

# PYTHON SCRIPTING FOR INSTRUMENT CONTROL AND ONLINE DATA TREATMENT

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## Abstract

Scripting is an important feature of instrument control software. It allows scientists to execute a sequence of tasks to run complex experiments, and it makes a software developers' life easier when testing and deploying new features. Modern instrument control applications require easy to develop and reliable scripting support.

At ANSTO we provide a Python scripting interface for Gumtree [1]. Gumtree is an application that provides three features; instrument control, data treatment and visualisation for neutron scattering instruments. The scripting layer has been used to coordinate these three features. The language is simple and well documented, so scientists require minimal programming experience. The scripting engine has a web interface so that users can use a web browser to run scripts remotely.

The script interface has a *numpy*-like library that makes data treatment easier. It also has a GUI library that automatically generates control panels for scripts. The same script can be loaded in both the workbench (desktop) application and the web service application for online data treatment. In both cases a GUI will be generated with similar look and feel.

## INTRODUCTION

The Gumtree scripting interface has a *numpy*-like Python library that makes data treatment easier. It also has a graphical user interface library that automatically generates control panels for scripts. The generic GUI rendering feature allows the same scripts to be loaded in both the desktop applications and the web service applications. The scripting interface benefits both the users and the developers. Users can easily make scripts to run experiments or treat the data, with a graphical interface automatically created for these scripts. Developers save a lot of time deploying new products when using this feature since they don't have to recompile. The total cost of operating this framework is therefore significantly reduced

## SYSTEM ARCHITECTURE

It is always important to provide a decent scripting feature in scientific software. When users want to run an experiment, it is a more flexible and direct way to write a script to finish some complex experiment steps. A smart graphical user interface such as software wizard is very useful, but has limited scope. Once users become more familiar with the instrument and the software, they may want to write ad hoc scripts to run complex experiments. In another scenario, when users want to do data treatment on the experimental results, experienced users write their

own scripts to do it. In this way they know exactly what will be done on their data and the scripts are always under their control. Many users love to write the scripts themselves. Other users who don't do programming still agree on the importance of scripting. And they will seek support from the instrument team to write scripts for them.

Gumtree is an application that provides general framework for building scientific software [2]. It is customised at ANSTO for neutron scattering experiments. It provides experiment control and data treatment services for 9 neutron scattering instruments in the Bragg Institute, ANSTO. It is designed to provide a simple and reliable scripting feature for instrument users.

Gumtree software is written in the Java programming language. But the scripting feature is provided in Python language. As shown in Figure 1, the Python engine is a core service of the application.

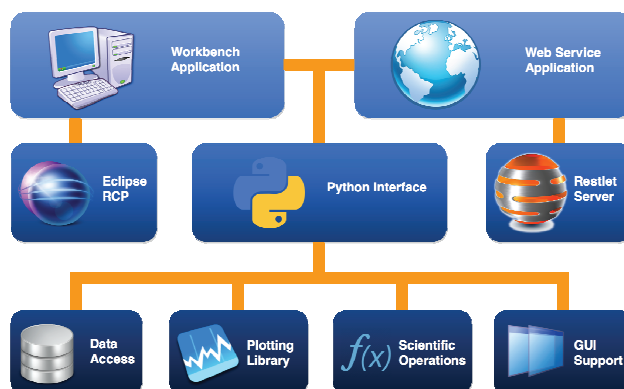


Figure 1: Gumtree system architecture.

## MULTI-DIMENSIONAL ARRAY OBJECT

One of the most important scripting packages in Gumtree is the multi-dimensional array object package. It is a *numpy*-like library that provides convenient access to array operations, the Dataset interface. However it is more than just *numpy*. It provides functions for treating experiment data, such as error propagation, carrying axes information, carrying metadata, and so on. These functions make it easier for users to write scripts for data manipulation and visualisation.

### Categories of the Scripting Interface

The Dataset interface borrows a number of *numpy* function names. Besides that, it also has exclusive function names to make Nexus data reduction easier.

In implementation, the python Dataset is a wrapper of a Java CDMA object [3]. The greater part of the logic

happens in Java. An object wrapped with Dataset can be referenced in Java.

The Dataset interface functions can be classified into the following categories:

- Constructing
- Indexing, Iterating, Slicing and Modifying
- Arithmetic operations
- Mathematical and statistical functions

The following *numpy* methods have been implemented in the Dataset package:

- Array attributes: shape, ndim, size, dtype, tolist
- Array methods: copy, fill, flatten, reduce, take, put, max, min, sum, prod
- Array creation: instance, zeros, ones, linspace, arange, zeros\_like, ones\_like, as array, rand
- Array manipulation: tile, concatenate, take, column\_stack, vstack, hstack, dstack, array\_split, split, vsplit, hsplit, dsplit
- Array modification: fill, append, delete, put
- Maths: add, subtract, multiply, divide, negative, power, exp, ln, log10, sqrt, divide, remainder, sum
- Trig: sin, cos, tan, arcsin, arccos, arctan
- Stats: Random: rand, engine, seed

The following methods are exclusive to the Gumtree Dataset package:

- Error propagation – quick access to var and err
- Normalisation – normalising against nexus metadata
- File access – Nexus HDF file access
- Nexus metadata – quick access to nexus metadata
- Rich axes information – carry Nexus axes

### The Analysis Interface

The Dataset is mapped to a Nexus file either stored in the physical drive or in memory. One can efficiently load a Nexus file into a Dataset. The Dataset is the subject of data analysis scripts, so it carries interfaces for data reduction and analysis.

The following features are designed to help analyse neutron scattering experiment data.

**Error Propagation:** a Dataset normally carries the error information. By default this is setup for Poisson count statistics which are commonly used in neutron scattering. It gets stored as variance in the memory. To access the Dataset variance, use `dataset.var`. To access the error of the Dataset, use `dataset.err` or `dataset.error`. To get the error from the Dataset will call a square root function (Poisson statistics) and hence is costly in compute time. When initialising the Dataset, one can choose to set the variance or not. If no variance is set, by default it will use a copy of the data storage as the variance.

**Nexus Axes:** if the Dataset is loaded from a Nexus file, it carries axes information provided by the file. If a Dataset is created from a helper function, one can initialise the axes in the argument list. If no axes information is provided, by default it creates an integer index as axes for the Dataset.

**Nexus Metadata:** Dataset provides interfaces to access Nexus metadata. Nexus metadata are treated as public

fields of the Dataset. For example, to get the wavelength value of a Dataset, simply call `dataset.wavelength`. To expose metadata in the Nexus file as an easy accessible property, a path table is provided. Before a Dataset is created, one can set a dictionary file that contains the path table information to the Dataset class.

**Normalisation:** the Dataset can be normalised against certain metadata. For example total counts or counting time. To enable the normalisation, set the normalising factor in the Dataset factory.

**Nexus Import and Export:** There is a helper function to help you load Nexus data. The requirements are to set the folder path and instrument prefix, and the use of the Nexus 'signal=1' attribute. Then use `df[index]` to access a file that follows the ANSTO naming convention of [instrument prefix][seven digit index number].nx.hdf. This shortcut can be customised to the naming convention of any facility. Dataset interface supports exporting to a Nexus HDF file.

## PLOTTING LIBRARY

The Python interface for plotting in Gumtree provides scientific plot functionality for one-dimensional curve plot and two-dimensional image plot.

**Curve Plot:** The curve plot is also called plot 1D. The plot takes vector Datasets as input. If the Dataset has axis information, the axis will be used to scale the horizontal axis of the plot. It is allowed to plot multiple Datasets in the same plot. The interface provides functions for managing the Datasets and how they are rendered. Below is an example of the curve plot, as shown in Figure 2.

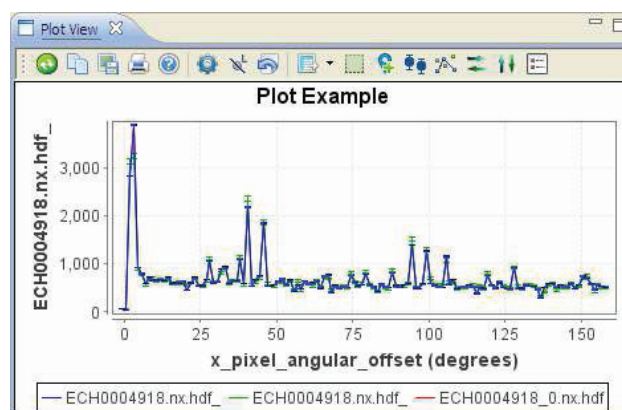


Figure 2: Example of curve plots in Gumtree.

**Image Plot:** the image plot is also called image 2D. The image plot takes a single two-dimensional Dataset as input. The Dataset may have up to two axes. The axes will be used to scale the vertical axis and horizontal axis of the plot. The plot renders the Dataset as a 2D histogram image.

**Plot Control:** The following scripting functions are provided for controlling the plots:

- Axis Control – quick access to axes of the plot, such as zooming in and out, reversing axis, and switching to logarithm axis.
- Rendering Control – change rendering colour, shape, and weight, or add markers, legends and titles.
- Mask Control – add, remove, and change masks.
- I/O Control – import and export data to the plot.
- Event Control – add event handlers to the plot to handle mouse and keyboard event.

### INSTRUMENT CONTROL INTERFACE

Gumtree Python scripting feature provides a library package for instrument control. This package helps users to write scripts that seamlessly combine experiment control and data treatment. For example, a calibration script for the 3-Axis Spectrometer uses the instrument control package to drive instrument devices and collect data. It uses the analysis package to calculate the offset, which will be used to calibrate energy and sample stage.

The instrument control package has two layers. The generic layer has functions for driving devices, setting parameters and collecting data. The instrument specific layer has helper functions for some unique procedures, such as driving the high voltage down on a detector before moving and ramping it up after the move.

### AUTO GUI CREATOR

One of the most advanced features of the scripting application is the auto GUI creator. This feature creates a graphical user interface for scripts automatically. When users are writing scripts for their experiments, they don't need to worry about what the interface looks like in the application. They simply follow a template to create arguments and procedures. When scripts are loaded, Gumtree automatically generates GUI for the scripts. For example, Figure 3 shows the GUI automatically created by a data reduction script for the Strain Scanner instrument 'Kowari' at ANSTO.

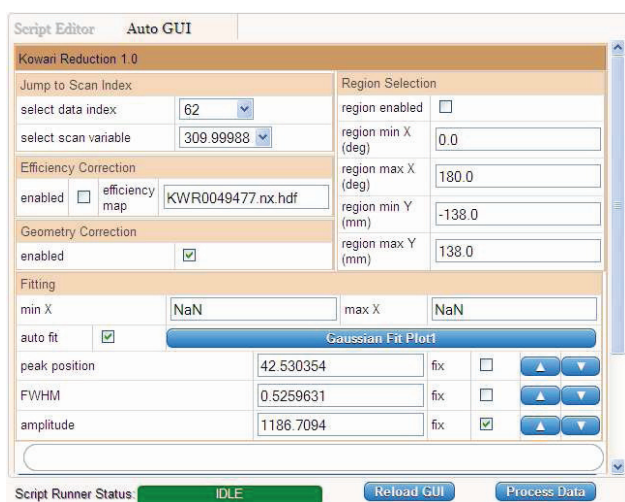


Figure 3: HTML auto-GUI created for a script.

When the user creates this script, all he needs to do is to define some arguments, and to use these arguments in procedures defined in the script. Such a facility minimises the learning requirements of programming with Python scripts. Even a novice user that doesn't have any programming experience with the Python language can make scripts that renders a rich, professional graphical interface.

The value of the feature is enhanced with the ability to execute the scripts on both the desktop application and online web application. Both applications provide similar graphical interfaces for the Python scripts. For example, in Figure 3, a data reduction script is rendered in the Gumtree web service application. The same script can also be used in the Gumtree desktop application for data treatment purpose.

When an argument is defined in the script, it can be defined in a list of types. The argument will be rendered differently according to its type. Table 1 shows a list of allowed types of argument for the Python scripts.

Table 1: Auto GUI Components

Python Type	SWT Widget	HTML Input Type
string, int, float	Text Widget	Text Input
bool	CheckBox	CheckBox
option	ComboViewer	Select
file	BrowseButton	Text Input
action	Button	Button
Group	MenuGroup	Table
progress	ProgressBar	jQuery widget
label, space	Label	Plain text

The Python scripting feature provides more GUI controls for advanced users. Users can define arbitrary table grid for the control panel to make the outlook more straightforward and more concise. Users can also have direct control of the widgets such as folding a group, enabling or disabling control widgets, and changing widget status.

### WIDELY USED IN ANSTO

The Python scripting feature has been widely used for experiment control and data treatment in neutron scattering experiments at ANSTO. Software developers of Gumtree applications write python script modules for complex experiment control tasks. For example, the calibration task of the Thermal 3-Axis Spectrometer was written in Python scripts. The scripts combine instrument control and data analysis together, so that the calibration procedure is highly automated. Figure 4 shows an example of using the script to do Nickel calibration routine.

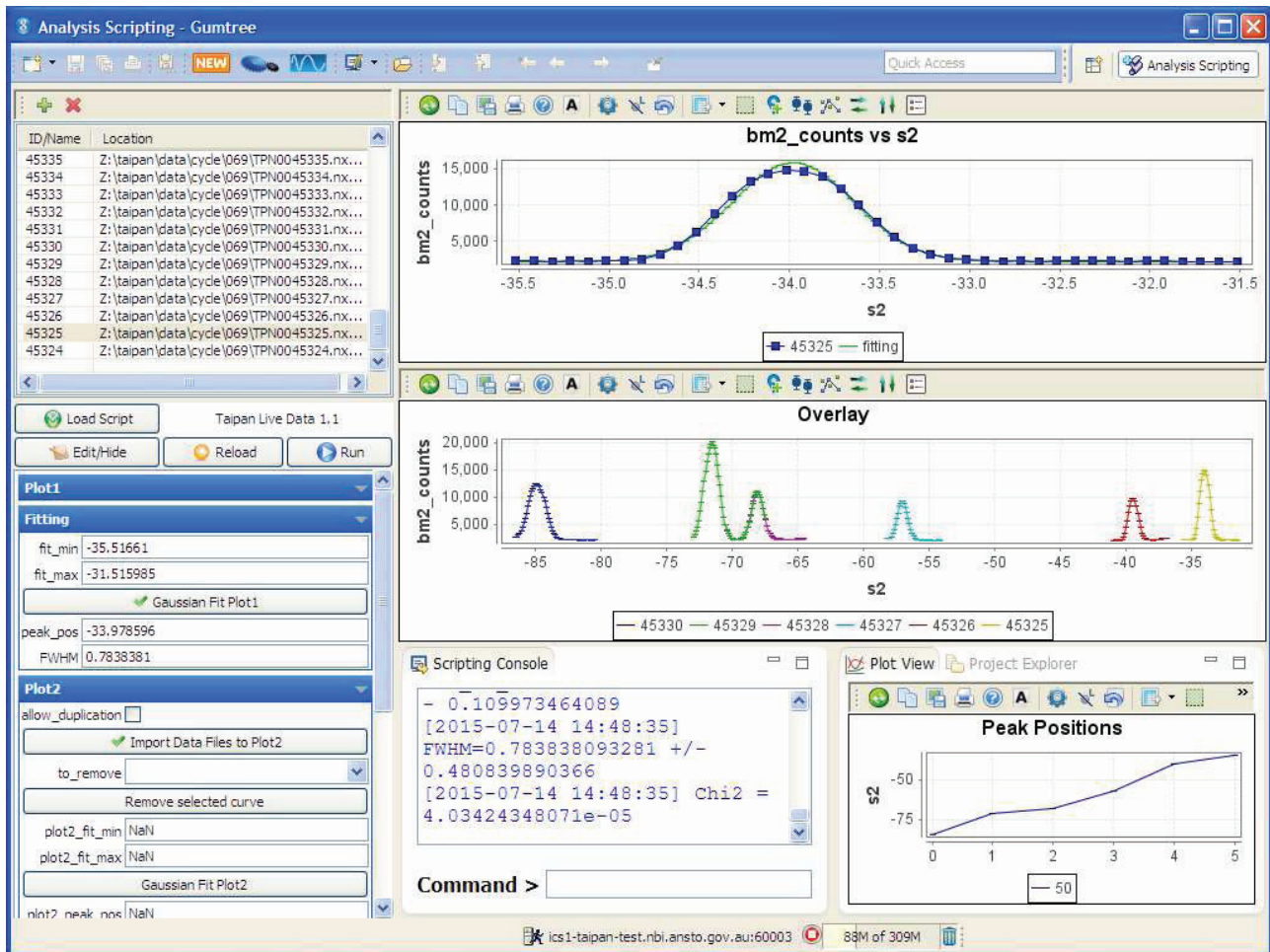


Figure 4: Calibration script for Thermal 3-Axis Spectrometer in Gumtree application.

Another example of using Python scripts in Gumtree is the implementation of the multi-sample workflow feature. This feature significantly improves the usability and efficiency of the Small Angle Scattering instruments in ANSTO. Python scripts play key technical roles in the software engineering of this feature.

Besides software developers, instrument scientists and users can quickly write Python scripts to do some ad hoc tasks on the instruments. For example, when new sample environment components are added to the instrument, it is more convenient to write a script on the fly to use them in experiments.

Python scripts are also used to provide data treatment features in both the Gumtree desktop applications and the Gumtree web applications. Data reduction applications of the Powder Diffractometer, the Strain Scanners, the Ultra-SANS, etc., are written in Python scripts.

In conclusion, Python scripts are used in the following actions:

- Preview data and send feedback to experiment
- Treat data on a local computer or on the server
- Align instrument
- Create quick experiment interfaces
- Make highly customisable features

## CONCLUSION

The Python scripting feature in the Gumtree software plays an important role in experiment control and data treatment for neutron scattering experiments at ANSTO. The *numpy*-like interface to Dataset, auto-GUI creator and the generic rendering feature are often used features that make it easier for users to write powerful scripts that can run in both desktop and web applications. The development and operations of Gumtree client and server for 9 instruments are supported with approximately 1 FTE with capacity to support more instruments in the future.

## REFERENCES

- [1] Gumtree website: <https://github.com/Gumtree>
- [2] T. Lam, N. Hauser, A. Gotz, P. Hathaway, F. Franceschini, H. Rayner, "GumTree. An Integrated Scientific Experiment Environment", *Physica B* 385-386, 1330-1332 (2006)
- [3] S. Poirier, A. Buteau, M. Ounsy, C. Rodriguez, N. Hauser, T. Lam, N. Xiong, "Common Data Model Access; A Unified Layer To Access Data From Data Analysis Point Of View", *Proceedings of ICALEPCS 2013, Grenoble, France*, pages 1020-1023 (2013).