Using WOMBAT

The wombat manual is a 'living document' please do note any corrections and suggestions for content within the manual printed at the instrument. These will be reflected on the next update.

1. Definitions and Abbreviations

SICS – Swiss Instrument Control Software/System. This is the control software used to operate the instrument.

HIPD – High-Intensity Powder Diffractometer WOMBAT.

Instrument Enclosure – Area enclosing the WOMBAT instrument. Access controlled by Saftey Interlock System (sometimes referred to as SIS). This interlock has to be enabled for neutrons to enter the area.

Instrument Cabin (Cabin or hutch) – room adjacent to instrument containing the instrument control computer and is the primary location to monitor and organise experiments.

ACNS - Australian Centre for Neutron Scattering (formally known as the Bragg Institute).

NBI – Neutron Beam Instrument

NBI Operator – A trained and authorised person who operates a Neutron Beam Instrument or experiment. (Authorised User in *AG 2471 - ANSTO OHSE Practice - Safe Management of Licensable Sources*).

NGH – Neutron Guide Hall. Central area in Building 82 containing many NBI.

OPAL Neutron Beam Facility (OPAL NBF) – The OPAL Neutron Beam Facility consists of Building 80 level 00 (the Reactor Beam Hall) and Building 82 (Neutron Guide Hall) and all their contents (NBI, X-ray instruments, laboratories and workshops) under the control of the Australian Centre for Neutron Scattering.

OPAL NBI Source Officer – Is nominated by the Head Australian Centre for Neutron Scattering and is responsible for compliance with the OPAL NBF Source Licence.

Sample Environment Equipment – Is a device which fits onto an instrument for modifying the sample state or environmental conditions such as temperature, pressure, electric and magnetic field, sample changers, Eulerian Cradle, etc.

SWMES - Safe Work method and environment statement. This is the pro-forma for risk assessments at ANSTO. If your experiment uses a novel process or equipment then it is likely that you will need to provide this for consultancy before your experiment starts. Liaise with your Instrument Scientist on this.

Gumtree – a combined instrument control and data analysis environment. Gumtree can be used to run SICS commands and much much more!

2. Operation

2.1. Opening and Closing the beam

The sample shutter may only be opened after going through the interlock procedure and ensuring no one is in the instrument enclosure. The interlock procedure is:

1. Search the instrument enclosure, check that no one is working on the instrument.

2. Once you are happy that no one is in the enclosure, activate the interlock by pressing the lockup initiation (exit) button near the door.

3. Visible and audible warnings will indicate the sequence has been initiated.

4. You must move to the instrument cabin and within 20 seconds the door must be closed. This is locked by the SIS. Only then will it be possible to open the sample shutter and allow the neutron beam onto your sample.

5. Emergency stops are in the instrument area or control cabin. Do use in an emergency but be aware that they also close the secondary shutter. In a non-emergency, an abort button may be used to stop the exit procedure.

6. The sample shutter is then opened using the safety control panel.

2.2. Swiss Instrument Control System (SICS)

PLEASE NOTE Most of the time you will be running your experiment in Gumtree, a windows interface for SICS that is installed on all of the neutron beam instruments.

SICS (Swiss Instrument Control Software/System), is a computer program running on Linux. SICS is a command line program that is responsible for keeping track of all motors, moving the motors, starting data acquisitions, etc. There are specific commands that SICS accepts, referred to as SICS commands. SICS is located on the SICS server:

ics1 wombat.nbi.ansto.gov.au

SICS can be accessed directly (using PuTTy or similar connection) and through Gumtree. The login is wombat and password is wombat. To access SICS use the SICS client by typing sicsclient and use the login Manager with password ansto.

Connecting to SICS via PuTTy:

- Choose the **Wombat ICS** account
- Load and open
- Usr: wombat, pwd: wombat
- At the prompt type
  >> sicsclient
  >> manager ansto

If SICS is not working/running, or if something has changed in the configuration files, then in the PuTTy window (***not*** logged into the SICS client) type:

>> runsics stop
>> runsics start

2.3. Gumtree

Gumtree is a combined instrument control and data analysis environment. SICS can be accessed through Gumtree, which is located on a Windows box at dav1-wombat.nbi.ansto.gov.au To launch Gumtree, double click on the icon on the desktop, then use the login ansto and password ansto when prompted.

In Gumtree, the most commonly used motors and their attributes can be seen in the SICS Instrument tab.

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You connect Gumtree to SICS by clicking on the little person at the bottom of the screen. They will be standing still when not connected and running when connected.

2.4. Wombat Beam Monitors

Wombat has two beam monitors:

- BM1 - is located just after the sample shutter, and is the default monitor loaded into LAMP for normalisation
- BM2 - is located downstream, after the flight tube and filter position (if used). It is more sensitive than BM1, and often used for normalising when Wombat is set up for polarisation

2.5. Controlling WOMBAT

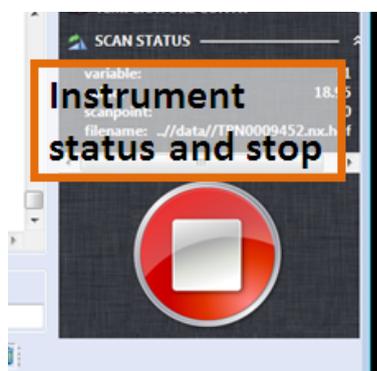### 2.5.1. Interrupting Data collection

To interrupt data collection in the batch file execution panel in Gumtree press the interrupt button or in putty or through a command line:

>> INT1712 3   (batch command interrupt)

>> INT1712 2   (regular command interrupt)

Or

Press the Big Red Button

2.5.2. Motion Control

There are two main SICS commands used to move motors:

>> run *mot value*

Runs the motor *mot* to position *value*. For instance, if you wish to move the sample stage sy to 0.5 – you would type

>> run sy 0.5

into the SICS command line.

>> drive *mot value*

Is the same as run but blocks the SICS client from issuing commands until the motion has finished. This is useful in batch commands where you wish for the motion to be completed before data are collected or the next line in the batch is executed. For instance if you were to type

>> drive tc1_driveable 280

this would set the temperature on channel A of tc1 (usually used for CF8) to 280 K. You would not be able to control WOMBAT until it had reached that temperature.

Other useful motor SICS commands include:

>> *mot* list

This lists all the attributes of the motor *mot*. There's a list of motors that can be called in this fashion on the cupboard in the WOMBAT cabin.

Useful note: If you want to find out where a motor on wombat is at - but can see it reported on the Gumtree dashboard, you can call on the motor in the tcl command prompt. For instance if you want to know the stth (detetor angle) positions you just type:

>> stth

and the position of the motor will be printed.

2.5.3. Data collection

Once you are ready to start collecting data (ie, sample is loaded in container and into the sample environment which is configured along with the instrument), you can start

collecting data.

There are several SICS commands used to acquire data, either directly through the SICS client, through the Gumtree interface or from within a batch file.

Collecting data in tandem with the collimator (most collections): Most data is acquired as a function of the tertiary collimator, which must be set prior to these scans. To set the radial collimator:

>> SetRadColl *time range*

Sets the radial collimator to do a full oscillation in (approximately) seconds. *Range* is the angular range the collimator will oscillate over (in one direction) in degrees. A range of 2 oscillates the collimator from +1 to -1 degrees and back again. *Time* is seconds per oscillation.

Standard Wombat operation: SetRadColl 60 2, radial collimator takes 60 seconds to scan 2 degrees back and forth.

Radial collimator runs are the standard data acquisition method and allow the option of doing multiple oscillations per run (called *oscno*). The time per run will scale accordingly.

>> RadCollRun *oscno reps*

This is a simple radial collimator run where, for each pattern, the collimator goes back and forth *oscno* times. If *reps* is 1 then a simple 2D file is created. If *reps*>1 then a 3D file is created with *reps* number of datasets in it. The time it takes to do each oscillation is set using SetRadColl. If *oscno*>1 then the time for each oscillation is a multiple of the time set in SetRadColl.

For instance:

>> RadCollRun 1 1

This does one run where the radial collimator goes back and forth once

>> RadCollRun 2 5

Do 5 runs, for each run the collimator goes back and forth twice. This means the time for each run would be twice what was set using SetRadColl.

>> RadCollTimed *oscno time*

Does a timed radial collimator run. The run will consist of one or more datasets, where the collimator has gone back and forth *oscno* times for each dataset. After each run the elapsed time is checked and if it is greater than *time* (in minutes) where the run can go for slightly longer than *time*.

For instance:

>> RadCollTimed 1 60:

This does multiple runs where each run consists of one radial collimator oscillation. Run will last for ~60 minutes

>> RadCollScan *motor start step numsteps oscno*

Scans the *motor* beginning at *start* with a step size of *step* for the number of steps *numsteps* where each step in the scan consists of *oscno* radial collimator oscillations.

For instance:

>> RadCollScan som -1 0.1 11 1:

Scans the sample omega (som) from -1 in 0.1 degree steps for 11 steps (ie until +1 inclusive). Data is acquired for 1 oscillation at each point

Collecting data without the collimator

Simple commands, usually only used for quick data acquisition or without the oscillating collimator (non-standard)

>> SimpleRun *steptime numsteps*

Does a simple timed run, with fixed radial collimator position. The timed run lasts for *steptime* seconds. *Numsteps* is the amount of times the timed run is repeated.

For example:

>> SimpleRun 180 1

One 180 second (3 minute) run.

>> SimpleRun 10 15

15 runs of 10 seconds each, saved in a single 3D file

>> SimpleScan *motor start step numsteps steptime*

Does a simple motor scan run with fixed time for each step and fixed radial collimator position (including for no tertiary collimator). Scans the motor beginning at *start* with a step size of *step* for the number of steps *numsteps*. *Steptime* is the time at each position in seconds.

For example:

>> SimpleScan som -1 0.1 11 10

Scans the sample omega (som) from -1 in 0.1° steps for 11 steps (i.e. until +1 inclusive). Data is acquired for 10 seconds at each point

At times in a batch script, you may want the instrument to pause while (for instance) a temperature or voltage 'settles'. This is done with the 'wait' command, which will pause the instrument for the required amount of time (in seconds).

>> wait 60

Will instruct the instrument to pause for 60 seconds.

2.6. Viewing data 'live' – The histogram memory server

The Wombat detector has 8 modules that are electronically tuned for response by 4 servers (2 modules per server). Data are seamlessly united (stitched) and binned in x and y through the histogram memory server (using the configuration files). The server is located at das1-wombat.nbi.ansto.gov.au. The binning is controlled through the server directly and can be changed if necessary.

Data can be viewed directly through the histogram memory server, through a web-browser at: http://localhost:8081/admin/viewdata.egi use the user name User and password Sydney (should be default).

Within this viewer you can change the view by disabling auto refresh:
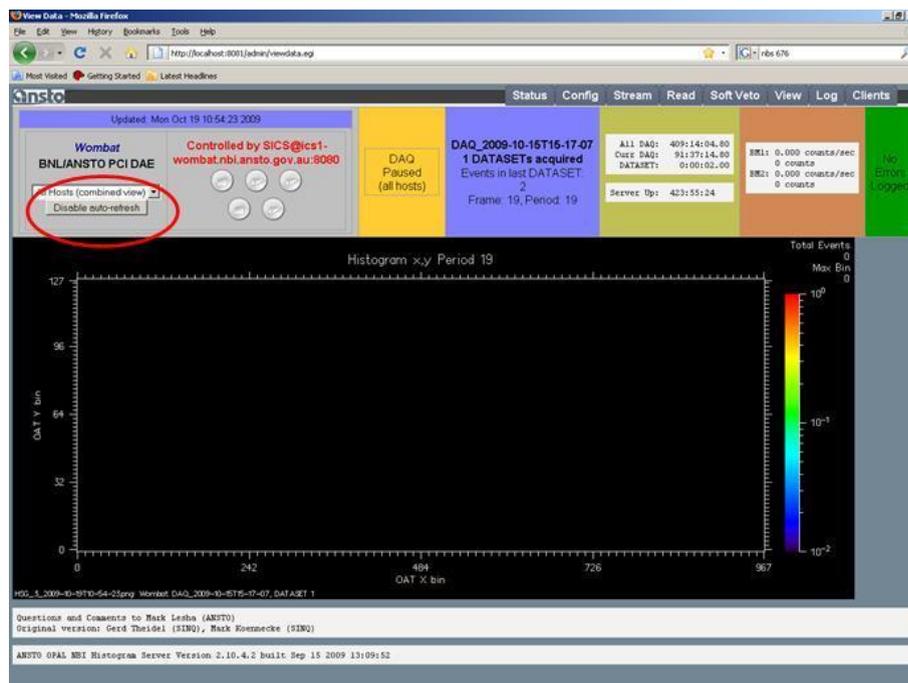
You can choose to change options such as the view (through the view tab):
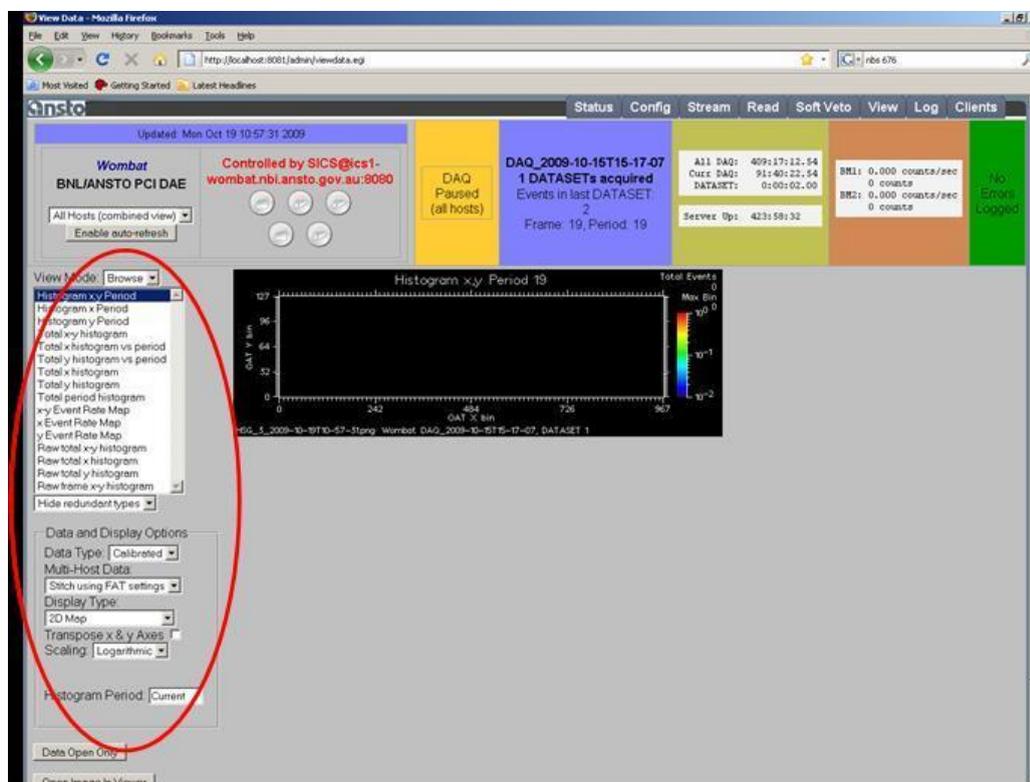
We recommend that you use linear scaling, total x histogram for a 1D view, or total x-y for 2D.

If you go home early, you can check the status of the WOMBAT instrument (to see that you're still running) at http://www.nbi.ansto.gov.au/wombat/

3. Sample Environment Controls

3.1. Using the CryoFurnace (CF7/CF8/CF16/CF17)

CF8 (and its sisters CF7, CF16 and CF17) can control sample temperatures with a standard stick between ~4 K and 300 K. With a 'full-range' stick, they can control sample temperatures between ~30 K and 750 K (base temperature can be achieved, but the sensors on this stick do not read below ~30K), however above 300 K the exchange gas must be removed to avoid damaging the cold head.

The most commonly used sample environment on WOMBAT is a cryo-furnace. SICS is capable of reading and driving the temperature on this device. Typically the cryofurnace is set up on WOMBAT so that the coldhead (or wall temperature) and sample temperature (through heaters positioned close to the sample) can be controlled.

The coldhead (cryo-furnace walls) is controlled with a lakeshore controller, and usually will be configured for control by SICS depending on your experiment. This is your means of cooling the sample. The sample temperature can be further controlled with heaters on the stick you are using, and is also controlled with a lakeshore, with up to two inputs for above and below your sample. Normal operation (for a variable temperature experiment) it is suggested that the temperature of the cryo-furnace will be set about 20 K lower than your sample.

Control and data collection with a CryoFurnace

We now have a number of hardwired commands that can be used to control and collect data with our cryofurnaces. These all have a common start (the letters 'cf') and are CASE SENSITIVE.

>> cf UseWall *wallset wallcontrol*

This informs the instrument if you wish to control the walls (coldhead) of the cryofurnace during your experiment. For instance if you wish to just control just the sample temperature you would type >> cf UseWall false false

The options here are **true** and **false** and must be in lower case. By default (eg if SICS restarts) the options are **true true**.

The two true or false settings have subtly different uses. The first true/false controls whether or not the temperature is set at all. The second true/false controls whether or not a drive command will wait for the wall temperature to be within tolerance. Note that the only combinations that make sense are **true true**, **true false** or **false false**.

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For example if you wanted to keep the walls at a specific temperature while setting the sample temperature, you would start with >>cf UseWall true true, then set the desired temperature, then type >> cf UseWall false false.

There is an important situation where you would need to use cf UseWall true false. If you are doing a full range (50-800K) stick run, the maximum temperature of the wall will be set to 300K but it might drift a bit over that when the stick is at high temperatures. As a result the run will stall because it's waiting for the stick to cool down.

>> cf UseBase *baseset basecontrol*

Similarly to UseWall, you can tell the instrument if you wish the bottom sample temperature control to be used. e.g. to prevent the instrument from controlling the bottom sample heater you would type >> cf UseBase false false

>> cf RampOn *rate*

Sets a temperature ramp for the Cryofurnace (rate in K/minute)

>> cf RampOff

Will stop any ramp underway.

>> cf WallParams *lag max tolerance*

Sets the parameters of the cryo-furnace (wall) controls. Variables are:
        lag temperature – interval (in K) that the coldhead temperature is set under that of the sample temperature.
        max – maximum temperature that can be set for the wall. This is usually 300K and you should only change this value under special conditions after consultation with the instrument scientist.
        tolerance – a value in Kelvin that the reported temperature has to be in relation to the set temperature for 30 seconds before the next step can proceed.
These parameters default to lag = 20, max = 300 and tolerance =2 every time sics is restarted.

>> cf TempSet *temperature*

Use this command to set the temperature of the cryofurnace. This uses the parameters set by the cf WallParams command. In default setting, using >> cf TempSet 50 will set the sample temperature (top and bottom) to 50 K and the coldhead temperature to 30.

>> cf TempDrive *temperature*

This will set the temperature of the cryofurnace in the sample way as TempSet EXCEPT using the drive command. i.e. the instrument will not proceed until the

temperature is achieved. Mainly for use in batch files.

>> cf Tolerance *sample_tolorance*

Set the tolerance of the sample temperature controllers for the sample stick only. (The tolerance for the walls is set using the WallParams command above). Defaults to 1 K on restart of SICS.

>> cf MakeCold

Sets the cryofurnace to cool to base temperature (4 K).

>> cf TempRun *temperature delay reps oscno*

Controls the cryofurnace to a specified temperature and collects WOMBAT data at the same time. Needs to be used in conjunction with a SetRadColl command.
      temperature – temperature you would like to collect at.
      delay – time in seconds after setting temperature before collection
      reps – number of repetitions of data collection
      oscno – defined with SetRadColl, number of oscillations of collimator during collection.

>> cf StepRun *start step fin oscno delay*

Controls the cryofurnace to a number of steps in temperature and collects WOMBAT data at the same time. Needs to be used in conjunction with a SetRadColl command.
      start – start temperature for the collection
      step – steps between temperature intervals (in K)
      fin – last temperature for sequence
      oscno – defined with SetRadColl, number of oscillations of collimator during collection.
      delay – time in seconds between reaching temperature and starting data collection.

>> cf StepWaitRun *start step fin oscno delay*

Pretty much the same as StepRun, except it executes the drive command (rather than run) so will wait for the sample to reach temperature before progressing. Useful if making large temperature steps.

Two things to be careful of when using this command: firstly, the drive command has a 30 second delay in it already, so if you have lots of temperatures you will need to factor this into the timing. Secondly, if you include very low temperatures (<10K) it might be worth setting the tolerance (using the cf Tolerance command) to a large enough value to make sure the run starts.

>> cf RampRun *start rate fin oscno*

Sets data collecting during a temperature ramp. Needs to be used in conjunction with a SetRadColl command.

    start – starting temperature
    rate – rate of ramp in K per min
    fin – temperature for the end of the ramp
    oscno – defined with SetRadColl, number of oscillations of collimator during collection.

>> cf HeaterOn

Turns on the heaters on the sample, useful to put in a batch file before running temperature control commands.

>> cf HeaterOff

Turns the heaters on the sample off.

>> cf GetTemp

Reports the temperature channels that are being controlled.

3.2. Using the Vacuum Furnace (VF1)

The vacuum furnace has a West controller require scans to be executed using:

>> RadCollRampWest *temp rate oscno*

This does a series of runs while ramping up the West controller. Each run consists of *oscno* oscillations with *temperature* in Celcius, *rate* in degrees per hour.

>> ResetWest

This 'resets' the furnace and puts the set temperature to 0 Celcius. To be used with caution at high temperature (over 1000C). It may be better to use the RadCollRampWest command to ramp to a lower temperature before executing this. It's also common practice to put a ResetWest command at the beginning of a script when the furnace is heating from room temperature.

Additional information on the Vacuum Furnaces

- There are actually two of these (VF1 and VF2) and control is identical, though calibration is a little different for each (but sample environment/instrument scientists will deal with that).
- When using 1.54 A, there can be background from the furnace - from Niobium diffraction peaks (Niobium is the element of the furnaces).
- Beam position is 380 mm from the stick flange

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- You may also need to pay attention to the Max Power setting in SICS, your instrument scientist will advise if that is an issue.

3.3. Using the Orange Cryostat (OC1)

To control OC1 a number of SICS 'motor' variables are used (see page 6). For instance typing:

>> tc1_driveable

into the SICS command line will show the sample temperature from channel A on tc1.

>> run tc1_driveable 200

This will set the temperature of channel A on tc1 to 200K.

>> wait 600

causes OC1 (and WOMBAT to wait in seconds, in this case 600))

>> drive tc1_driveable 200

Will drive the regulation temperature (B) to 200K and (as default) waits for it to be within 1K of this value before continuing to the next command.
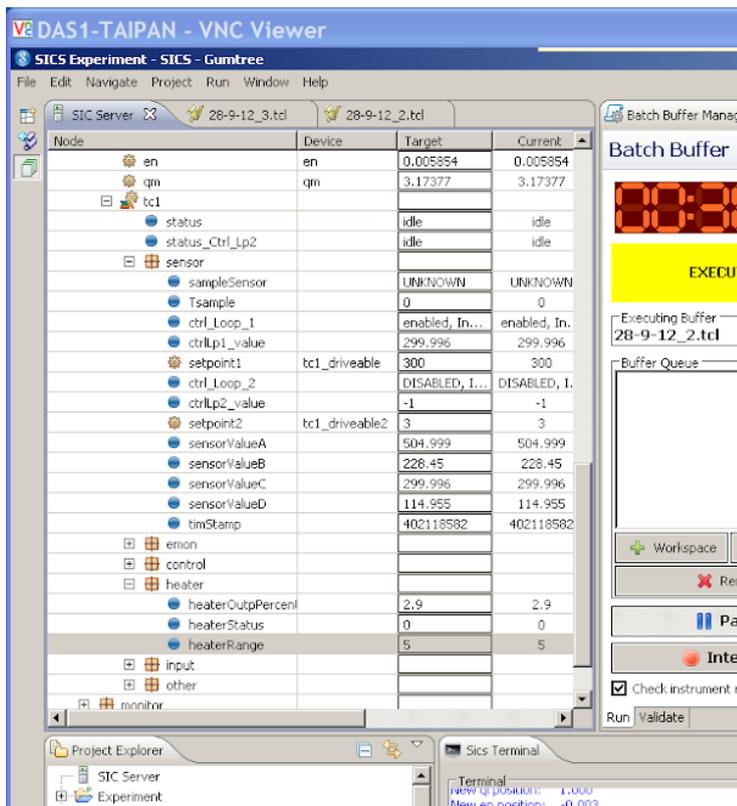
>>sct_ls340_tc1 send "RANGE?"

Query the heater power range – (0 = off, 5 = 100W)

>>sct_ls340_tc1 send "RANGE 1"

sets the heater power range – set to a value between 0-5.

In addition the fine control of the temperature parameters, such as tolerance, heater power range, etc, can be adjusted by clicking on the SIC Server tree view.

To heat the sample relatively quickly you need to have the heater range to 5.

These detailed commands can be used (also in batch files) to control the temperature parameters:

>> hlist –val /sics/tc1/sensor   shows set points and sensors etc

>> hget /sics/tc1/sensor/setpoint1   to show the temperature

>> hset /sics/tc1/sensor/setpoint1 200

Sets the temperature to 200K – there is no blockage of the drive functions when this command is used)

>> hset /sics/tc1/heater/heaterRange 5   for 100W power, or 4 for 10W power

>> hset /sics/tc1/control/tolerance 1 5

Sets the tolerance of 5K to reach desired temperature

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Steps for a Helium full of the Orange cryostat (only if authorised by Sample environment and Instrument team)

1. Remove the one-way valve
2. Release pressure using the red lever
3. Open the Helium entry port
4. Close overpressure on the dewar, remove dustcap
5. Insert transfer line into dewar **slowly**
6. When liquid is visible (like a white flame) insert the other end of the transfer line into the cryostat **slowly**
7. When you reach the bottom in either dewar, lift a bit and tighten to keep in place
8. Control pressure in supply dewar to be 3-6 PSI, 3 is good when using gas bottle He and inlet lever

WHEN FULL

9. Open pressure release valve on supply dewar
10. Loosen and remove transfer line from both cryostat and supply dewar simultaneously
11. Close dewars
12. Replace one-way valve

3.4. Using the 12 T Magnet (ASM-1)

The distance from the top of the stick flange to the beam centre is 1261 mm (or 1265 mm considering the O-ring). As of 2021, the 12 T magnet has been limited to 10 T.

Coordinate with your instrument scientist on writing scripts for controlling the magnet as there are a number of things to pay attention to. In order to change field the heat switch of the magnet needs to be on, and stay on while the field is ramped. The rate of the field ramp may also have to be changed depending on what field strength you are driving too (generally slower rate at higher fields).

A summary of useful magnet TCL scripts (Magnet_scripts.tcl) can be found in the W:\users\scripts folder.

Temperature of the magnet can be controlled with a SICS driveable (similar to OC1).

The rotation stage within the magnet can be controlled with the 'msom' motor in SICS

3.5. Batch Commands

SICS commands can be batched together in a text file, or created using Gumtree.

The text file can be stored in w:/user/scripts, in that file you'll find examples of previously run batch commands.

Only use the *drive* command within batch files, as this instructs SICS to wait for the command to finish before progressing onto the next instruction.

Batch files can be dragged into the buffer queue or loaded from the file system (see the *Gumtree* section).

4. Data

4.1. Format

The raw instrument files from WOMBAT are output in **nx.HDF** format into Z:/data/current/sics/data. In addition to your diffraction data this file contains important metadata – the position of all motors for the instrument (so we can always determine approximate wavelength and resolution functions) and output from any configured sample environments

You can open these in HDFview (freeware and does not need installation) that HDF Group produces, but you need to know where to look in the file for the details.

To produce a 2D plot of your data, or to output at 1D individual data file you can use the Gumtree analysis scripting, or the ILL program LAMP. Instructions for how to undertake both of these are described subsequently.

4.2.Processing

To process any data you will need:

- efficiency calibration file (your instrument scientist will provide you with this)

- Your data file

If you have run WOMBAT in a non-standard configuration (i.e. without the collimator or running other than SetRadColl 60 2, or running at an extra-long wavelength) you

will likely need to collect data for vanadium and generate a new efficiency calibration file. Depending on the flux in your configuration this could take between 2 and 12 hours.

4.3. Processing data in Gumtree

General description of the interface

The Gumtree data processing window is accessed by clicking the 'Analysis Scripting' button at the top right of the Gumtree window. If no such button is present, you can start the 'Analysis Scripting' view by selecting the small square button at the left of the row of buttons at the top right of the Gumtree window and choosing 'Analysis Scripting' from the drop-down menu. The Experimental view can likewise be redisplayed by clicking on the 'Wombat Experiment' button at the top right. The following description assumes that you have clicked on the 'Analysis Scripting' button.
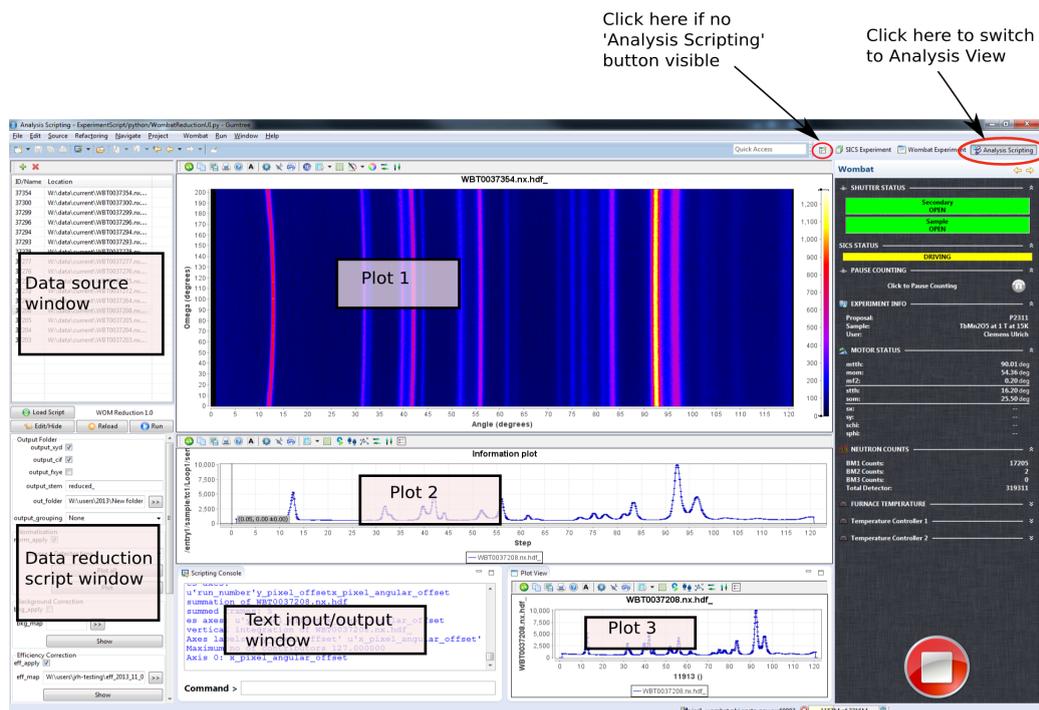
At the top left is the 'data source' window. You should add datafiles to this window by clicking on the green 'plus' icon. Note that only files that are in this window *and selected* will be processed. Underneath the data source window is the data reduction control window. You can select the type of data reduction by clicking on the 'Load Script' button and selecting from the list of recently used reduction scripts. See the individual sections below for the names of appropriate scripts to load.

To the right of the data source and data reduction control windows are three plotting

areas. 'Plot1' is at the top, 'Plot2' is in the middle and 'Plot3' is at the bottom. An optional text input/output window may also appear next to Plot3. This text window reports on the progress of calculations, and allows interactive processing of your data using Python (beyond the scope of this manual). If this window has been minimised, it can be brought back by clicking on the small icon at the top left of the main Gumtree window.

Powder data reduction

Select the 'WombatReductionUI' script from the 'Load Script' button. In general, powder data reduction proceeds by normalising the frames in the input datafile according to monitor counts, optionally subtracting a background, applying a gain ('efficiency') correction, and then summing the resulting frame(s) vertically to obtain a 1D pattern.
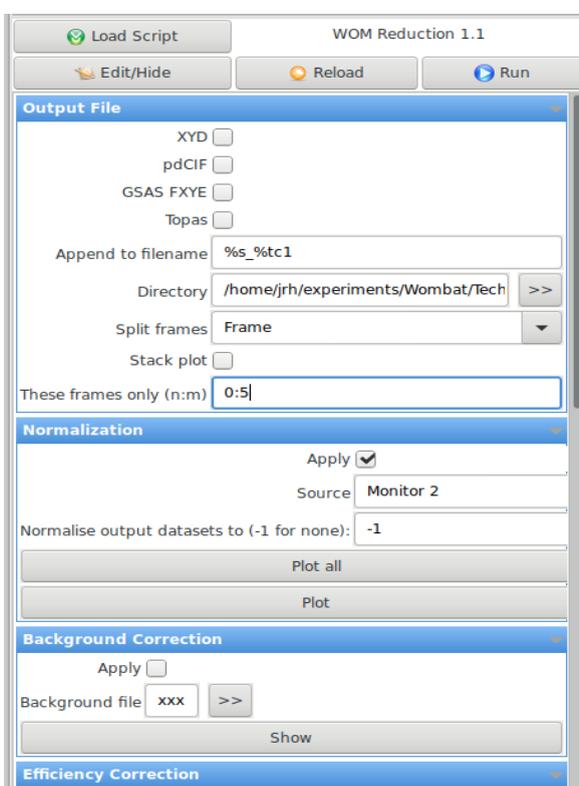
The powder data reduction script will produce an output file for every file that is selected in the data source window. These files will be written to the directory specified in 'out_folder', and will have a name of form 'WOMnnnnnn_<tag>_mm.yyy'. The initial part of the filename is simply the file number on the system. <tag> will be whatever has been entered as the 'output stem', and mm is a frame number for files that have been split into separate frames during data reduction. The extension 'yyy' will be chosen according to the output format.

Wombat datafiles may contain frames that have been collected under different conditions (e.g. during a temperature ramp), or else multiple frames that should be summed together, or both. By choosing 'None' for 'Output grouping', all frames will be summed together. Choosing instead 'Frame' will output each frame as a separate reduced datafile. Choosing 'TC1' will sum frames with the same TC1 setpoint temperature.

A number of "magic format instructions" exist to embed more than just the data frame number in the file name using the "output_stem" entry. These are:

- %s: substitute the sample name
- %t1: substitute measured value of cryofurnace stick top temperature sensor (sensorValueA)

- `%t2`: substitute measured value of cryofurnace stick bottom temperature sensor
- `%vf`: substitute measured value of vacuum furnace temperature

So, for example, if output stem is `%s_reduced_%t1` and the sample name is `Al2O3`, a measurement at 125K will produce a filename `WOM012345_Al2O3_reduced_125.xyd.`

Efficiency maps are usually stored under the 'W:/calibration' directory. Ask your instrument scientist to set the appropriate file for your experiment.

You are able to restrict the range of vertical integration by changing the lower and upper boundaries, and can optionally rescale such that the maximum intensity is equal to the 'rescale target' value.

Data reduction is initiated by pressing the 'Run' button. Plot 2 will show the final 1D pattern(s), which can be copied to Plot 3 for further investigation or comparison using the widgets at the bottom of the data reduction script window. Use the green button at the top left of each plot to unzoom, and select with the mouse to zoom.

If the 'Stackplot' option is ticked, at the end of data reduction all output 1D patterns will be shown stacked in Plot 1, with frame number as the vertical axis. If 'Output grouping' is 'Frame', the 1D patterns for each frame from all files selected for reduction will be sequentially stacked. If 'Output grouping' is 'None', the 1D patterns for each file selected are stacked.

Note that it is possible to check monitor count behaviour using the buttons in the 'Normalisation' area. Clicking on 'Plot All' will plot all monitor counts to Plot2, and clicking on 'Plot' will plot only the monitor counts currently selected for normalisation. If 'norm_apply' is ticked, monitor counts will be displayed on the same arbitrary scale by dividing each measurement by the average value for that monitor.

Gain re-refinement
Relative pixel efficiencies can be redetermined if powder data have been measured by stepping the detector position and collecting multiple frames. Typically this is useful if an oscillating background appears in parts of the collected powder patterns. To refine and apply pixel gains determined using this algorithm, tick the 'Apply' button in the "Recalculate Gain" section of the Powder Data reduction GUI and select the number of iterations. Typically 5 iterations are sufficient. You may also save the resulting gains in a file and load that file. To load a file instead of re-refining gains, check the 'Apply' box as well as the 'Load gain from file' box. Obviously you will need to have saved a gain file at some point to be able to do this!
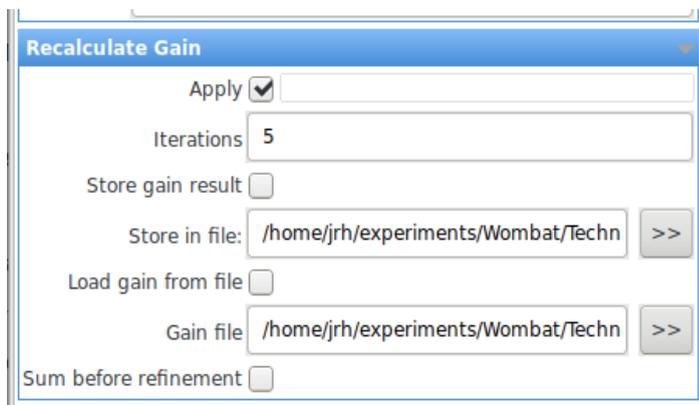
The 'Sum before refinement' check box is only relevant when the detector step is less than the horizontal separation between pixels (0.125 degrees in single mode/0.0625 in double mode). In this case checking this box will result in a faster refinement, but there should be no effect on the final results.

The 2D plot displayed in Plot 1 when using gain re-refinement is obtained by simple summation of each measured frame, offset according to detector position, that is, no re-refined gains have been applied. The final values of the individual gains and the progress of reduction in χ^2 are given in Plots 4 and 5, which are usually minimised and can be opened by clicking on the plot icons in the border of the Gumtree window.
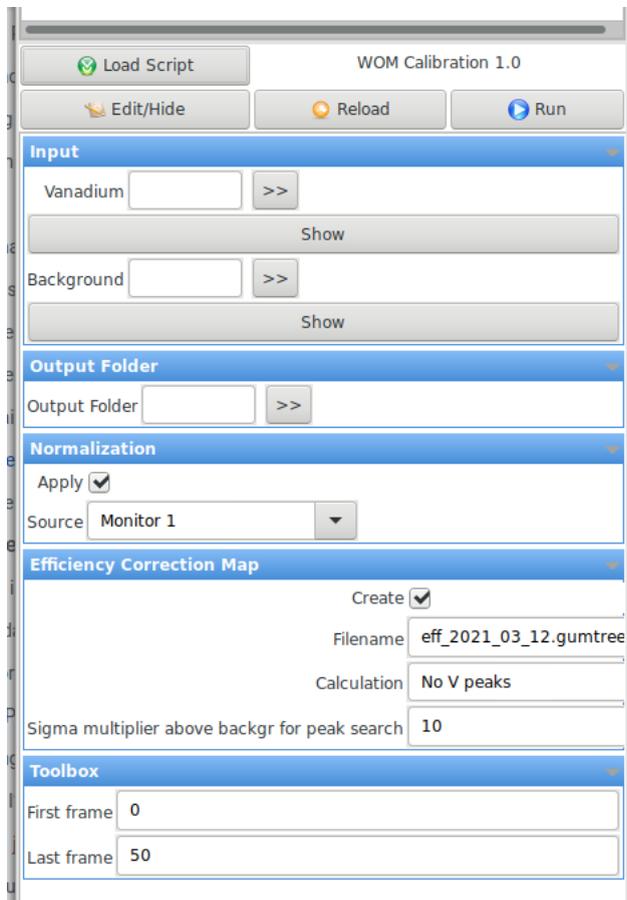
Details of the algorithm used for gain re-refinement are given in Avdeev, M and Hester, J. R. (2019) *J. Appl. Cryst*. **51**, 1597-1604.

Creating a calibration file
Efficiency calibration files are created via selection of the "WombatCalibrationUI" script from the "Load Script" button. The raw data consist of a Vanadium and Background exposure. The raw data files corresponding to these runs should be selected, and can optionally be displayed in Plot 1 (to make sure you've chosen the right file) by clicking "Show". Use "Output Folder" to select the directory to write the result file,

whose name is given in the "Filename" entry of the "Efficiency Correction Map" section.

"Normalisation" should be applied, using whatever monitor you trust at the moment.

Options for the type of calculation for the efficiency correction map are either "No V peaks" or "Naive". "No V peaks" will search for peaks in the Vanadium measurement and ignore all points within 3 FWHM of the peak position when determining pixel efficiency. The final option adjusts the sensitivity of this peak search: in the screenshot, a peak is only found where an intensity is at least 10 times background. If this fails to find a peak, the number can be reduced. A "naive" calculation will not search for V peaks and so the final option is ignored.

The "Toolbox" options allow some frames at the beginning or end of the Vanadium and Background files to be ignored, for example, if the beam went off. Ordinarily, these should be set to the first (0) and last frame numbers.

Single crystal reduction

Select the 'SingleCrystalUI' script from the 'Load Script' button. Single crystal reduction at present simply sums all frames in the input file vertically (after normalisation and efficiency correction), then stacks them in sequence to form a 2D display in Plot1. The 'axis setup' entry box allows you to select which axis in the datafile should be used to label the vertical axis on the 2D plot. This would normally be sample rotation ('som').

Toolbox

Select the 'ToolboxGUI' script from the 'Load Script' button. This GUI is a collection of independent widgets for quickly looking at different aspects of the datafile(s) selected in the data source viewer. One particularly useful widget allows you to plot the value of TC1 and TC2 for each frame in the input datafile. It is also possible to plot arbitrary values by giving the properly capitalised, full location in the HDF5 file: for example '/entry1/sample/tc1/Loop1/sensor' will plot the sample temperature on stick 1 of the 12T magnet.

4.4. Processing Data in LAMP

The ILL program (written in idl) LAMP (Large Array Manipulation Program) can be used to process the data. Your data can be re-processed at any time if you have an efficiency correction file and either full LAMP or the idl runtime version of LAMP. For details on LAMP, and to download the program please go to

http://www.ill.eu/?id=3463

For standard processing to produce 1D data (powder diffraction patterns) with LAMP the procedure on the wombat instrument is:

1. Launch LAMP and "extend to classical"

2. Set working path to the location of your data file

3. Import data (as hdf) into workspace 1

4. Import efficiency correction data (as lamp hdf) into workspace 60

5. correct for detector efficiency using "w2=womcal(w1, calibration = w60) - this assumes that you have the correct calibration file loaded into workspace 60.

6. Optionally straighten Debye-Scherrer cones using "w3=straight_2D(w2, distance = 728), or window central third of the detector using "w3 = w2(*,44:84)"

7. vertically integrate to create a 1D pattern using w4 = total(w3,2).

8. change the working directory to where you want your data to be. Export as gsas using "wom_gsas_save, w4, "filename", where filename must begin with an integer. User wom_txt_save,w4,"filename" for ascii output or wom_xye_save,w4,"filename" for xye output.

Please note: If you are re-processing at home, the 'wom' commands will only work if you have these routines saved on your own computer, these are available should you want (ask your instrument scientist). However, it is probably a good idea to process all of your files before the end of your experiment.

At any point you can save your lamp session, with the inputted workspaces. This would be a good idea once you have loaded your efficiency calibration file as if LAMP crashes at any point you can relaunch it with the calibration in place.

There is also the lamp.jou file, which is a useful journal files that LAMP produces which lists the commands used to process the data.

Summary of the 'wom' commands

Wombrowse

wombrowse, xxxxx,p='w'

Wombrowse starts up an HDF file viewing program that lets you look around the data that's saved in the wombat raw data file. These files (more or less) conform to the NEXUS data standard for neutron data (google "NEXUS neutron" to learn more) These files have the format "WBT000xxxx.nx.hdf." Here xxxxx is the number of the

raw data file, and the optional p='w' allows you to point to where the raw data lives. The format for this can be any legal directory name, so something along the lines of p='C:\womdata\expt\' in Windows or p='/usr/data/wombat/' for Unix/Mac works fine. Note that the path information is in single quotes. If you're at the Wombat instrument on one of the data analysis PCs, then p='U' is a shortcut for the current data directory on the instrument. Note that there's a delay between when the data gets saved and when it shows up to be read in.

Wombrowse is useful to find out where sample environment data has been saved. For example, temperature data for CF8 might be saved in something like /entry1/sample/tc1/sensor/sensorValueA. You can work out what the path is then use it in womload

Wombrowse comes up as a separate window in lamp, you can just close the window (usual x top right corner) when you don't need it any more.

Womload

W1 = womload(xxxxx, p='w', z='msom',/noerr)

Womload is the best way of loading in raw datafiles into lamp. It makes sure the 2theta and y axes values are correct.Here xxxx is the number of the file you want to load, p is the path (as explained in the wombrowse command above) and z is the extra data for the run you want to load in. This can be any path within the hdf file (which you can use wombrowse to find out) and is very useful for loading sample environment data like temperatures from CF8 or VF1.

The z value can be a full hdf path (like z='/entry1/sample/tc1/sensor/sensorValueA') or if you want to use a standard wombat motor, that will work (like z='som' or z='ephi'). Note the path or motor name has to go in quote marks.

The /noerr flag is optional and useful for very large files. It stops errors from being calculated and stored when the hdf file is loaded.

Womcal

W3=womcal(w2,calibration=w60)

Sorts out the detector normalisation. The convention is to load in a calibration file in w60 but you can use any workspace. Use file->open hdf to import the calibration file, choose a workspace with the slide and hit the "load" button. You only have to load the calibration file once

Wom_gsas_save

Wom_gsas_save, w5, "filename"

Saves workspace in gsas format. Actually saves the file as "filename.gsa", you don't

have to add the ".gsa" suffix. If you have a 1d powder pattern (ie just the single intensity vs 2theta graph) it saves as a single file. If you have a 2d file it saves as "filename_1.gsa", "filename_2.gsa" etc which is the correct format for sequentioal refinements in fullprof and gsas.

Wom_xy_save

Works the same way as wom_gsas_save but saves the data as x,y,error format with the extension .xy.

Wom_xye_save

Works the same way as wom_gsas_save but saves the data as x,y,error format that is suitable for loading into TOPAS - with the extension .xye.

Wom_map_save

Saves a 2d image as a (very large) text file of equally spaced values- perfect for loading into programs like matlab. Note: it can be a bit slow and don't be surprised if the textfiles created are megabytes long.

Straight_2D

W10=straight_2d(w9,distance=728)

Corrects the curvature in the wombat detector. If the file starts out as a 3d file, it stays a 3D file. If it starts a 2d file, it stays a 2d file.

Straight_1D

Does the conversion like "straight_2d" but then also follows it up with a "total" command, so it will reduce a 3d file to a 2d map of intensity vs 2theta, and a 2d image to a 1d intensity vs 2theta graph

Womnorm

w2=womnorm(w1, mon=10000)

Normalises detector counts to beam monitor (defaults to BM1, if you wish to normalise to BM2 you need to load this in at the 'womload' stage. Works best on files before they have been run through total or straight (so just after womcal is usually good).

This does not work for a single frame collection, or between workspaces - If one wants to normalize a data of single frame, you can use w2=w1*mon_target/mon_real. Need to open the hdf file for mon_real.

Other useful LAMP commands

Summing along axes in lamp with the "total" command

One of the most common tasks in lamp is to sum up the elements in an array. For example, you might have done multiple 15 minute runs to make up a very long 2 hr run, rather than just run a single 2 hr run and risk something going wrong and losing the whole lot. Or you may wish to sum vertically in the detector and not straighten the peaks

The general formal is

W4 = total (w3,2)

Where the second number is the choice of axis. If you load a 3d dataset then axis 1 is twotheta, axis 2 is the detector height and axis 3 is whatever you scanned in the run (temperature, som or just doing multiple runs with radcollrun). However if you are summing multiple runs together you may want to do this:

W4 = total(w3,3) & n4 = total(n3)

The second part with total of n4 preserves the beam monitor count (and actually sums it together into one big beam monitor)

Combining runs together using square brackets

It may be that there are separate wombat runs that need to be combined together, for example if they are separate parts of a temperature run. The usual convention is to reduce them to 2d images in separate workspaces (ie get as far as using straight_1d or total) and then using a command that looks something like this:

W10 = [[w1],[w2],[w3]]

This is a command to stack runs together in the second dimension ("on top of one another") However, if you have temperature data or some other y axis data you want to keep, you may wish to do this:

W10 = [[w1],[w2],[w3]] & y10=[y1,y2,y3]

 The second part stacks the y axis data.

Putting data into q space

W10= qxqynew(w9, lambda=2.41, dQ=0.01, omega=45)

Lambda is the wavelength, dQ is the mesh size (0.01 s a good value, anything smaller than 0.005 is probably overkill) and omega is the rotation if the map in q space. Don't put omega=0, that may crash things.

This assumes that the data you are converting is a 2d image with correct 2theta and y axis values (usually som, but could have come from eom or ephi if you used the Euler cradle)

5. Troubleshooting

5.1. SICS is not responding

Interrogate SICS by typing: status. To be able to execute further commands sics needs to return a status of "eager to execute commands". If it is:

"driving" you must wait until the previous drive command has completed, or cancel this. The easiest way to check is to go into Gumtree and refresh the instrument control panel to see which motors are driving: (a green arrow will appear). A common problem is driving temperature. To fake reaching the temperature without interrupting the setpoint change the tolerance on the setpoint to outside the range, and then wait 30s to settle.

"counting" then data collection is underway and you should interrupt this (or not, depending on what you want to do)

"busy" you may need to interrogate SICS through another connection – use PuTTy or relaunch Gumtree

Restarting the Histogram Memory server sometimes fixes all the above:

1. login to das1-wombat.nbi.ansto.gov.au through putty using login: ansto password: ansto123

2. type runsics stop, then wait 10 seconds

3. type runsics start, then wait 20 seconds

4. typing runsics status will return "running" or stopped"

5.2. The data from the histogram memory server looks funny:

- The 2D view has a configuration other than 127 x 967 (standard Wombat

configuration, this will be different if you have configured the histogram memory server to non-standard binning).

- One section (module) of the histogram memory server is missing. This may be an intermittent issue, wait until the next frame before querying this with your instrument scientist.

- There are low counts.

    o Check that TG123 and TG1 shutters are open (status red above the bunker). If they are closed this status will be green. This will happen if those working on wombat or echidna trip the interlock system (for instance, through the light curtain). In all eventualities you will need to contact your instrument scientist to investigate this for you.

    o Check the reactor status (check the light indicator on the other side of the guide hall). If the reactor is off, and does not come back in ~30 minutes then it is likely to have poisoned out (build up of Xenon) and power will not return for ~36 hours. Please note the power indicator on Gumtree is not always reliable (can read 0 W when power is up).

    o You have not blocked the beam (slits closed or shielding in the way)

    o Check that the high voltage (HV) is on – the light on the front of the detector. Call an instrument scientist if it is off.

Restarting the Histogram Memory server sometimes fixes all the above:

5. login to das1-wombat.nbi.ansto.gov.au through putty using login: ansto password: ansto123

6. type runhistmem stop, then wait 10 seconds

7. type runhistmem start, then wait 20 seconds

8. typing runhistmem status will return "running" or stopped"

You may need to reconnect to SICS.

5.3. I've brought an extra sample, can I run that?

Is this sample on your experimental data sheet? If so, then it's been checked by our lab manager and you're good to go.

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If not – no you can't. We are regulated by ARPANSA, and have to have documented what is in the neutron beam (and considered the risks) at all times. We can be spot checked at anytime, and if a sample is not on the experiment data sheet and being collected this can have serious implications for you and the Australian Centre for Neutron Scattering. If **up to two weeks BEFORE** your experiment you wish to add some samples to your proposal, please let your instrument scientist know and they will progress this for you.

5.4. LAMP had just crashed.

Yes, it does that. Hopefully you would have saved your session when you set it up (recommended) with your calibration file in w60. If you didn't you will need to find the calibration file to use – these are usually located in w:\calibration\YEAR_MONTH

Pick the most recent file and then the appropriate calibration file (either *v_cal_154* or *v_cal_241* depending on the wavelength you are using). Any specialist calibrations you have prepared will probably be stored in your home folder.

5.5. Can I just take samples straight from the beam back to my lab?

No, you can't. Your samples may have activated in the neutron beam, opening them and emptying their contents could cause a serious contamination. There is a procedure for when and how powdered samples can be taken from the enclosure (your instrument scientist should have run you thought this – ask if you are not sure). There is a further procedure to follow for unloading samples from vanadium cans. This is displayed in the furnace lab fume hood (the one for handling powdered samples).

6. Suggestions for future inclusions in the wombat manual

Please use this space in the printed copy of the manual in the wombat cabin to note what future instructions/explanations you would like in this manual.