Using WOMBAT Version 4 - August 2025



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.

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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, the official name for 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 - 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:

- 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 15 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)

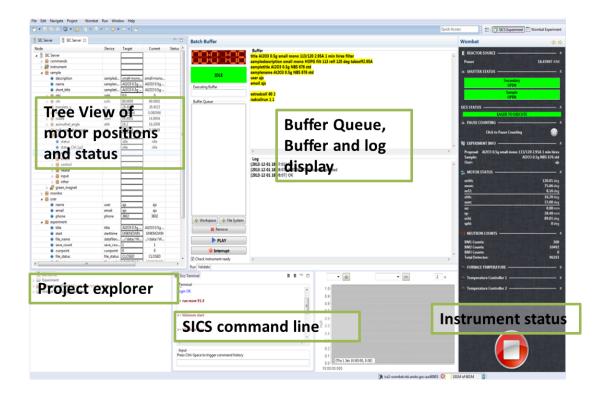
PLEASE NOTE Most of the time you will be running your experiment in Gumtree, a windows interface for SICS that is installed on all of the neutron beam instruments.

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.

2.3.Gumtree

Gumtree is a combined instrument control and data analysis environment. SICS can be accessed through Gumtree.

In Gumtree, the most commonly used motors and their attributes can be seen in the SICS Instrument tab. The image on the next page shows the basic layout.





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. 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.

2.5.2. 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



2.5.3. 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 moving 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).

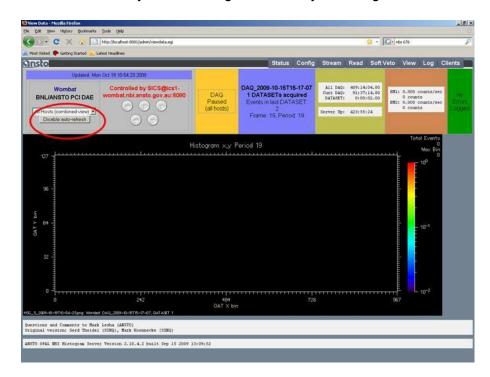
>> wait 60

Will instruct the instrument to pause for 60 seconds.

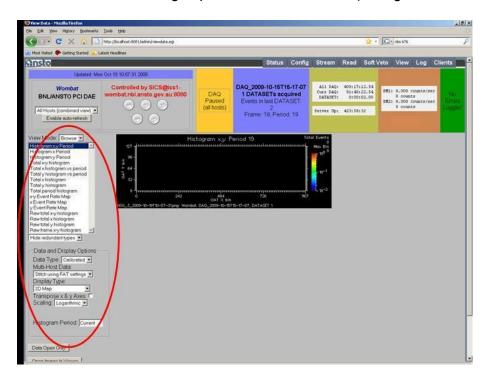
2.6. Viewing data 'live' - The histogram memory server

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

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. 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.Batch Commands

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

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).

3.2. Using the Cryofurnace (CF8)

CF8 (and its sister CF7) 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 below 30 K 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 cryofurnace is the most commonly used sample environment on WOMBAT and SICS is capable of reading and driving the temperature on this device. Typically the cryofurnace is set up on WOMBAT so that the variable temperature insert (VTI or 'wall temperature') and sample temperature (through heaters positioned close to the sample) can be controlled.

The VTI (cryofurnace 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 1-2 K lower than your sample.

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/ VTI) 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.

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

>> cf RampOn rate

Sets a temperature ramp for the Cryofurnace (rate in K/minute). Note, there is a time delay on setting this rate, if using with a batch command we recommend also using a 'wait 180' which will instruct the instrument to wait 3 minutes while the ramp is set.

>> cf RampOff

This will turn off the ramp setting, it will not pause any ramp underway however.

>> 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 tolerance

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). This needs to be negative if temperature is cooling

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.

3.3. Using the Vacuum Furnace (F1/F7)

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.

- There are actually two furnaces (F1 and F7) 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
- You may also need to pay attention to the Max Power setting in SICS, your instrument scientist will advise if that is an issue.
- Typical cooling rates:
 - 'Freefall from 700 to 350 °C take ~45 minutes
 - Cooling profile in VF1 from 700 °C is temp(t) = 751-121In(t)

3.3.1. Sample Change Procedure for VF1

Step 1. Turbo Off (<350 °C)

At temperatures below 350 °C the vacuum turbo can be turned off off 350 C

- Rightmost button on grey turbo panel, with status LEDs above
- Verify turbo RPM decreases from 1000 to 999 or 998 after pressing

Step 2. Bleeding Helium (<200 C + turbo <300 RPM)

Only if discussed with Instrument Scientists and Sample environment, cooling can be sped up by bleeding helium into the chamber. This is not appropriate for all samples.

- This cannot be done if the turbo is too fast or it will damage the turbo
- This cannot be done at high temperatures or it will damage the element
- Flush the helium line before connecting by opening the main valve on the bottle and having flow when you connect.
- Connect press fitting to bleed line on furnace
- Turn vacuum valve (black) clockwise all the way
- Open bleed line on furnace (right hand side blue valve) slowly
- Check furnace vacuum display shows "OR" (over range)
- Furnace relay should turn off at this point
- Close bleed line on furnace
- Remove helium bleed line and close helium bottle valve
- Turn furnace off by lifting toggle switch and switching

Step 3 Extracting Sample (<100 C)

IMPORTANT: Check that 1 min post run has actually been completed, in case sample removal results in damaged sample

- Air cannot be allowed into the chamber above 100 ₀C or it will damage the elements
- Open helium vent valve slowly to let air in
- Unplug temp sensor cable by turning anticlockwise
- Undo clamp
- Pull sample straight up very carefully, do not handel without correct PPE until it is verified that the samples is cool and not active.

Step 4 Installing Sample

- Close helium vent valve to stop air getting in
- Insert sample straight down very carefully
- Tighten clamp not too tight
- Plug temp sensor cable by turning clockwise, supporting from underneath when plugging to prevent sample stick creep

Step 5 Vacuum drawdown

- Open vacuum pump valve all the way
- Wait for furnace vac readout to show 100 mbar
- Press turbo on button
 - Rightmost button on grey turbo panel, with status LEDs above
 - o Verify on screen RPM readout increases
 - If 'actual RPM' not shown, use right arrow key to change display views
 - o If 1000 RPM is not achieved within 15 mins, will automatically turn off

Step 6 Prepare furnace for OK to start

- Wait for turbo OK condition (1000 RPM)

- Wait for vacuum OK condition (<2e-3 mBar)
- Wait for furnace self check (no red lights)
 - Reset button to run fault re check
- When all are good, furnace is OK
- Verify setpoint is 0
- Turn furnace ON by lifting toggle switch and switching

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

The distance from the top of the stick flange to the beam centre is 1261 mm (or 1265 mm considering the O-ring). Though it is named the 12 T magnet, the magnet is currently only capable of reaching 11 T.

Magnet essentials:

- Only non-ferrous metals (including screws) to be used at the sample position
- NO rotation of sample while field is ramping
- Sample changes ONLY at ZERO field

3.4.1. Changing magnetic field

Coordinate with your instrument scientist on writing scripts for controlling the magnet as there are a number of things to pay attention to. For the vast majority of cases the command

>> drive magnet1 magnet setpoint field

is sufficient for changing magnetic field to field in Tesla. This command automatically

- 1. Ramps the power supply current if needed to match the existing field of the magnet
- 2. Turns the heat switch on. Power supply current = current in magnet coils. The heat switch must be on for the duration of the ramp.
- 3. Ramps the power supply current to the new field value.
- 4. Turns the heat switch off.
- 5. Ramps down power supply current back to zero.

There are settling times associated with each 'flick' of the heat switch, and of course, time needed for the ramp itself.

Some relevant *read-only* parameters to watch while ramping the field are:

sample/magnet1/magnet/setpoint is the setpoint of the magnetic field (the value you are ramping to/the value you have ramped to most recently).

sample/magnet1/magnet/field is the reported value of the magnetic field based on the current circulating in the coils.

sample/magnet1/magnet/he level is the helium level % of the magnet i.e. 100 % is a full magnet. In real life, when the magnet is full, the helium level is 101.6 %! Ramping the magnet uses more helium. Keeping the magnet in persistent mode (i.e. steady state field) uses little helium. A quench will use all the helium...

sample/magnet1/magnet/ramp setpoint tesla is the ramping rate of the field in tesla per minute. It is usually set to 0.5 T/min.

sample/magnet1/magnet/ramp_setpoint_amps is the ramping rate of the power supply current in amps per minute. It is usually 8.482 A/min (equivalent to 0.5 T/min).

Consult with Sample Environment if you think you need to change the ramp rate (the default ramp rate of 0.5 T/min is fine for the majority of cases).

sample/magnet1/magnet/htr sw is the status of the heat switch which will be 1 (ON) while the actual ramping of the field is happening, and 0 (OFF) when the magnet is in persistent mode (steady state).

sample/magnet1/magnet/htr timer msec this is the waiting time for the heat switch to stabilise before beginning to ramp the field up or down. It is set to 60000 msec.

sample/magnet1/magnet/settle_timer_sec this is the waiting time for the field to stabilise after ramping. It is set to 30 sec.

You must wait for htr timer msec and settle timer sec to return to zero at the completion of the ramp BEFORE sending another ramp command!

sample/magnet1/magnet/psupp field shows the power supply "field", which is calculated based on the current in the magnet power supply. It should be zero unless ramping.

If the power supply field does not return to "zero" (i.e. less than 10^-4) after ramping the magnet, the drive command will not complete, and the magnet will remain in ramping purgatory. Get in touch with your local contact who will contact Sample Environment.

sample/magnet1/magnet/temperature is the temperature of the superconducting coils ~ 5.5 K is normal.

Please note that depending on a few factors it may not be possible to complete your scheduled experiment if we need to recover from a guench.

3.4.2. Temperature control of your sample in the magnet

There are three "temperatures" involved in an experiment with AVM-1:

- 1. the temperature of the superconducting coils i.e. the magnet itself sample/magnet1/magnet/temperature, obviously we never want to warm these up during the experiment, ~ 5.5 K is cool and normal!
- 2. the temperature of the VTI, cooling power comes from adjusting the needle valve (Mercury iTC, usually sample/tc1 on Wombat)
- 3. the temperature of the sample (Lakeshore 336, usually sample/tc2 on Wombat).

The usual magnet sample probe does not have a heater on it, so temperature control is done through the VTI plus exchange gas. The sample temperature is sample/tc2/sensor/sensorValueA and sample/tc2/sensor/sensorValueB. The sample temperature setpoints are sample/tc2/sensor/setpoint1 and sample/tc2/sensor/setpoint2.

Needle valve pressure for the VTI is controlled with the Mercury iTC. The relevant parameter in SICS is sample/tc1/pres8/setpoint. 20 mbar is good for cooling while 5 mbar is good otherwise for the standard magnet sample probe (if using the dilution insert, the pressure will likely be higher for base temperature, 10 - 15 mbar). The measured pressure is sample/tc1/pres8/sensor and the valve position in % is sample/tc1/pres8/valve (100 % corresponds to the valve being completely open, ~ 15 % is normal for 5 mbar needle valve pressure).

Using the 'hset' command works well for adjusting temperature control parameters, e.g. to set the needle valve pressure to 20 mbar

>> hset sample/tc1/pres8/setpoint 20

3.4.3. Sample rotation in the magnet

If using the standard magnet sample probe, your sample can be rotated about msom "magnet sample omega". The command is

>> drive serotabs position

where position is between -179 and 179 degrees. The name serotabs comes from "sample environment rotation absolute". The position of the sample is at instrument/msom.

3.5. Using the Kelvinox dilution refrigerator insert (DL-1/DL-2)

Dilution / condensing won't be achieved without the dilution insert sitting in a VTI comfortably below 2 K. The measurements are usually conducted upon the warming process from the base temperature (~ 25 mK). The sample temperature is determined by the temperature of the mixing chamber (sensor name: T5). The units for this are Kelvin. To change the temperature setpoint, the command is

>> hset /sample/ghs1/dev/loop/tset val

Heating power needs to be adjusted gradually on heating, the units for range are **mA**. the command for changing the heater range is

>> hset /sample/ghs1/dev/loop/range val

The value of the heater range is not arbitrary. Below are recommended heater ranges for different temperatures.

T < 100 mK: 0.316 mA , T < 250 mK: 1.00 mA

T > 250 mK: 3.16 mA, T > 900 mK: 10.0 mA

Do not increase temperature in large steps. Breaking down into multiple smaller temperature steps is recommended. For example, warm up the sample from the base temperature (~ 25 mK) to 0.5 K, the below commands are recommended.

hset /sample/ghs1/dev/loop/tset 0.1

wait 300

hset /sample/ghs1/dev/loop/range 1

hset /sample/ghs1/dev/loop/tset 0.2

wait 300

hset /sample/ghs1/dev/loop/range 3.16

hset /sample/ghs1/dev/loop/tset 0.3

wait 300

hset /sample/ghs1/dev/loop/tset 0.4

wait 300

hset /sample/ghs1/dev/loop/tset 0.5

wait 600

Because of the way the multiplexing works on the resistance bridge, certain temperature sensors can become frozen / won't update regularly. We want to avoid this when controlling the temperature of the mixing chamber T5 away from base. This is why the other temperature sensors such as T2 & T4 are usually set to disabled / OFF when operating above base temperature.

To assist Sample Environment with diagnostics, here is a list of relevant sensors on the dilution insert under the 'sample/ghs/dev/' tab in SICS:

- T1, T3, TA: usually disabled / OFF.
- T2: condenser a.k.a. "1 K pot", should be 2 K or below.
- T4: still, should be 2 K or below.
- T5: mixing chamber, base temp ~ 25 mK. This is the temperature you are controlling.
- P1: tank pressure in the gas handling unit.
- P2: pressure at the condenser, a nice operating pressure is 200 mbar to 300 mbar (600 mbar is too high!).
- P3: pressure at the still.
- P5: backing pressure at the Adixen forepump.

The dilution insert is typically installed in the AVM-1 magnet or in CF-11. The VTI temperature (should be happily below 2 K) is controlled by its own Lakeshore and the needle valve pressure (typically 10 mbar to 15 mbar) for the VTI will be controlled via a Mercury iTC. Do not change the temperature / needle valve settings for the VTI when operating with the dilution insert!

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 with HDFview software - we like the web-base https://myhdf5.hdfgroup.org/ which will display your file and even plot out quantities within it.

To produce a 2D plot of your data, or to output at 1D individual data file you can use the Gumtree analysis scripting (or a legacy option was the ILL program LAMP). You can also use WombatDMCpy to look at single crystal data. Instructions for how to undertake any of these data analysis options 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

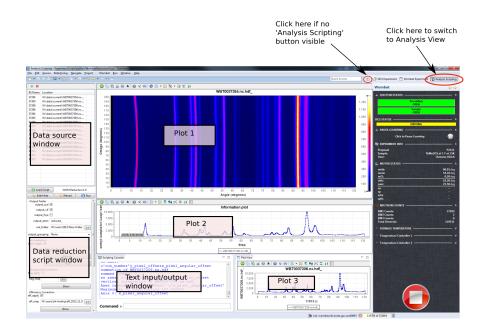
If you have run WOMBAT in a non-standard configuration (i.e. without the collimator or running other than SetRadColl 60 2, or running at an extra-long wavelength) you will likely need to collect data for vanadium and generate a new efficiency calibration file. Depending on the flux in your configuration this could take between 2 and 12 hours.

4.3. Processing data in Gumtree

4.3.1. 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.

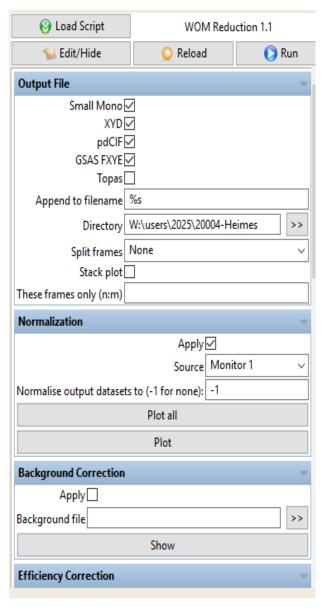


At the top left is the 'data source' window. You should add datafiles to this window by clicking on the green 'plus' icon. Note that only files that are in this window and selected will be processed. Underneath the data source window is the data reduction control window. You can select the type of data 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.

4.3.2. Powder data reduction

Select the 'WombatReductionUI' script from the 'Load Script' button. All the necessary metadata for data reduction are already present in the raw data file, except for the monochromator that was used: the "small mono" checkbox at the top of the data reduction GUI should be selected whenever the small, flat Ge mono is in use. Otherwise, this box should be unticked. An incorrect monochromator selection will affect the wavelength output to the pdCIF file and the d-spacing calculation when using the d-spacing plot option.



In general, powder data reduction proceeds by normalising the frames in the input datafile according to monitor counts, optionally subtracting 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 'WOMnnnnn <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 A1203, а measurement at 125K will produce filename WOM012345 Al203 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. The "straighten" option remaps every pixel to its true 20 value before vertically integrating. While this produces more symmetric peaks, particularly at low angles, it may worsen structure refinement results from many packages, which typically model unstraightened peak asymmetry correctly.

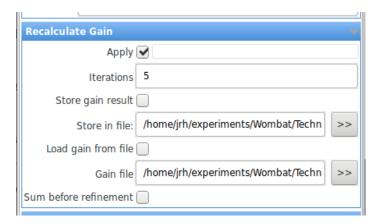
Data reduction is initiated by pressing the 'Run' button. Plot 2 will show the final 1D pattern(s), which can be copied to Plot 3 for further investigation or comparison using the widgets at the bottom of the data reduction script window. Use the green button at the top left of each plot to unzoom, and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

4.3.3. 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.

When straightening has been requested (see above), the refined gains are back-applied to the 2D data, which is then straightened and summed. Note that this is different to the non-straightened case, where the final 1D dataset is an output of the refinement process.

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.

4.3.4. 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.

4.3.5. 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' or 'msom').

4.3.6. **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 single crystal data with wombatDMCpy

DMC at PSI is a very similar instrument to Wombat, and we have a variation of the 'DMCpy' software developed by Jakob Lass, Samuel Harrison Moody, and Øystein Slagtern Fjellvåga (https://doi.org/10.1016/j.softx.2025.102237) called wombatDMCpy. It can be used to have a quick look at single crystal data from Wombat (we have not implemented any of the powder functionality of DMCpy for Wombat).

wombatDMCpy takes .nx.hdf files as input (no need to reduce the data). If you want to combine data from different run numbers, these runs must all have the same number of steps.

The necessary Python is currently set up only on DAV8 (not on DAV7) - which is the additional computer in the wombat cabin (ie the one not used for instrument control). There are example scripts at

C:\Users\wombat\Desktop\example wombatDMCpy scripts which you can copy into your own working directory and then modify (these already point to the most recent version of the wombatDMCpy module). The scripts have lots of comments to guide you.

There is a pdf which provides a basic how-to also in the example scripts directory (WombatDMCpy so far.pdf). Additional documentation for the original DMCpy package can be found at https://dmcpy.readthedocs.io/en/latest/index.html

The wombatDMCpy module is at C:\Users\wombat\wombatDMCpy

It is also available at

https://github.com/queenofthefairies/Wombat DMCpy/tree/wombat WIP#

Any questions or comments about wombatDMCpy? Please contact Siobhan.

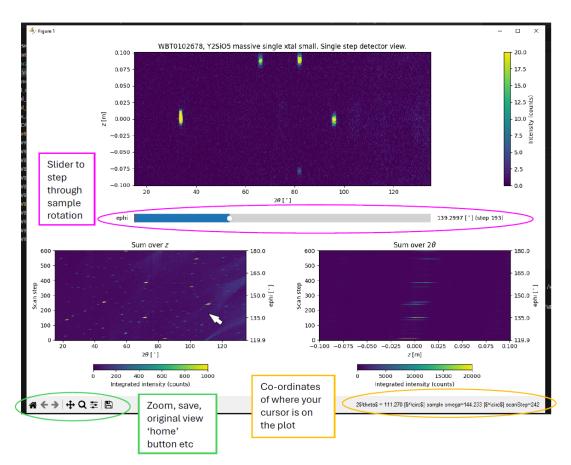
4.4.1. Launching python on DAV8

- 1. Open Miniforge Prompt (it's in the taskbar). A terminal window will appear.
- 2. Run the command conda activate wombatsinglecrystal
- 3. Run the command code .
- 4. MS Visual Studio code will open. Then you can open your working directory by clicking "Open folder" in the start options.
- 5. All the files in the working directory will be on the left hand side. Choose a script to edit/run.
- 6. Press the play button (top right) to run the script. You need to save it first.

4.4.2. **Detector view**

Example script: Detector_View_Wombat_example.py

The 'detector view' script allows you to look at Wombat's 2D detector for one run, step-by-step. You specify the crystal rotation axis as one of: som, msom, eom, ephi, epsi. The middle plot has a slider allowing you to scroll through the steps. At the same time the lower left plot shows the data after integrating the entire detector vertically (each row is a different step). The lower right plot shows the data after integrating the entire detector horizontally - useful for quickly seeing whether your peaks are in the scattering plane of the detector (i.e. about z = 0). On any of the plots, you can zoom in using the magnifying glass, and also see the position of your cursor in terms of the data coordinates (i.e. two theta, omega/step number etc.) in the bottom right corner.

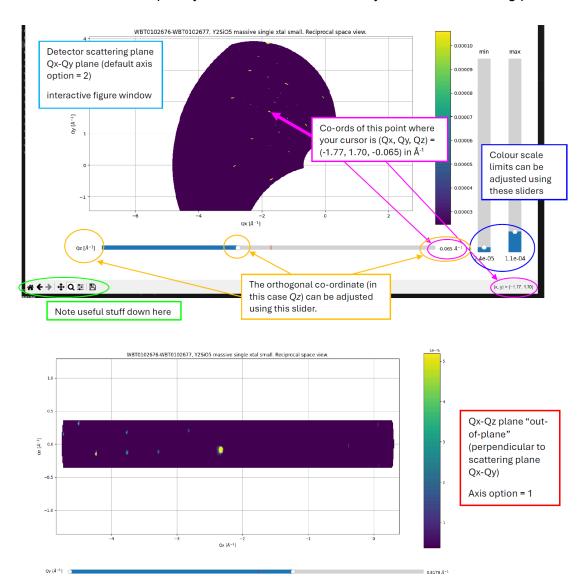


4.4.3. Reciprocal space view (inverse Angstroms)

To combine different run numbers in reciprocal space view, all run numbers must have the same number of steps!

Example script: Reciprocal_Space_View_invAA_Wombat_example.py

Reciprocal space view allows you to combine different runs and view the aggregated data in the scattering plane of the detector (Qx-Qy plane = axis option 2) or out-of-plane (Qx-Qz = axis option 1, or Qy-Qz = axis option 0). This gives you an idea of how much Q space you have covered and then you can start indexing peaks.

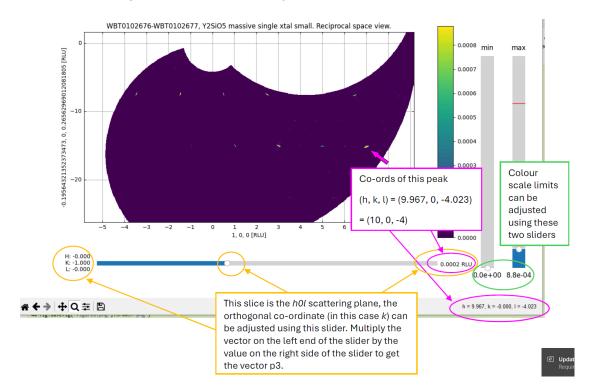


4.4.4. UB matrix and reciprocal space view in r.l.u.

Example script: Reciprocal_Space_3D_align_Wombat_example.py

With single crystals on Wombat, typically one plane is measured at a time (e.g. hk0 plane = scattering plane of detector). Alignment of data with reciprocal lattice axes in this script is based on determining a UB matrix from peaks in the same plane.

You need to determine coordinates (Qx, Qy, Qz) in inverse Angstrom of different peaks, and index those peaks. Lattice parameters for your unit cell are also required. More details are given in WombatDMCpy_so_far.pdf



wombatDMCpy can then plot the plane of your choosing based on the orthogonal basis vectors you have defined.

4.5. Processing Data in LAMP

The ILL program (written in idl) LAMP (Large Array Manipulation Program) is our legacy way of reducing WOMBAT data and is no-longer updated.

We recommend that you use the Gumtree reduction process outlined above. At present a runtime version of LAMP is installed on the WOMBAT data computers (DAV7 and DAV8). Data can be re-processed at any time after your instrument 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 integer. User wom txt save,w4,"filename" 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 seguentioal 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. 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.

5.2. 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.

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.

5.3. 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).

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.

