

## QUOKKA user manual

*This guide is not intended to replace your local contact, but to jog your memory if you are operating independently. Anything strange, call your local contact...*

Numbers for QUOKKA local contacts:

Elliot Gilbert, office – 9470, mobile – 04 09 03 43 05

Katy Wood, office – 7100, mobile – 04 17 47 35 37

Jitendra Mata, office – 7221, mobile – 04 30 19 30 21

Chung-Ming (Charlie) Wu, office – 7213, mobile – 04 21 13 53 67

Andrew Whitten, office – 3582,

An image of the QUOKKA detector is visible from outside ANSTO at the following webpage:

<http://www.nbi.ansto.gov.au/quokka/>

Reactor status and cold source temperature visible at (do not leave this webpage open for long periods of time):

<http://prism.nbi.ansto.gov.au/reactor/ReactorInfo.swf>

Other useful numbers:

Emergencies – ERT: 888

ERT(not emergency, working alone form etc...): 3434

Health Physics: 9779

IT helpdesk: 9200

<b>1. PERFORMING AN EXPERIMENT</b>	<b>3</b>
<b>1.1. LOGIN TO DATA ACQUISITION COMPUTER</b>	<b>3</b>
<b>1.2. START GUMTREE</b>	<b>3</b>
<b>1.3. STARTING A STANDARD EXPERIMENT</b>	<b>3</b>
I. SELECT 'MULTI-SAMPLE WORKFLOW':	4
II. INSERT SAMPLE DETAILS	5
III. SELECT CONFIGURATIONS	7
IV. SELECT ENVIRONMENT – EXAMPLE OF TEMPERATURE CONTROL	8
V. SELECT ENVIRONMENT – EXAMPLE OF DUMMY MOTOR AND TEMPERATURE CONTROL	9
VI. ACQUISITION TAB – EXAMPLE WITHOUT ANY SAMPLE ENVIRONMENT CONTROL	10
VII. ACQUISITION TAB – EXAMPLE OF TEMPERATURE CONTROL	12
VIII. ACQUISITION TAB – EXAMPLE OF TEMPERATURE CONTROL AND DUMMY MOTOR	13
IX. ACQUISITION TAB – EXAMPLE USING DETECTOR COUNTS INSTEAD OF TIME	14
<b>1.4. WHERE IS THE DATA?</b>	<b>14</b>
<b>1.5. IS MY EXPERIMENT RUNNING OK?</b>	<b>15</b>
<b>1.6. COMMON ISSUES</b>	<b>15</b>
X. I HAVE STARTED A WORKFLOW, BUT WOULD LIKE TO STOP IT.	15
XI. I HAVE STARTED A WORKFLOW, BUT WOULD LIKE TO PAUSE IT.	15
<b>1.7. 'ON THE FLY' DATA INSPECTION WITH IGOR</b>	<b>15</b>
<b>1.8. BEFORE YOU LEAVE</b>	<b>19</b>
<b>2. INSTALLING DATA REDUCTION MACROS ON YOUR OWN COMPUTER</b>	<b>19</b>
<b>2.1. INSTALL IGOR</b>	<b>19</b>
<b>2.2. REMOVE ANY OLDER VERSIONS OF THE MACROS.</b>	<b>19</b>
<b>2.3. INSTALL QUOKKA SPECIFIC MACROS</b>	<b>20</b>
<b>2.4. SWITCH TO NIST MACROS</b>	<b>21</b>
<b>3. QUICK GUIDE TO QUOKKA DATA REDUCTION</b>	<b>22</b>
<b>3.1. CHOSE A WORKSPACE AND COPY ACROSS REPORT FILES</b>	<b>22</b>
<b>3.2. OPEN IGOR MACROS</b>	<b>22</b>
<b>3.3. SELECT WORKING DIRECTORY</b>	<b>23</b>

<b>3.4. CALCULATING TRANSMISSIONS.</b>	<b>23</b>
XII. READ THE REPORT FILE & CREATE TABLE	23
XIII. CALCULATE TRANSMISSIONS	23
<b>3.5. REDUCE DATA</b>	<b>23</b>
<b>3.6 PATCH THE DATA (IF REQUIRED)</b>	<b>25</b>

## **1. Performing an experiment**

Your local contact will train you in how to enter the enclosure and load samples. Please note safety aspects of the stairs and platform in the QUOKKA sample area. There should be no gap between the platform and instrument sample stage. Going down the stairs you should stay facing the instrument (as you would going down a ladder) and hold onto the hand rail. If you have any concerns please speak to your instrument scientist.

Before you change samples independently you must sign the training form to acknowledge you have received the training. The following describes how to run the acquisition software.

### **1.1. Login to data acquisition computer**

*Login and password will be given to you by your local contact*

### **1.2. Start gumtree**

Link on desktop

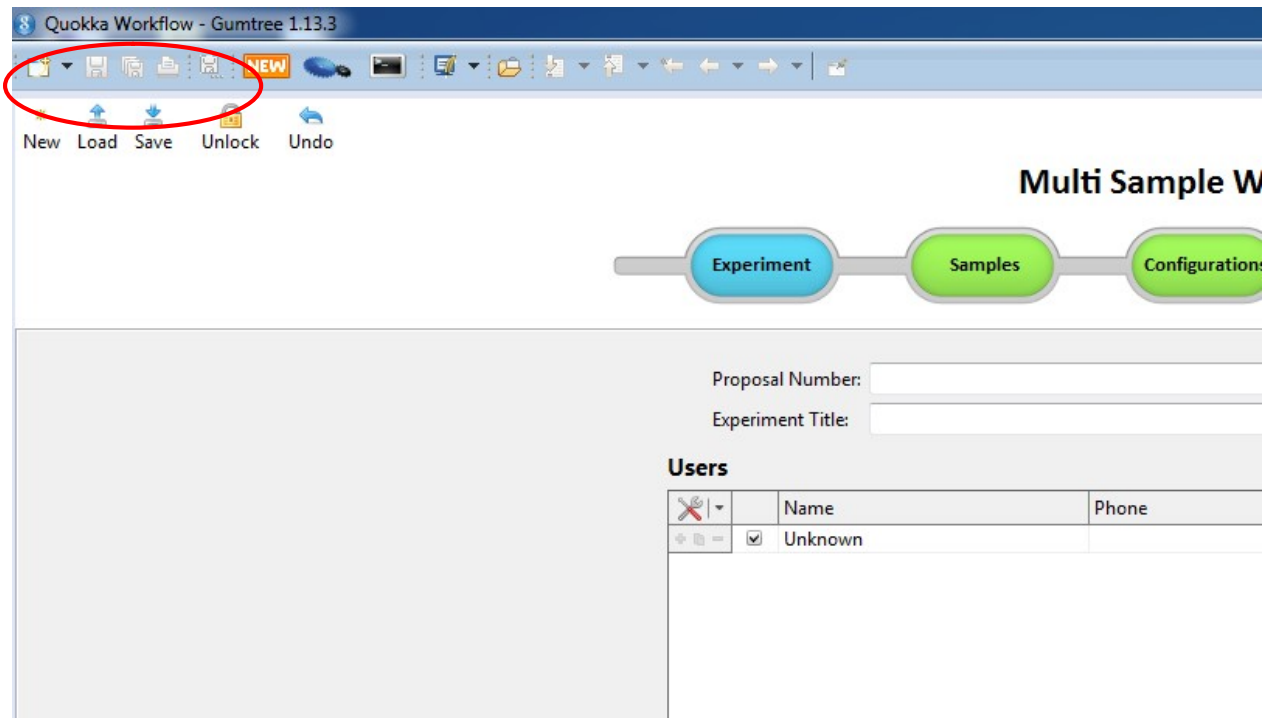
*Login and password will be given to you by your local contact*

(Normally this would already be open).

### **1.3. Starting a standard experiment**

Below describes starting an experiment with the 20 position sample changer.

i. Select 'multi-sample workflow':

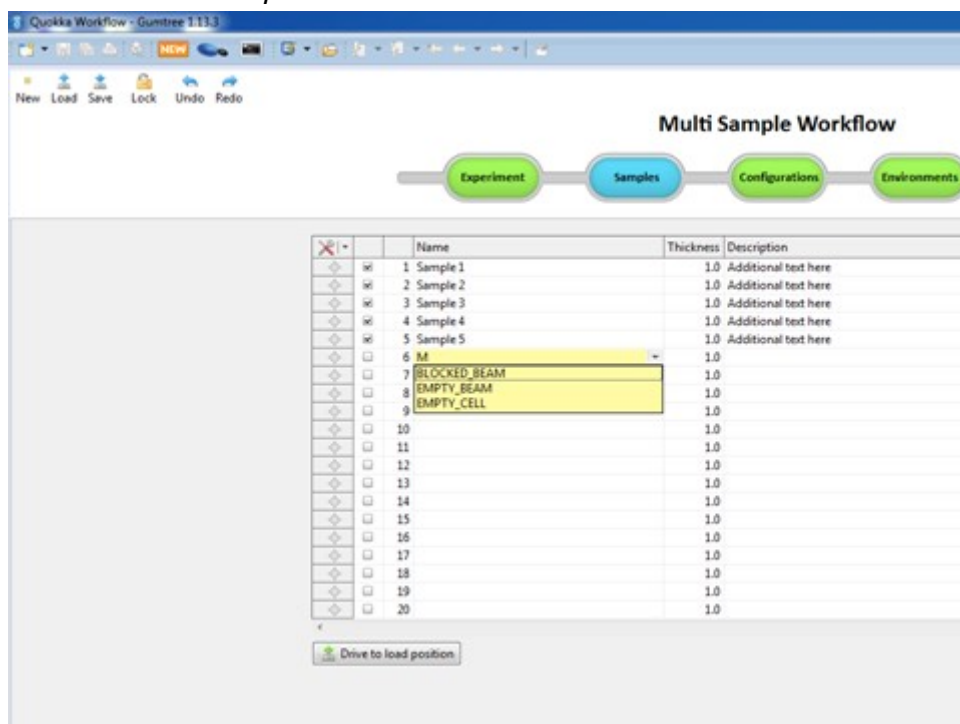


The 'Experiment' tab is highlighted in blue. In the 'Proposal Number' box enter the proposal number and then click on 'Autofill'. The experiment title and experimental team will be loaded automatically. Changes can be made to these fields if required.

The upper left buttons circled in red in the above figure allow the following:

- 'New', start a new blank workflow (this will delete any of the workflow currently active).
- 'Load' can be used to load a previously saved workflow
- 'Save' saves the state of the workflow and you will be prompted to choose a name. This can be used if you would like to save the entire workflow (configurations, samples, count-times etc...) and may be useful if you return and run similar experiment in the future.
- 'Unlock', only your local contact can unlock this button. When locked the workflow will not allow you to modify any configurations, but you may still run the workflow, label samples and change count-times.
- 'Undo' to undo the last action performed.

## ii. Insert sample details



Click on the 'Samples' tab to insert sample details (now highlighted in blue).

Fill in the 'Name' column with the names of your samples in the different positions. Additional text may be entered in the 'Description' column (optional).

Type the thickness in the thickness column.

To select Blocked Beam/ Empty beam/ Empty Cell enter some text and click the downwards arrow that appears. This will ensure the correct file associations occur and simplifies data reduction. Samples need to have the check box ticked on the left to be run (this is checked automatically but can be unchecked if you do not wish to run the sample).

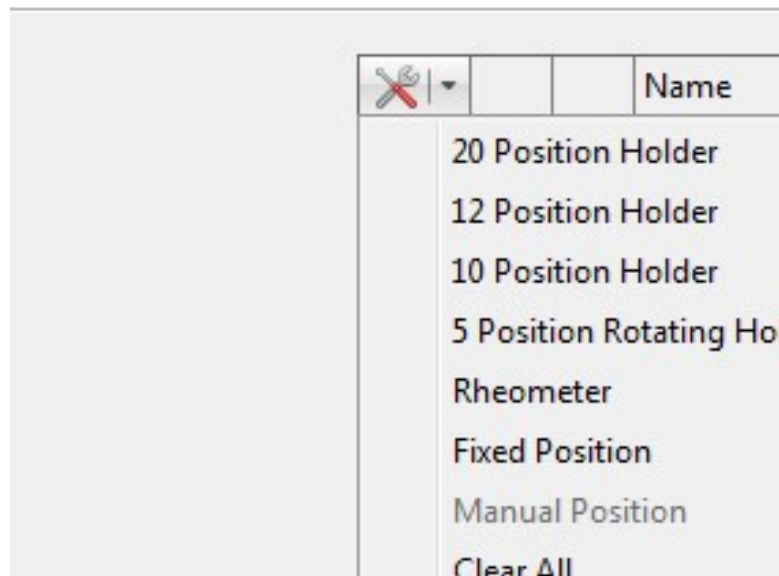
The 'drive to load position' button allows you to move the sample changer in the enclosure to a position where you can easily load your samples. Once in this position insert your sample blocks into the changer. The workflow automatically drives the changer to the load position at the end of a run so generally it is not necessary to hit the 'drive to load position'. If you wish to drive to a different sample position for any reason, the button to the left of the sample can be pressed, shown below with a red arrow below:

Undo Redo



By clicking on the drop down tools menu, circled in red above, brings up other useful options:

Undo Redo



The first options allow to change between different sample environments: 20 positions sample changer, 12 position etc... Your local contact will select the appropriate sample environment this up for you and it should not be changed.

'Clear All' allows you to delete all sample names.

'Enable all' and 'Disable all' check or uncheck all samples. Only checked samples will be run.

'CSV Import' allows you to import a previously saved list of samples.

'CSV Export' allows you to save the current list of sample names to a CSV file.

### iii. Select configurations

Navigate to the 'Configuration' tab.

Your local contact will discuss suitable instrument configurations with you prior to starting the experiment and these will be listed in the column on the left.

The configurations you wish to run need to be checked on the left, those that are not run unchecked.

Redo

## Multi Sample Work

Experiment Samples Configurations

	Name
<input checked="" type="checkbox"/>	1 L1=12m_L2=1p3m
<input checked="" type="checkbox"/>	2 L1=L2=8m
<input checked="" type="checkbox"/>	3 L1=L2=20m_lens_med

Configuration

Group: Katy

Name: L1=L2=20m\_lens\_med

Description: New fast scripts

Scripts

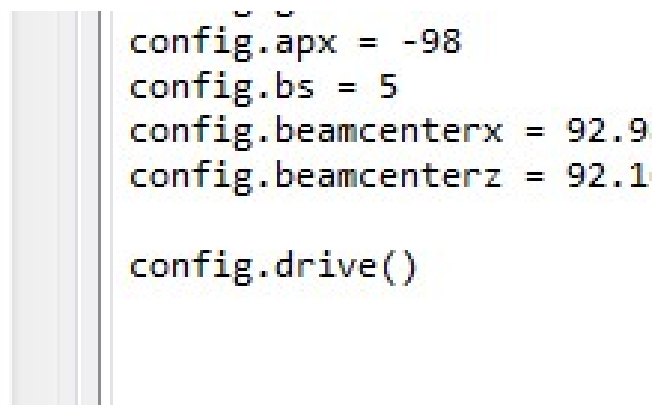
Initialize Pre-Transmission

```
config.wavelength = 8.1
config.wavelength_sprea
config.det = 19250
config.det_offset = 0
config.srce = 30
config.guide = 'lens'
config.apx = -98
config.bs = 5
config.beamcenterx = 92
config.beamcenterz = 92
config.drive()
```

The only parameters that should be changed by the user on this page are the acquisition times circled here in red on the bottom right. On the left is the acquisition time for the transmission measurement, generally 120 seconds is suitable. On the right is the acquisition time for samples. The number inserted here (in the example 600 seconds) will be used for all samples, but can be changed for individual samples later.

The red arrow on the above screen shot shows where configurations can be re-ordered by changing the number to the left of the configuration name.

More options for choosing counting times can be found by clicking the 'Advanced Options'.



```
config.apx = -98
config.bs = 5
config.beamcenterx = 92.9
config.beamcenterz = 92.1

config.drive()
```

You can then specify how many monitor counts or detector counts you would like in the data files rather than defining a count time. A minimum time and maximum time are also given to make sure counting times do not become unreasonable.

Enter counting times in all the different configurations on this page, navigating to the different configurations is done by simply clicking on the title in the left and column.

#### *iv. Select environment – example of Temperature Control*

Once you are happy with configurations and counting times, select the 'Environment' tab. If you are not running any temperature control or repeating measurements do not change anything here and simply skip to the final 'Acquisition' tab.

Below is an example of how to use the temperature bath (Huber). Select the 'tc1\_loop1' from the 'Template' drop down menu (upper right, circled in red below).

At the bottom of the page (circled in red below) enter a start and end temperature in the 'From' and 'To' boxes. The number of steps or temperature points is inserted in 'Steps', and a value in seconds of time to wait before the acquisition starts, then click 'Generate'. In the example below 5 temperature points are measured between 20 and 60 C. A table appears above listing the temperature points. The temperatures and wait times can be modified by writing directly in the table, and also re-ordered by changing the numbers next to them. Steps can be added /removed by using the tools drop down menu on the table.



## Multi Sample Workflow

	Name
1	Environment
2	Configurations
3	Samples

Environment

Name: Environment

Description: Temperature bath

Scripts

Initialize

Drive

```
sics.drive("/sample/tc1/
```

Values

- v. *Select environment – example of Dummy motor and Temperature Control*

Several different environments can be selected and embedded within each other. Below shows an example where a 'Dummy\_motor' is used from the Template menu. The dummy motor is used simply to collect data from your samples several times. In the example below, the same temperature series will be run twice (20C, 30C, 40C, 50C, 60C, 20C, 30C, 40C, 50C, 60C) . The sample environments 'Loop' and 'Temperature bath' can be re-ordered so that two separate data sets are collected at each temperature (ie, 20C Loop1, 20C Loop2, 30C Loop1, 30C Loop2 etc...)

## Multi Sample Work



The screenshot shows the 'Experiment' tab selected. On the left, a table lists configurations:

	Name
1	Loop
2	Temperature bath
3	Configurations
4	Samples

On the right, a panel shows configuration details for the selected 'Loop' configuration:

- Environment: Name: Loop, Description: (empty)
- Scripts: Initialize (empty), Drive (sics.drive("du...))
- Values: (empty)

vi. Acquisition tab – example without any sample environment control

# Multi Sample Work



Acquisition Tree						Max
<input checked="" type="checkbox"/>	1	L1=12m_L2=1p3m				
<input checked="" type="checkbox"/>	1	Transmission				<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	1	Sample 1	Position:	1	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	2	Sample 2	Position:	2	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	3	Sample 3	Position:	3	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	4	Sample 4	Position:	4	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	5	Sample 5	Position:	5	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	6	EMPTY_BEAM	Position:	6	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	2	Scattering				<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	1	Sample 1	Position:	1	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	2	Sample 2	Position:	2	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	3	Sample 3	Position:	3	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	4	Sample 4	Position:	4	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	5	Sample 5	Position:	5	<input checked="" type="checkbox"/>	
<input type="checkbox"/>	6	EMPTY_BEAM	Position:	6	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	2	L1=L2=8m				
<input checked="" type="checkbox"/>	1	Transmission				<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	1	Sample 1	Position:	1	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	2	Sample 2	Position:	2	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	3	Sample 3	Position:	3	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	4	Sample 4	Position:	4	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	5	Sample 5	Position:	5	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	6	EMPTY_BEAM	Position:	6	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	2	Scattering				<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/>	1	Sample 1	Position:	1	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	2	Sample 2	Position:	2	<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	3	Sample 3	Position:	3	<input checked="" type="checkbox"/>	

A final table is generated here with all the configurations selected and different samples, and it is possible at this point to finely control which measurements will occur for what time and in what order.

Unchecking boxes enables you to unselect either the entire configuration, all the transmission /scattering measurements or individual samples. Samples or configurations that are not going to be run become greyed out.

The order of configurations, Transmission/Scattering and the samples themselves can be modified by changing in numbers in the boxes on the

left. The count times on the right can also be modified for individual samples.

For ease of viewing levels can be 'collapsed' by clicking on the small triangle next to either the configuration or the Transmission/Scattering titles.

By default the transmission is recorded for the empty beam but not the scattering, as this is generally what is performed, but this can be changed if required.

At the bottom, a time estimation is given, the configuration times are currently overestimated.

Clicking 'run' then starts the run you have setup. If you have not opened the shutter, you will see a prompt 'shutter not open'. Check it's open and then 'OK' to start your run.

The workflow will then ask if you would like to optimise the order in which your experiments will proceed (ie it will measure samples 1,2,3,4,5 in configuration 1 and then 5,4,3,2,1 in configuration 2). It is generally advised not to optimise the order simply for ease of data reduction.

*vii. Acquisition tab – example of Temperature Control*

In the case where temperature control is used, these values also appear in the final table.

Acquisition Tree			
▲	☑	1	Value: 20 Wait: 1
	▶	☑	1 L1=12m_L2=1p3m
	▶	☑	2 L1=L2=8m
	▶	☑	3 L1=L2=20m_lens_med
▲	☑	2	Value: 30 Wait: 1
	▶	☑	1 L1=12m_L2=1p3m
	▶	☑	2 L1=L2=8m
	▶	☑	3 L1=L2=20m_lens_med
▲	☑	3	Value: 40 Wait: 1
	▶	☑	1 L1=12m_L2=1p3m

As with the above example, everything in this table can be modified, temperatures, wait times etc... In the above example the levels have been collapsed for ease of viewing. These can be re-expanded by clicking on the triangle next to the different configurations.

When the workflow is run, it will prompt if you would like to optimise the order of experiments with respect to samples and to sample environment. Generally it is best to optimise with respect to sample environment but not to samples.

viii. *Acquisition tab – example of Temperature Control and Dummy Motor*

## Multi Sample Work



Acquisition Tree			
▲	☑	Loop	
☑	☑	1 Value:	1 Wait: 1
▲	☑	Temperature bath	
☑	☑	1 Value:	20 Wait: 1
▶	☑	1 L1=12m_L2=1p3m	
▶	☑	2 L1=L2=8m	
▶	☑	3 L1=L2=20m_lens_med	
☑	☑	2 Value:	30 Wait: 1
▶	☑	1 L1=12m_L2=1p3m	
▶	☑	2 L1=L2=8m	
▶	☑	3 L1=L2=20m_lens_med	
☑	☑	3 Value:	40 Wait: 1
▶	☑	1 L1=12m_L2=1p3m	
▶	☑	2 L1=L2=8m	
▶	☑	3 L1=L2=20m_lens_med	
☑	☑	4 Value:	50 Wait: 1
▶	☑	1 L1=12m_L2=1p3m	
▶	☑	2 L1=L2=8m	
▶	☑	3 L1=L2=20m_lens_med	
☑	☑	5 Value:	60 Wait: 1
▶	☑	1 L1=12m_L2=1p3m	
▶	☑	2 L1=L2=8m	
▶	☑	3 L1=L2=20m_lens_med	
☑	☑	2 Value:	2 Wait: 1
▲	☑	Temperature bath	
☑	☑	1 Value:	20 Wait: 1
▶	☑	1 L1=12m L2=1p3m	

As with the above examples, temperature, dummy motor values, configurations and samples can all be re-ordered. The wait times and data acquisition times can also be changed for each temperature step sample.

Here the configurations have been collapsed for ease of visibility, they can be re-expanded by clicking on the arrows next to them.

ix. Acquisition tab – example using detector counts instead of time



## Multi Sample Workflow



Acquisition Tree		Min Time	Detector
1	L1=12m_L2=1p3m		
1	Transmission	<input type="checkbox"/>	1 <input type="checkbox"/>
2	Scattering	<input type="checkbox"/>	5 <input type="checkbox"/>
2	L1=L2=8m		
1	Transmission	<input type="checkbox"/>	1 <input type="checkbox"/>
2	Scattering	<input type="checkbox"/>	5 <input type="checkbox"/>
3	L1=L2=20m_lens_med		
1	Transmission	<input type="checkbox"/>	1 <input type="checkbox"/>
1	Sample 1	Position: 1	<input type="checkbox"/>
2	Sample 2	Position: 2	<input type="checkbox"/>
3	Sample 3	Position: 3	<input type="checkbox"/>
4	Sample 4	Position: 4	<input type="checkbox"/>

In this case, counting to detector counts has been selected in the Configurations tab. In the above example the transmission is counted for 120 seconds, but the scattering will be collected for each sample until 3e5 detector counts are recorded. Minimum and maximum times (here of 5 seconds and 600 seconds) are included to ensure count times remain reasonable.

### 1.4. Where is the data?

Data files are written and updated every minute in the directory in /experiments/quokka/data/current. This directory is read only.

Report files are in /experiments/quokka/data/current/reports

A read/write copy of the data is also copied to the directory named after the proposal number: /experiments/quokka/data/proposal/xxx. This data modified etc... and used to do data reduction (see section 3). It is updated approximately every 4 minutes.

At the end of the cycle the read only copy of the data and report files will be moved into a directory named after the cycle number, eg. /experiments/quokka/data/cycle/030

Links to these directories can be found on the desktop.

### **1.5. Is my experiment running OK?**

- As the workflow moves through your run, messages will be displayed at the bottom in the 'console' indicating progress. Any errors will appear in red.

- Approximate counts/rates on 'standard' samples. For each experiment, your local contact will record count rates on standard samples (ie empty cell, D2O etc...), which are printed and in a folder. You should have similar values to those recorded for the same configurations.

### **1.6. Common issues**

*x. I have started a workflow, but would like to stop it.*

Click on any of the 'Interrupt buttons'. A report file will be saved.



Multisample work flow will then go into 'cleanup mode', ie will drive the attenuation to a high value, protecting the detector from any possible over-exposure. By using the 'back' buttons, you can then modify the run and restart.

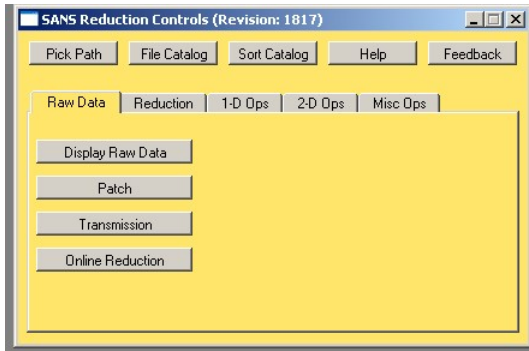
*xi. I have started a workflow, but would like to pause it.*

The workflow can be paused if the detector is counting by clicking on 'pause' in gumtree. If the detector is not counting (eg the instrument is moving between configurations, it is not possible to pause the workflow).

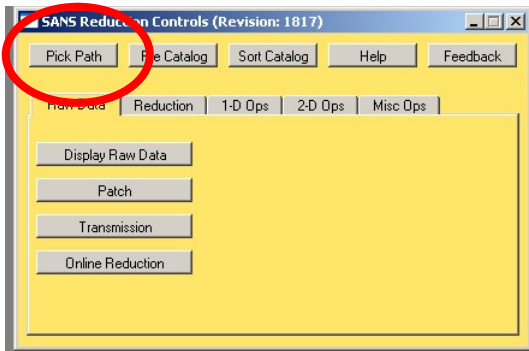
### **1.7. 'On the fly' data inspection with Igor**

It is now possible to look at data during collection, before the file is complete. Following the procedure below allows you to open the file and inspect the radial average, which will automatically be updated approximately every minute.

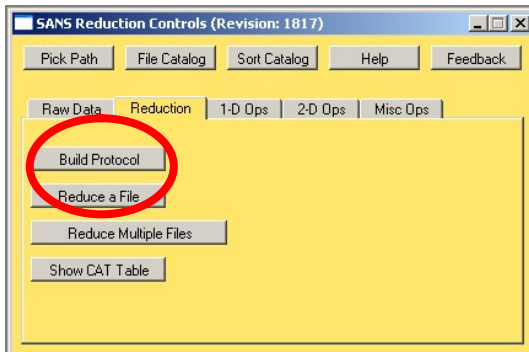
1. Open "Igor with Quokka macros", and in the macros menu select 'Load Quokka Sans Reduction Macros'. Following yellow panel appears.



2. Click on 'Pick Path' and navigate to /experiments/quokka/data/proposal/xxx

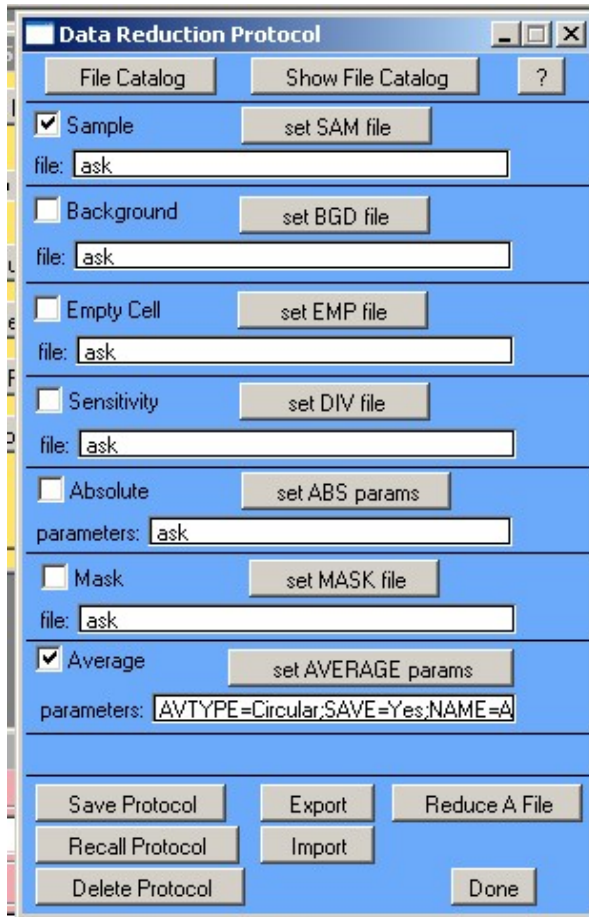


3. In the 'Reduction' tab 'Build protocol'.



Following appears:

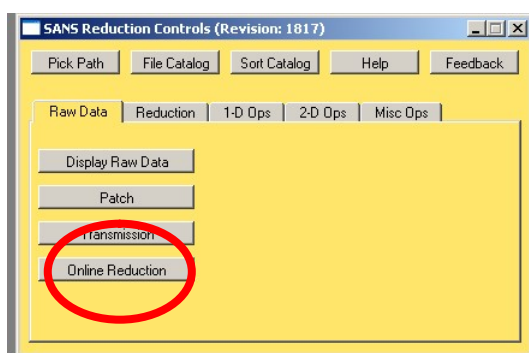




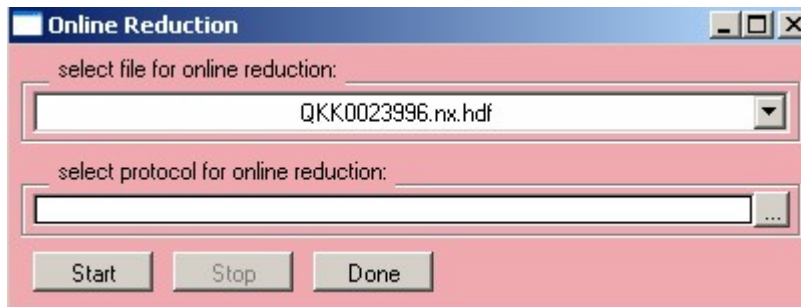
Uncheck all except Sample and Average and 'Save protocol'. Choose a name eg 'on\_line'.

(Note that it is not possible to put data on an absolute scale on the fly, as the transmission has not yet been calculated, you can however add in the other steps of the data reduction protocol if required).

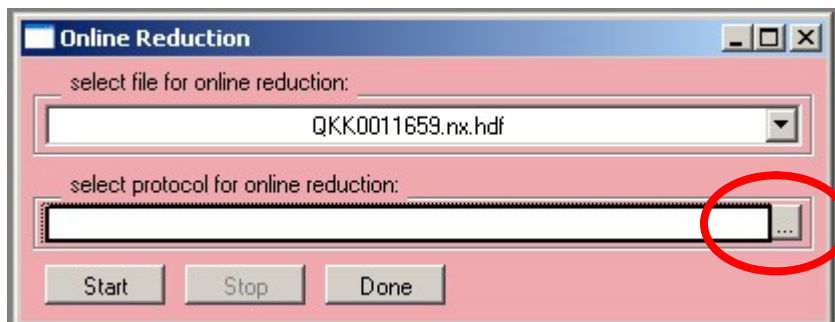
4. Select 'Online Reduction' on the 'Raw Data' tab



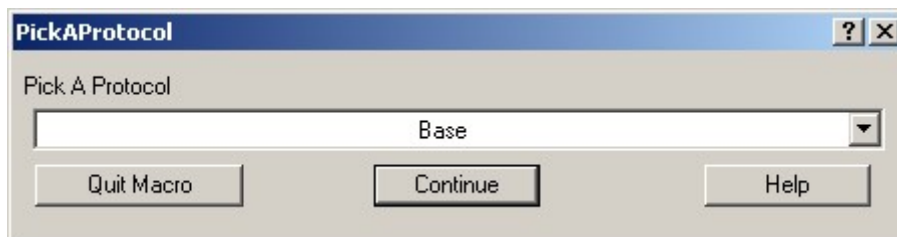
Following appears:



Select the file you would like in top drop down menu.  
In the second window click `...`,



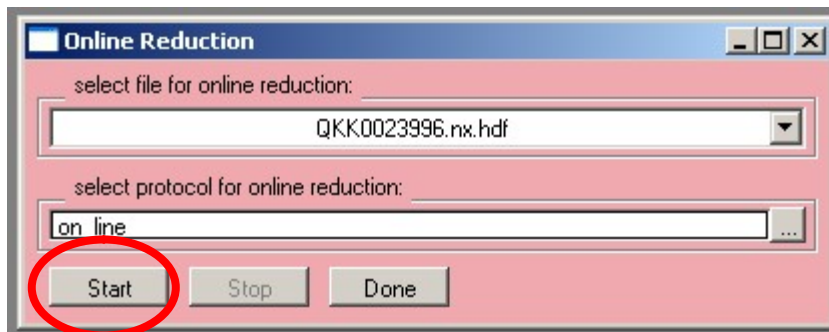
following appears:



Select the protocol you have just built in the drop down menu, eg `on\_line` and `continue`.



Then click `start` on the pink `Online Reduction panel`.



The radial average data will then be displayed and automatically updated.

### **1.8. Before you leave**

Before you leave the instrument, please:

- Clean and return your sample holders. Instructions in the 'instructions' section of the manual in the cabin. We will not lend sample holders to users who have a history of not returning them clean.
- Take all raw and treated using ANSTO sharefile (web-based system) at [sharefile.ansto.gov.au](http://sharefile.ansto.gov.au).

## **2. Installing data reduction macros on your own computer**

Note: Any data publication with QUOKKA data reduced with the NIST macros should cite: Kline SR (2006) Reduction and analysis of SANS and USANS data using IGOR Pro. *Journal of Applied Crystallography* **39**: 895-900

### **2.1. Install Igor**

If you don't already have it... A free 30 day demo version can be downloaded from the wavemetrics website. You need Igor version 6.2 or later.

### **2.2. Remove any older versions of the macros.**

Skip this step if you've never had any of the NIST or QUOKKA macros installed. If you've had any older versions of the NIST or QUOKKA analysis macros installed, it's important to remove completely/rename folder so there will be no conflicts. You will only have to do this once, as the future

updates will be done automatically as long as you are connected to the internet.

**! Caution** – once you have installed the newer versions of the macros, you will not be able to load any Igor project files made with the older ones. This means you should save all the treated asquii files you are likely to need before installing a newer version of the software.

1) Delete any old NIST and QUOKKA macros from the following directories (or move all macros elsewhere if you'd like to keep older versions of the macros):

- C:\Program Files\WaveMetrics\Igor Pro Folder\User Procedures
- C:\Documents and Settings\user\_name\My Documents\WaveMetrics\Igor Pro 6 User Files\User Procedures
- C:\Documents and Settings\user\_name\My Documents\WaveMetrics\Igor Pro 6 User Files\Igor Procedures

2) Delete the two shortcuts to HDF5.xop and HDF5 Browser.ipf in:

C:\Program Files\WaveMetrics\Igor Pro Folder\Igor Extensions

### 2.3. Install QUOKKA specific macros

Navigate to:

<http://www.nbi.ansto.gov.au/quokka/macros/IgorUserFilesSwitch.exe>

and download the executable 'IgorUserFilesSwitch.exe'. Double click on the executable.

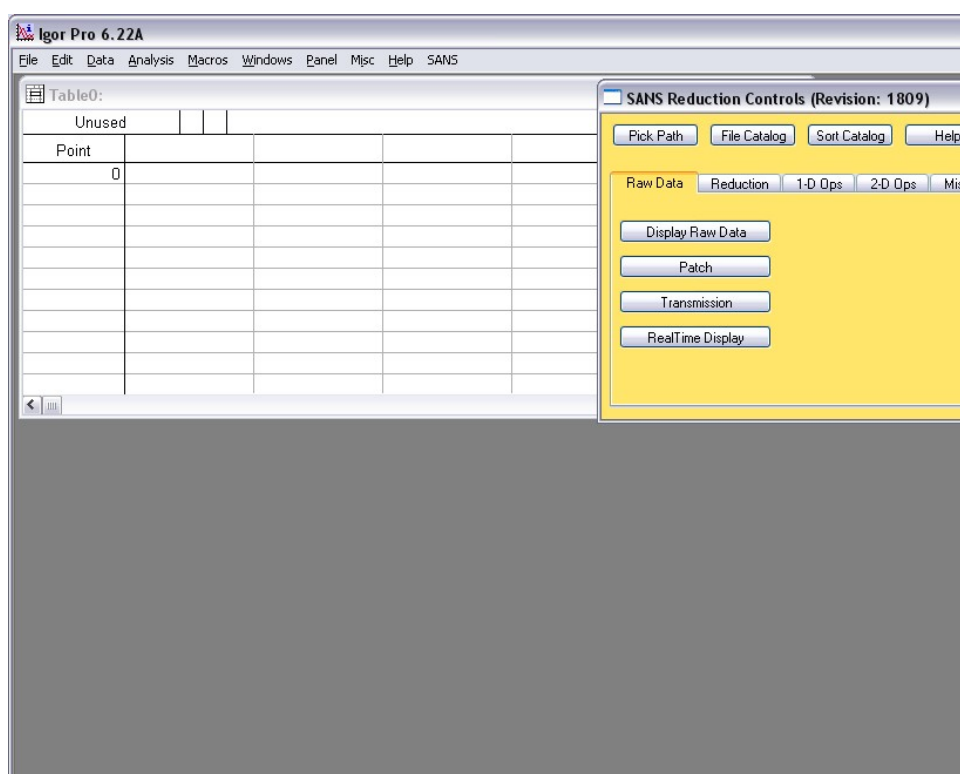


Select QUOKKA macros to install and click OK. You will be asked if it is OK to download the macros, select yes.

After installation 'continue' will launch Igor. Ticking the 'continue when done box' will automatically start Igor after you have used the switch.

Once this is done you should have a "Igor with Quokka macros" shortcut either under the Start>Igor menu OR on your desktop (depending on which version of windows you are running).

Once Igor Pro is open, the Macros menu should now contain 'Load Quokka SANS Reduction Macros'. Selecting this brings up yellow 'SANS Reduction Controls'.



Every time you open the "Igor with Quokka macros" shortcut, if you are connected to the internet, you will be prompted to install any updates as they become available.

## 2.4. Switch to NIST macros

Double click again on the executable 'IgorUserFilesSwitch.exe'. (Or select the "Igor Pro Macro Settings" shortcut under either under start>Igor or on the desktop). Select the NIST macros and click OK. As above, you will be asked if it is OK to download macros, select yes.

Once this is done you should have a "Igor with NIST macros" shortcut either under the Start>Igor menu OR on your desktop (depending on which version of windows you are running).

Both NIST and QUOKKA macros will now be on your computer and you can switch between by selecting the different shortcuts "Igor with NIST macros" and "Igor with Quokka macros".

### 3. Quick guide to QUOKKA data reduction

Note: Any data publication with QUOKKA data reduced with the NIST macros should cite: Kline SR (2006) Reduction and analysis of SANS and USANS data using IGOR Pro. *Journal of Applied Crystallography* **39**: 895-900

The following is a 'quick guide' to treating QUOKKA data. More detailed help about the macros is found in the 'help' buttons in Igor.

#### 3.1. Chose a workspace and copy across report files

Please work in your proposal directory:

/experiments/quokka/data/proposal/xxx

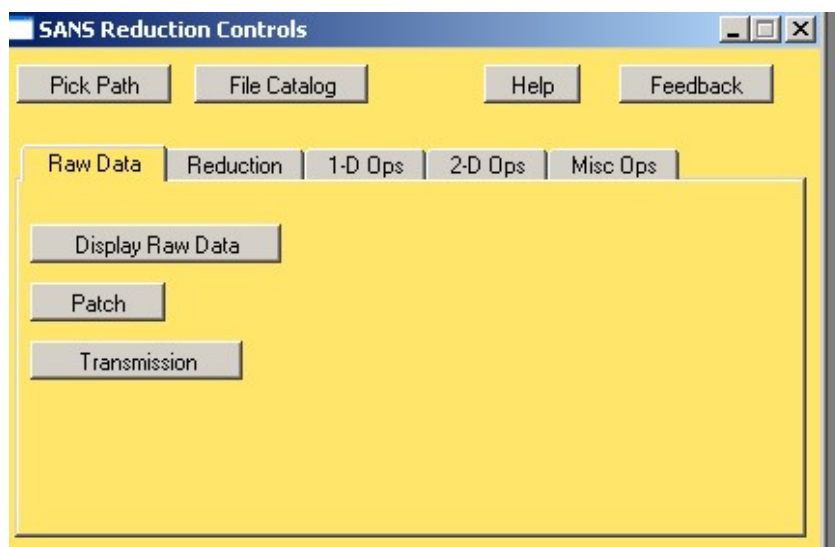
Report files are saved which associates the relevant transmission measurements with the scattering files – copy across the report files associated with your data to your working directory. These are under

/data/current/reports

Your local contact should give you the relevant sensitivity and mask files.

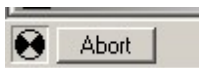
#### 3.2. Open Igor macros

Open "Igor with Quokka macros", then in the 'Macros' menu select 'Load Quokka data reduction'. You should be able to see the following window:



### 3.3. Select working directory

On the SANS Reduction controls, 'Pick path' (select path where all your data is), then 'file catalogue'. A table with all data files + characteristics appears, this table takes some time to appear the first time, the small sign on the bottom left of Igor tells you it's working....



### 3.4. Calculating transmissions.

*xii. Read the report file & create table*

Select 'transmission' in the 'raw data' tab. 'pick path' then select the xml report generated by gumtree, then 'List Files'. A table is then created with all the correct file associations.

*xiii. Calculate transmissions*

Select the 'empty beam' transmission file for the first configuration you want to treat by clicking on the appropriate box in the table (should appear in the column 'EMP\_Filenames'), and click 'set BCENT file' on the 'calculate transmissions' window (this sets this to beam centre). Click 'Set XY Box' and use the square to select the beam centre. Right click and select 'SetXY box coords'. Then highlight the scattering files in the 'scattering files table' at the configuration for which you've just set the empty beam transmission, and click 'calculate selected files' in the Calculate transmissions window. The S\_Transmission column in the 'ScatteringFiles' window should now be populated.

Repeat this step for the other configurations.

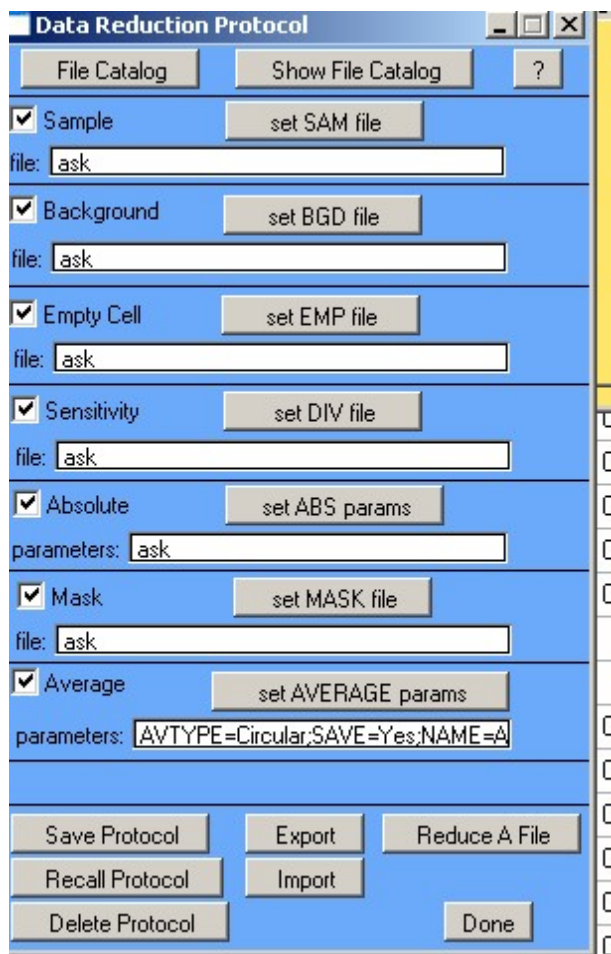
Click 'done' when finished with transmissions'. If you click 'File catalog' the data File catalog window will be updated, and you should be able to see the transmission values. These are 'patched' into the data files.

If your report is incomplete (ie you have stopped a MSW early and the different files are now in different reports) you can easily modify the report by opening it in a text editor.

### 3.5. Reduce data

This section is not complete, but gives a quick overview. More info is available in the NIST help document.

In the 'reduction tab' choose 'build protocol'. The following appears:



Leaving 'ask' will mean that during the reduction Igor will prompt you to select the file you wish to use:

'Sample' will typically remain 'ask'.

'Background' is a scan of the blocked beam.

'Empty Cell'. If you are always subtracting the same empty cell/buffer run this can be set to the empty file by clicking on the appropriate 'filename' in the 'Data File Catalog' table, then clicking 'set EMP file' (or the filename can be copied and pasted in). (If you are using an empty cell from a previous run, you need to copy the file to the current directory – these will have different beam centres, unless obviously far off warnings about this can be ignored).

'Sensitivity'. Take the sensitivity file in S:\Bragg\Quokka\Sensitivity and standards\

or one given by your local contact. Copy and paste the sensitivity file name or select it in the 'data file catalog', then 'set DIV file' on the data reduction window.

'Absolute' – for absolute scaling. Click 'set ABS params', then select method of absolute calibration 'Empty Beam Flux'. Select the empty beam transmission file, and draw a box around the beam with the cursor, then click 'continue'.



'Mask'. Take the mask file in S:\Bragg\Quokka\Sensitivity and standards\

or one given by your local contact, or make up your own!

'Average' can be left as is for isotropic data.

The data reduction protocol that you've now created can be saved 'Save Protocol'. You can now reduce a file by selecting 'Reduce a file' directly in the blue 'Data Reduction Protocol' panel, or if you have saved the protocol, directly on the yellow 'SANS Reduction Control' panel. Via the 'SANS Reduction Control' panel you can then select the protocol (useful if you want to make multiple protocols).

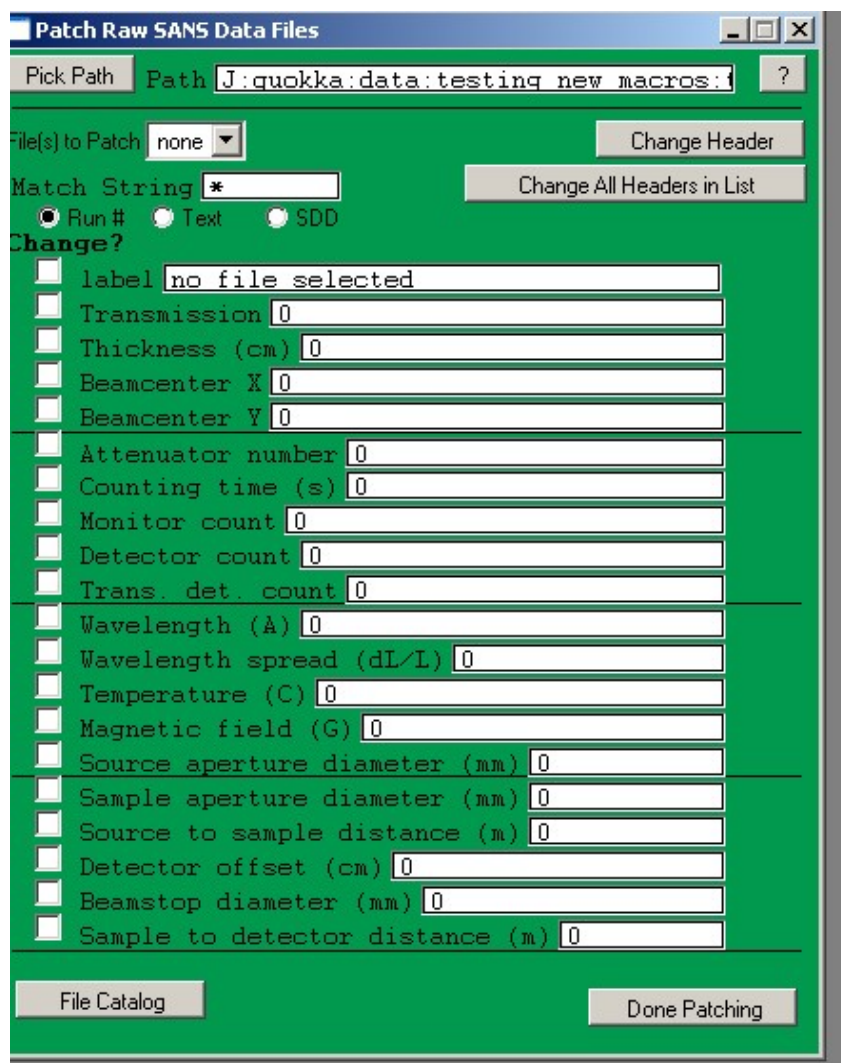
During the reduction, you'll be prompted to select files to use. Each time Igor asks 'Do you want to add another xxx file'? This is for if you wish to add multiple runs together, if you only have one run, select no.

Reduced data are then saved in the file: QKK00xxx.ABS

To merge several configuration together: 1D Ops, 'sort' button

### **3.6 Patch the data (if required)**

Most data should not require patching. If however a parameter has been entered incorrectly into the file header (eg, sample thickness, beam centre etc...) this can be changed via the 'patch' panel:



Select the file you wish to change from the drop down menu. Click the tick box on the left next to the parameter you wish to change, enter the value on the right. Then click 'Change header' to update the header in the file.