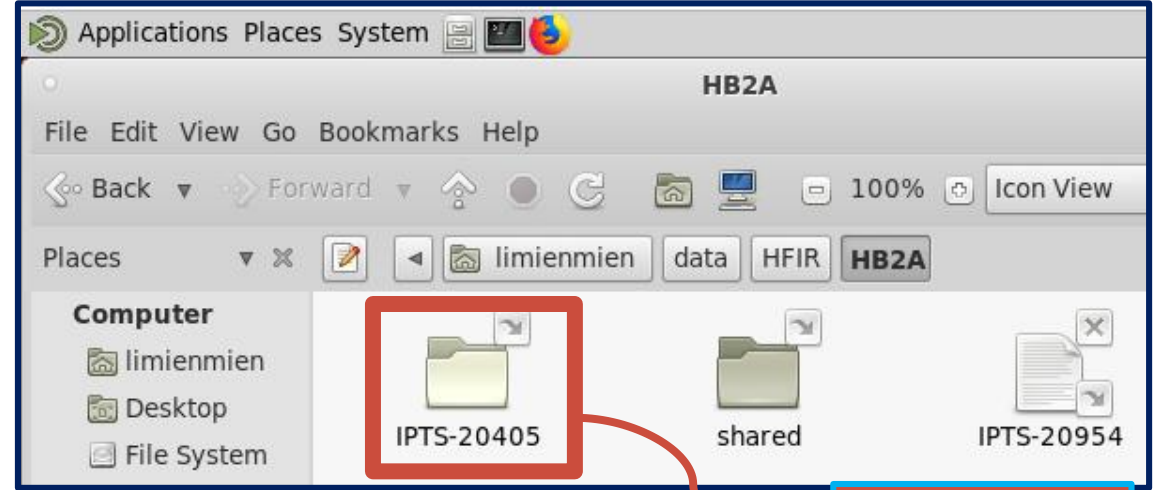
- Downloading your Autoreduced Data from ONCat
- Accessing the Analysis Cluster
- **Manual Data Reduction, Plotting and Saving with Mantid**
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Your data is stored on the analysis cluster under your IPTS number

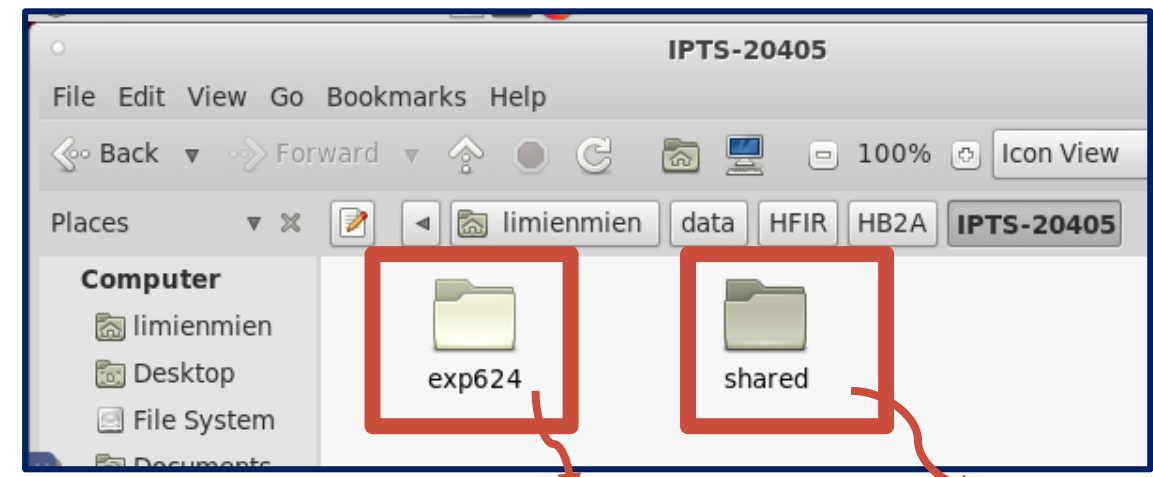




3) Click on HFIR

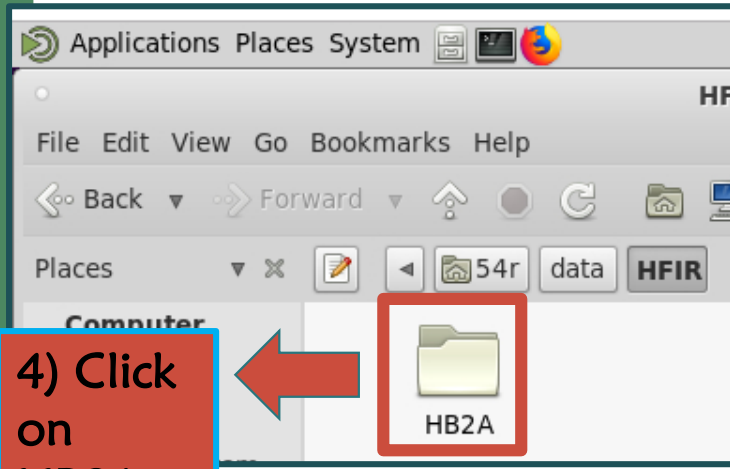


5) Click on your IPTS



6) The exp folder contains all the files from the HB2A instrument computer, including raw data, normalization files, excluded detectors, etc.

7) The autoreduced files are stored here.



4) Click on HB2A

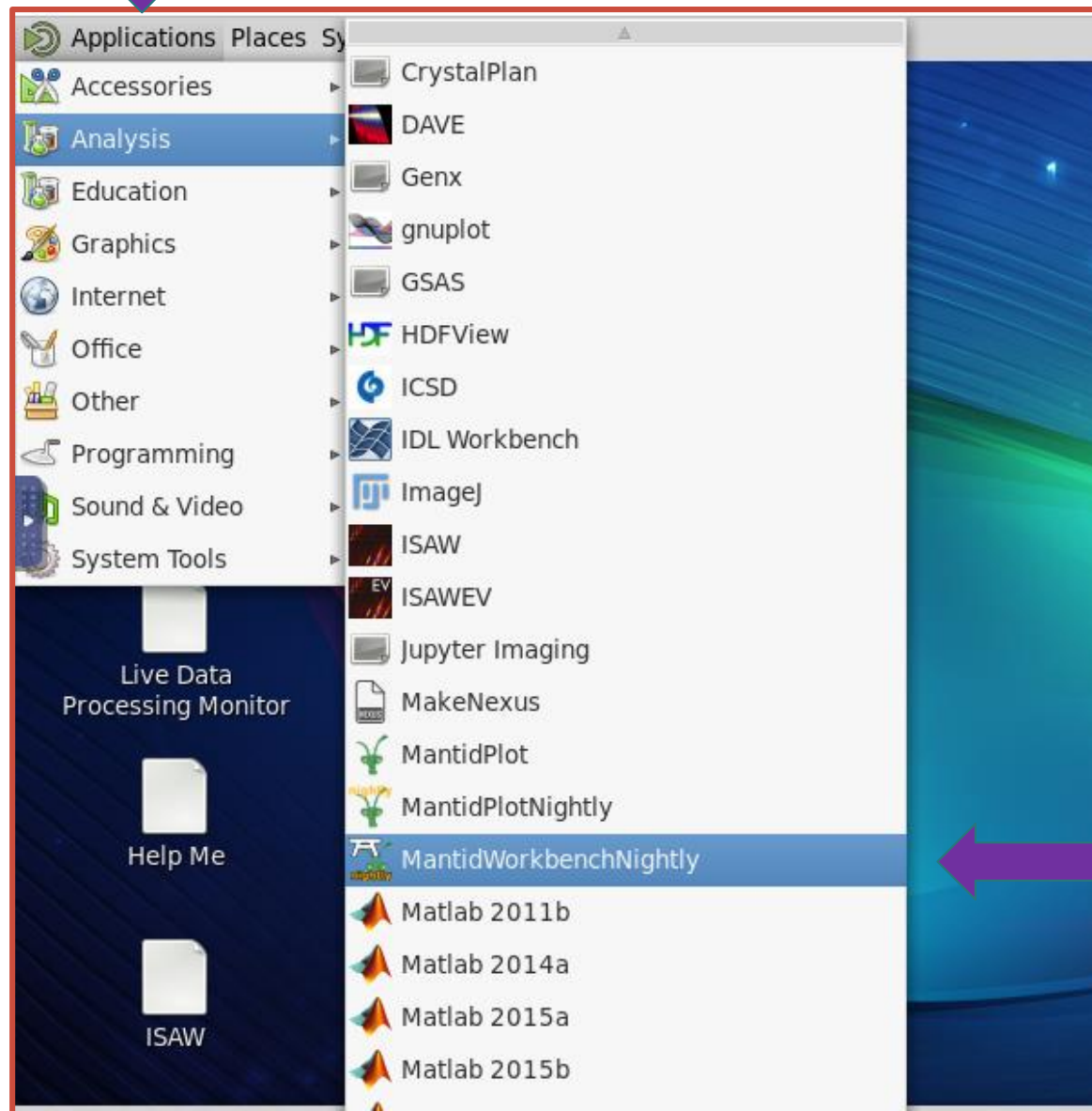
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Open Mantid

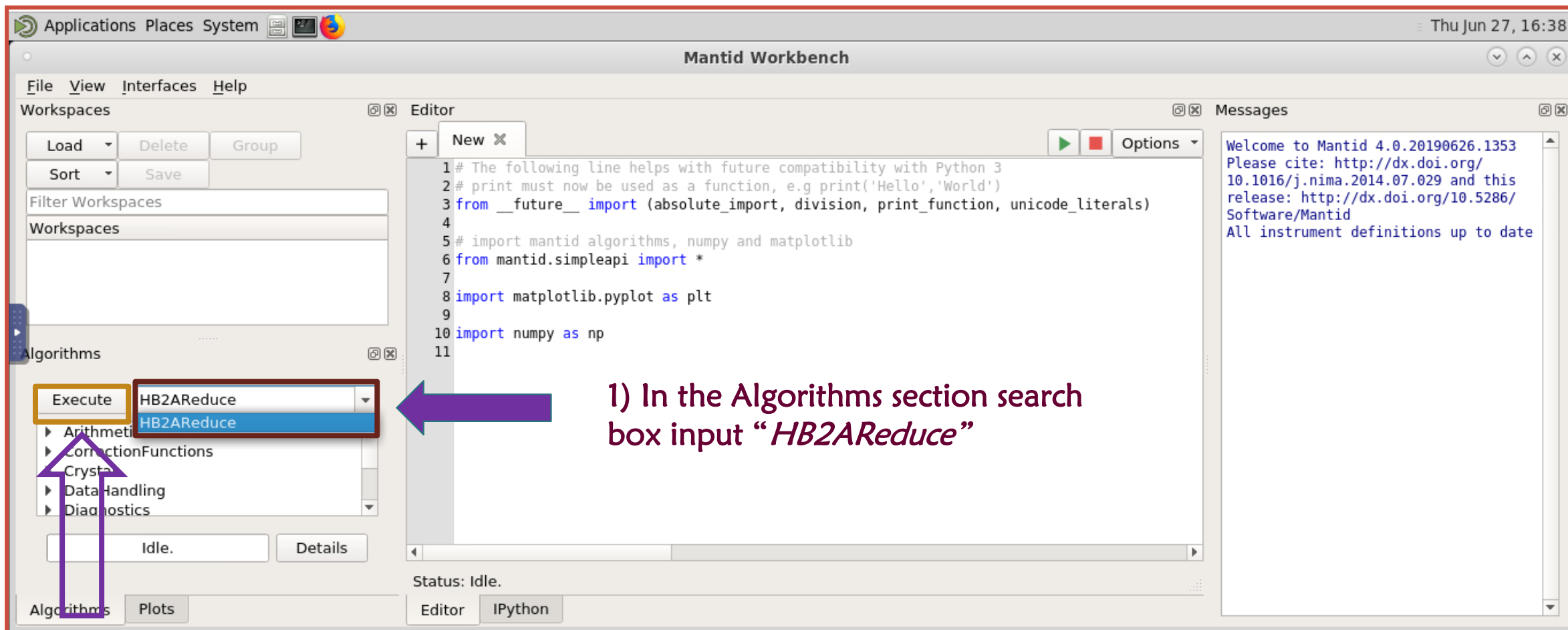
1) Click on Applications

2) Click on Analysis



3) Click on MantidWorkbenchNightly

Open the HB2AReduce input dialogue window



The screenshot shows the Mantid Workbench interface. The 'Algorithms' section is active, and the search box contains 'HB2AReduce'. The search results show 'HB2AReduce' selected. The 'Execute' button is highlighted with a yellow box. A purple arrow points to the 'HB2AReduce' entry in the search results. The Editor window shows Python code for the algorithm, and the Messages window shows a welcome message.

```
1 # The following line helps with future compatibility with Python 3
2 # print must now be used as a function, e.g print('Hello','World')
3 from __future__ import (absolute_import, division, print_function, unicode_literals)
4
5 # import mantid algorithms, numpy and matplotlib
6 from mantid.simpleapi import *
7
8 import matplotlib.pyplot as plt
9
10 import numpy as np
11
```

1) In the Algorithms section search box input “*HB2AReduce*”

2) Click Execute to start the Algorithm

***About Mantid:** There are many advanced capabilities in Mantid. The algorithm may be scripted, but we will use the GUI

HB2AReduce input dialogue window

Typically leave empty since we will supply the ScanNumbers

NOTE: If running Mantid on local computer and not analysis will need to browse for file

To plot data input IPTS and Exp and put a single or multiple ScanNumbers (e.g. 12,13,14,27 or 12-14,27). (Scan details can be found using ONCat, see earlier in guide for details)

Typically leave empty to use default vanadium normalization. Check Normalize.

Typically keep unchecked. Clicking this box allows you to view each separate detector. (The section on individual detectors will show what happens if this box is selected)

BinData: Check this combine detector counts and create diffraction pattern.

Put name to label output workspace file

The screenshot shows the 'HB2AReduce input dialog' window. At the top, it says 'Performs data reduction for HB-2A POWDER at HFIR'. The fields are: 'Filename' (empty), 'Browse' button; 'IPTS' (20405), 'Exp' (624), 'ScanNumbers' (12); 'Vanadium' (empty), 'Browse' button, and a checked 'Normalise' checkbox; 'ExcludeDetectors' (empty); 'DefX' (empty); 'IndividualDetectors' (unchecked checkbox); 'BinData' (checked checkbox); 'BinWidth' (0.05); 'Scale' (20000); and 'OutputWorkspace' (Sample 1). At the bottom, there is a '?' button, a 'Keep Open' checkbox (checked), a 'Run' button, and a 'Close' button.

Typically leave empty. Exclude detector only when advised by instrument team, otherwise leave blank

Typically leave empty and default will be used. Allows alternative x values to be defined

Define data bin size (0.05 is default)

Define arbitrary scale factor (default is 20000)

This button is FAQ, if you need any additional help click this

If you want this window to stay open after you run the program click this box

Clicking this to run the reduction

Running HB2AReduce

Applications Places System

Tue Aug 6, 13:45

File View Interfaces Help

Workspaces

Load Delete Group

Sort Save

Filter Workspaces

Workspaces

Algorithms

Execute HB2AReduce

- ▶ Arithmetic
- ▶ CorrectionFunctions
- ▶ Crystal
- ▶ DataHandling
- ▶ Diagnostics
- ▶ Diffraction
- ▶ Events

Idle.

Details

HB2AReduce input dialog

Performs data reduction for HB-2A POWDER at HFIR

Filename Browse

IPTS

Exp

ScanNumbers

Vanadium Browse

Normalise

ExcludeDetectors

DefX

IndividualDetectors

BinData

BinWidth

Scale

OutputWorkspace

Keep Open Run Close

Messages

```
Welcome to Mantid 4.1.20190801.2117
Please cite: http://dx.doi.org/
10.1016/j.nima.2014.07.029 and this
release: http://dx.doi.org/10.5286/
Software/Mantid
All instrument definitions up to date
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
IPTS-20405/exp624/Datafiles/
HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.09
seconds
```

Name your Workspace

*NOTE: For each analysis you run you **MUST** change your name or else the data will be overwritten

If you want this window to stay open after you run the program click this box

When ready click run

Workspace files created

Applications Places System Tue Aug 6, 13:45

File View Interfaces Help

Workspaces

Load Delete Group

Sort Save

Filter Workspaces

Workspaces

Sample 1

After clicking run your workspace will appear here

Algorithms

Execute HB2AReduce

- Arithmetic
- CorrectionFunctions
- Crystal
- DataHandling
- Diagnostics
- Diffraction
- Events

Idle. Details

Algorithms Plots

autoreduce Mantid Workbench HB2AReduce input dial...

HB2AReduce input dialog

Performs data reduction for HB-2A POWDER at HFIR

Filename Browse

IPTS

Exp

ScanNumbers

Vanadium Browse

Normalise

ExcludeDetectors

DefX

IndividualDetectors

BinData

BinWidth

Scale

OutputWorkspace

Keep Open Run Close

Messages

```

Welcome to Mantid 4.1.20190801.2117
Please cite: http://dx.doi.org/
10.1016/j.nima.2014.07.029 and this
release: http://dx.doi.org/10.5286/
Software/Mantid
All instrument definitions up to date
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
IPTS-20405/exp624/Datafiles/
HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.09
seconds

```

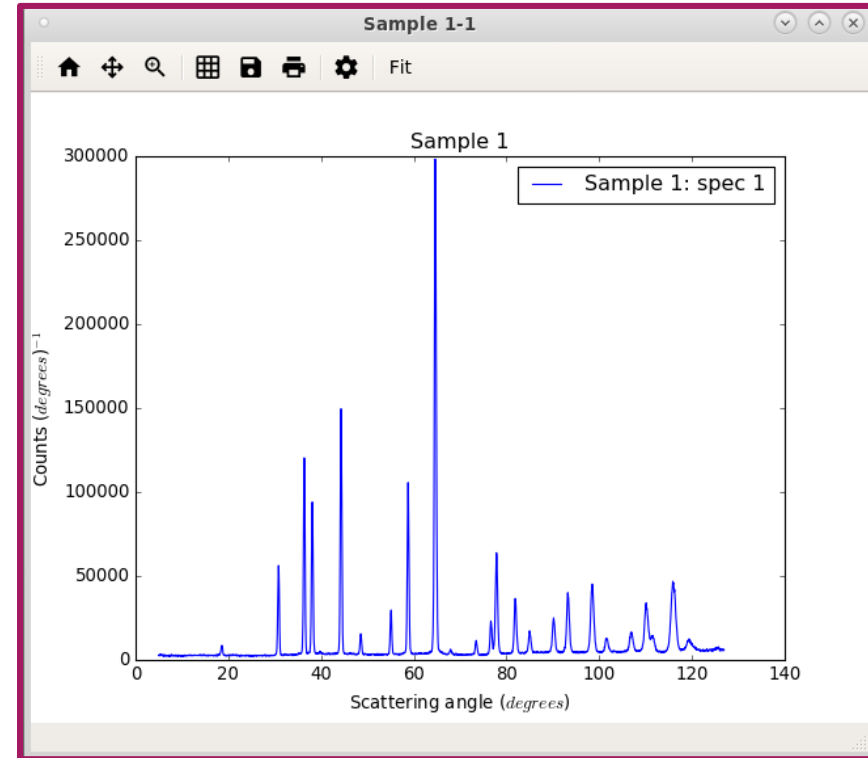
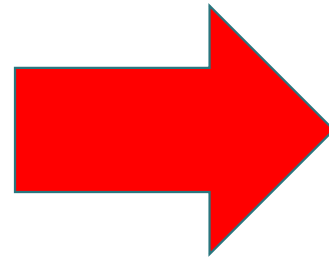
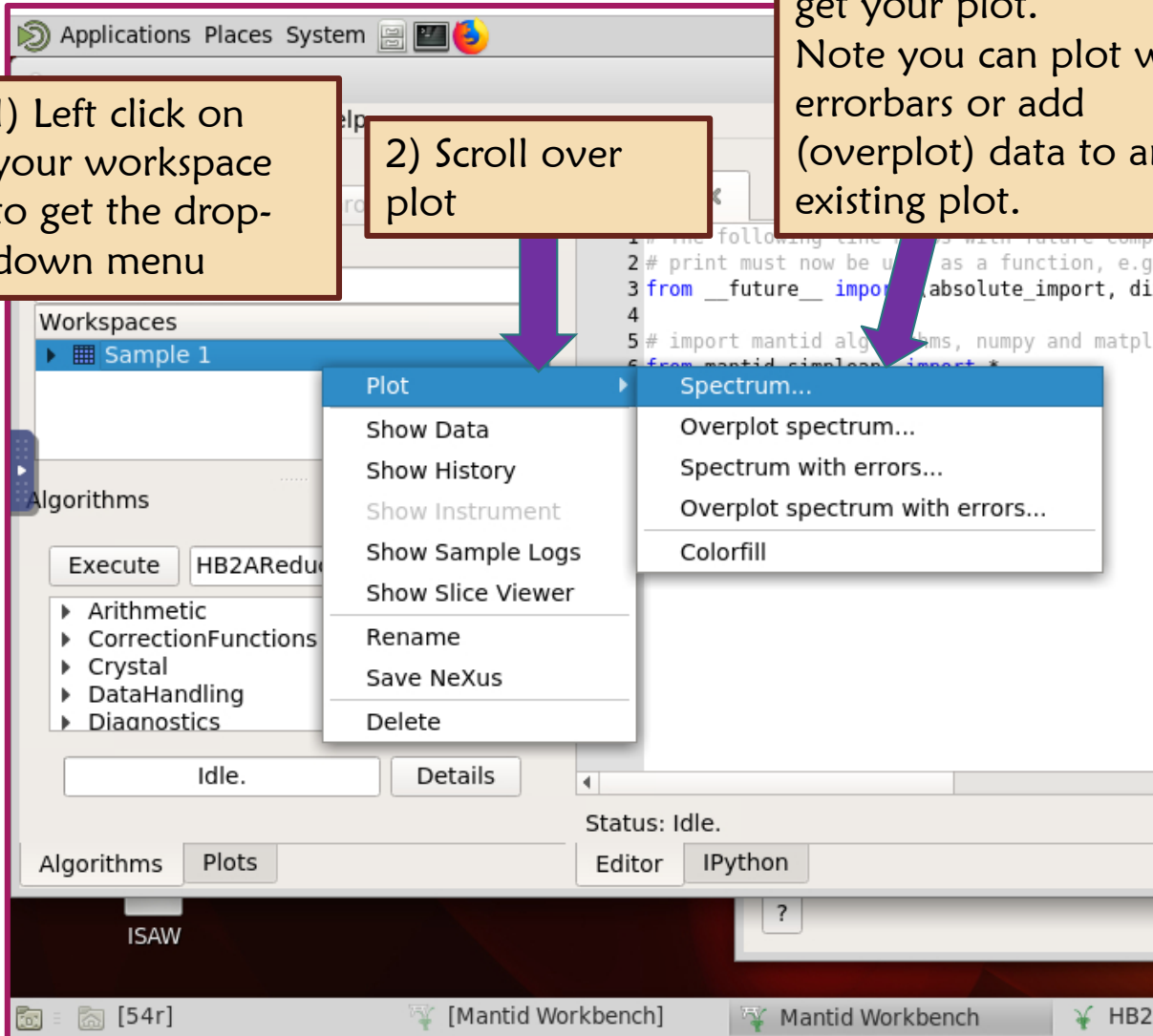
Plotting data from workspaces

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1) Left click on your workspace to get the drop-down menu

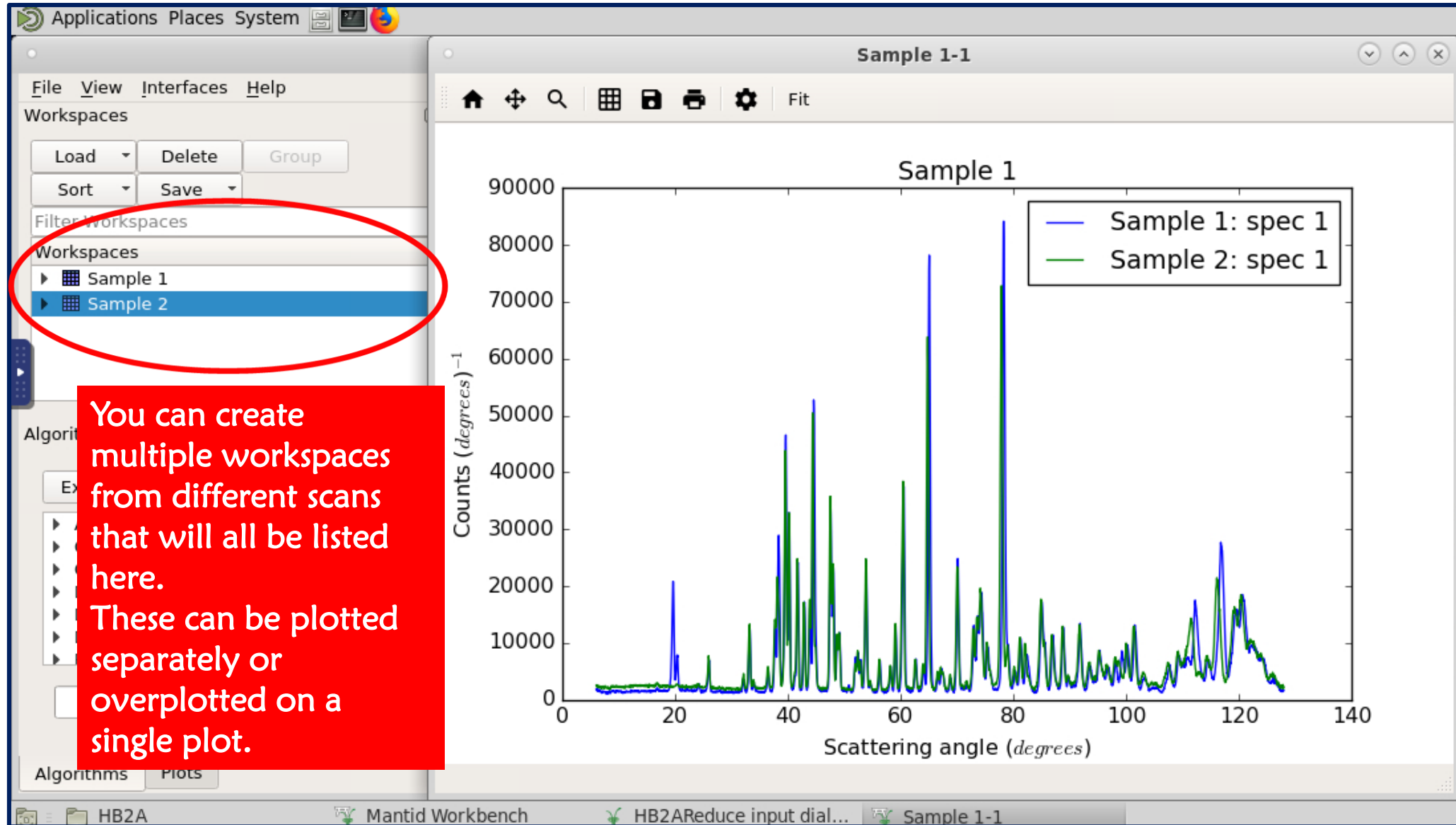
2) Scroll over plot

3) Click on Spectrum to get your plot.
Note you can plot with errorbars or add (overplot) data to an existing plot.



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Overlaid plots



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Plotting individual detectors

- Order parameter measurements on HB2A are run to follow the intensity of a single detector as the temperature (or field/pressure) is controlled.
- These can be plot using the same HB2AReduce dialogue window.
- The procedure is described in the following steps

Plotting a single detector

Load Delete Group

Sort Save

- Sample 1
- Sample 2

Execute HB2AReduce

- Arithmetic
- CorrectionFunctions
- Crystal
- DataHandling
- Diagnostics
- Diffraction
- Events

Idle.

Details

HB2AReduce input dialog

Performs data reduction for HB-2A POWDER at HFIR

Filename Browse

IPTS

Exp

ScanNumbers

Vanadium Browse

Normalise

ExcludeDetectors

DefX

IndividualDetectors

BinData

BinWidth

Scale

OutputWorkspace

? Keep Open Run Close

1) Make sure that this box is checked

```
seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
IPTS-20405/exp624/Datafiles/
HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.03
seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
IPTS-20405/exp624/Datafiles/
HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.03
seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
IPTS-20405/exp624/Datafiles/
HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.04
seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
IPTS-20405/exp624/Datafiles/
HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.04
seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
IPTS-20405/exp624/Datafiles/
HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.03
seconds
```

The screenshot shows the Mantid Workbench interface. The 'Plot' menu is open, and the 'Spectrum...' option is highlighted. The background shows the 'Workspaces' panel with 'Sample 2' selected and the 'Editor' window containing Python code for plotting.

```

1 # The following line helps with
2 # print must now be used as a f
3 from __future__ import absolut
4
5 # import mantid algorithms, num
6 from mantid.simpleapi import *
7

```

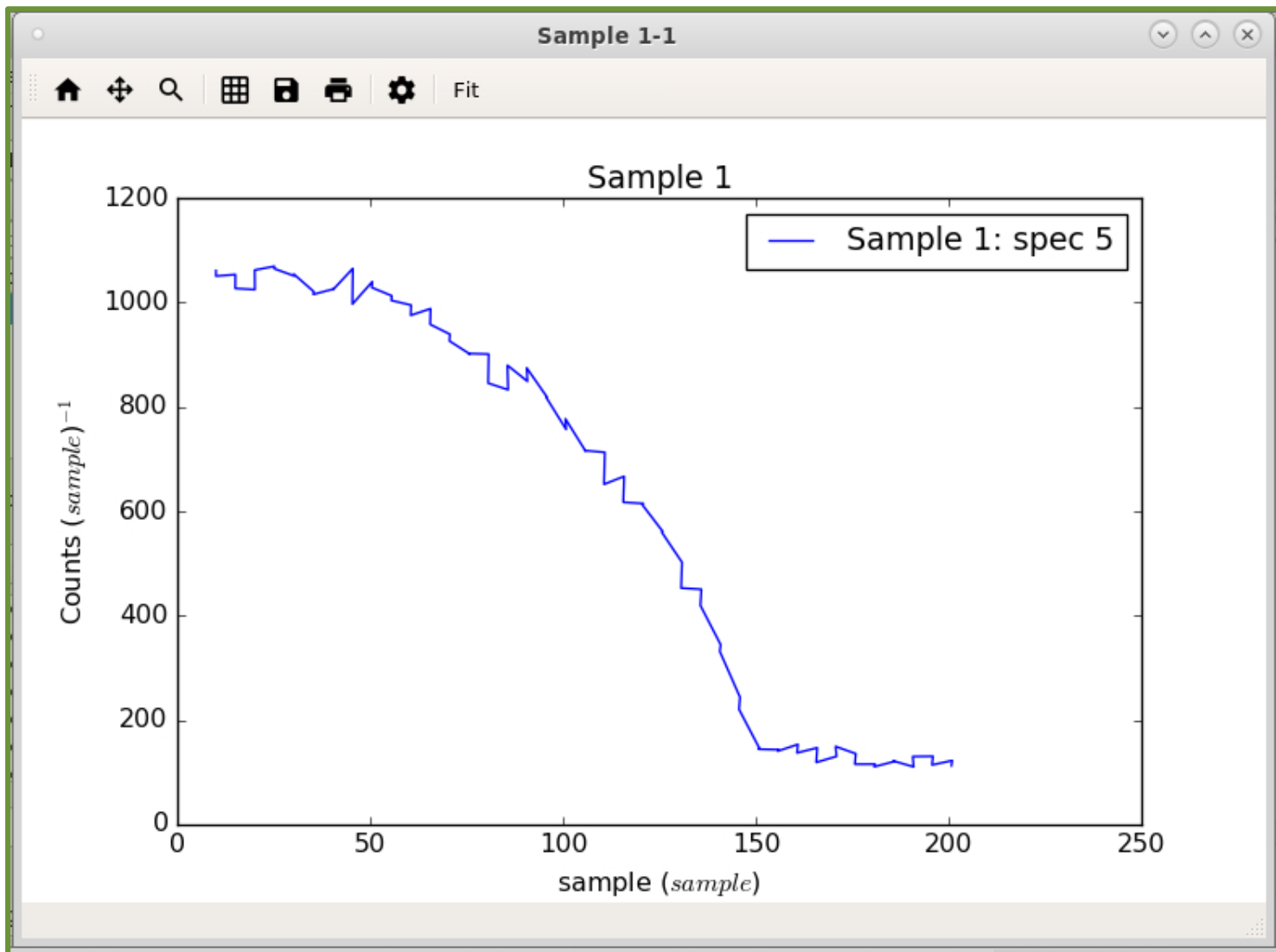
2) Follow the same steps you would as if you were plotting a standard diffraction pattern

The 'Plot 1D' dialog box is shown with the following settings:

- Spectrum Numbers: valid range: 1-44 *
- Workspace Indices: valid range: 0-43 *
- Plot type: Individual

Buttons: Cancel, OK, Plot All

3) This box should appear. Put the individual detector that you want
(This will be known to you and the instrument team when running the scan and id should be included in the scan title when the scan is run)



4) The detector you selected should appear.
Detector 5 in this case.

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How to manually save your data

The screenshot shows the Mantid Workbench interface. The 'Algorithms' panel on the left has 'SaveFocusedXYE' selected under the 'Execute' button. A yellow box highlights this selection. A yellow arrow points from a text box to the 'SaveFocusedXYE' algorithm. The 'Messages' panel on the right shows the output of the 'HB2AReduce' algorithm, indicating successful execution.

1) To save your plot search for *SaveFocusedXYE*

2) Click execute to execute the algorithm

```

1 # The following line helps with future compatibility with Python 3
2 # print must now be used as a function, e.g print('Hello','World')
3 from __future__ import (absolute_import, division, print_function, unicode_literals)

...
import *
...
plot as plt

```

Messages:

```

seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
  IPTS-20405/exp624/Datafiles/
  HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.03
seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
  IPTS-20405/exp624/Datafiles/
  HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.03
seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
  IPTS-20405/exp624/Datafiles/
  HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.04
seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
  IPTS-20405/exp624/Datafiles/
  HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.04
seconds
HB2AReduce started
Using vcorr file: /HFIR/HB2A/
  IPTS-20405/exp624/Datafiles/
  HB2A_exp0624_Ge_113_IN_vcorr.txt
HB2AReduce successful, Duration 0.03
seconds

```


3) This box should appear

This is where you name your data

This is the format you would like to save it in
*The next slide will show all the formats the file can be saved as

If you want to keep this box open, click this

When you are ready to run the algorithm click here

This is the workspace you want to save. If you have executed more than one workspace, there is a drop-down function to pick the workspace you want to use

SaveFocusedXYE input dialog

Saves a focused data set (usually the output of a diffraction focusing routine but not exclusively) into a three column format containing X_i , Y_i , and E_i .

InputWorkspace: Sample 1

Filename: Run 1

SplitFiles:

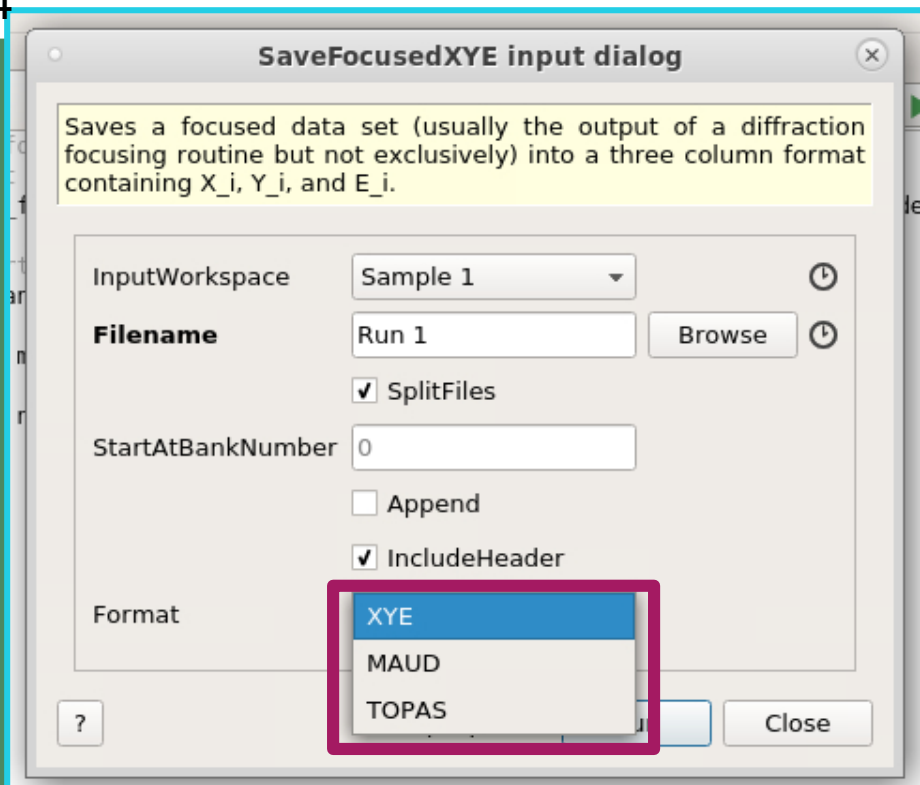
StartAtBankNumber: 0

Append:

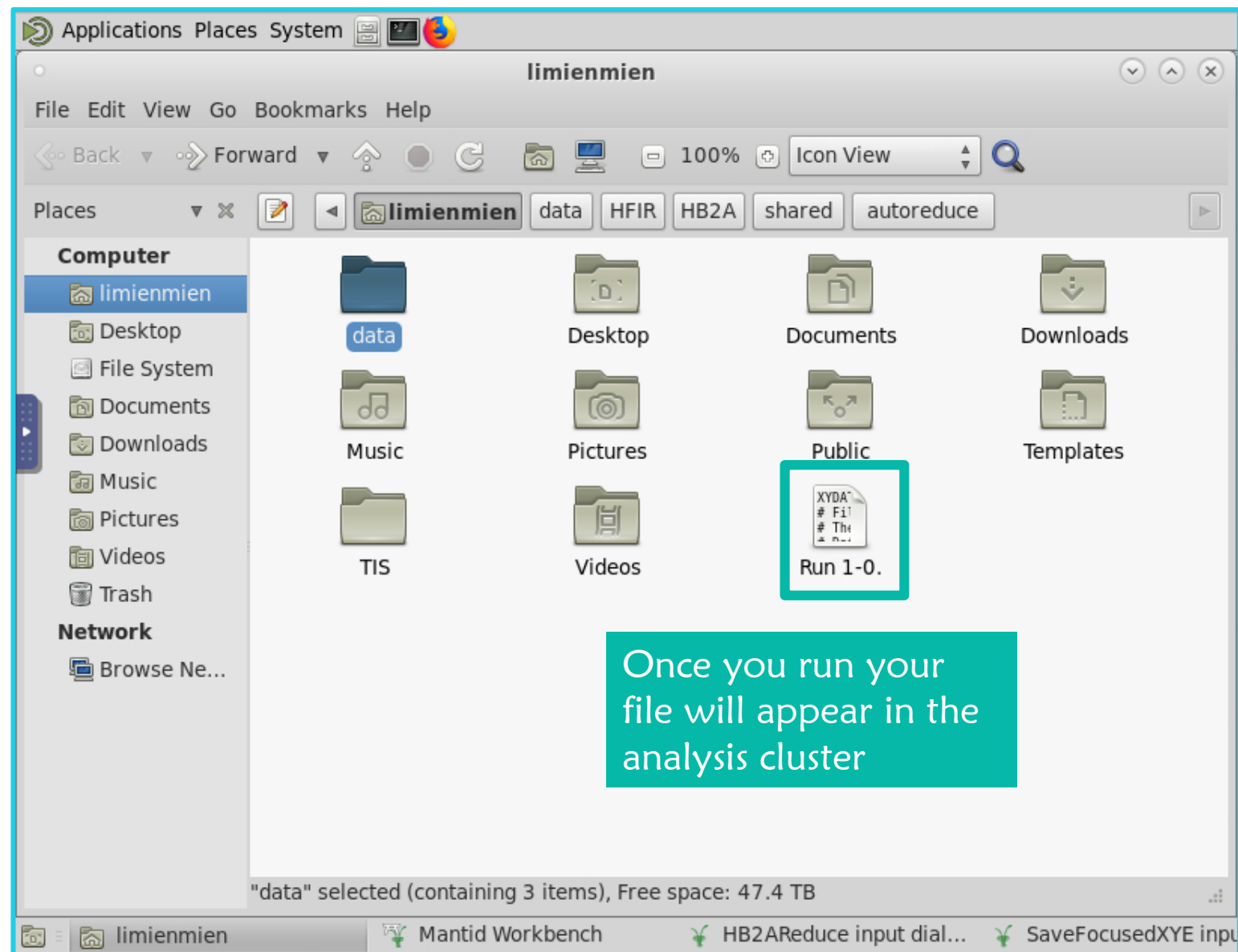
IncludeHeader:

Format: XYE

Keep Open: Run Close



This is a drop-down menu, and you can select the format you want to save your file in



Once you run your file will appear in the analysis cluster