Technical Report
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OSIRIS (The First Step) A User Guide

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COUNCIL FOR THE CENTRAL LABORATORY OF THE RESEARCH COUNCILS

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OSIRIS (the first step)

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This is the user guide for the first steps of the OSIRIS project. It contains information on how the instrument is working, what kind of experiment you can perform at present and how to do it.
RAL-TR-1999-068

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1 About this document

The OSIRIS Project will explore the instrumental horizons available with the cold neutrons from a pulsed source and especially the totally new avenues available to polarised neutrons on these sources. On pulsed sources, polarisation techniques offer great potential for high resolution studies, and only lack of opportunity has left the field unexploited. On OSIRIS, the fundamentally novel methods developed on IRIS will be combined with proven and extended neutron polarising techniques. The high flux available at ISIS, coupled to the advanced design of the OSIRIS guide, will provide the means to take this field to its next evolutionary stage. By exploiting the combination of sharp pulses, white beams and cold neutrons from ISIS, high resolution measurements, both dynamic and structural, can be carried out using both unpolarised and polarised neutrons. The OSIRIS Project is an international collaboration involving India, Italy, Spain, Sweden, Switzerland and the United Kingdom. The project has three well-defined phases; phase 1: Extraction of a second cold beam guide from the IRIS beam line; phase 2: large d-spacing powder diffraction, incident beam polarised powder diffraction; phase 3: high resolution spectroscopy, spectroscopy polarisation analysis, diffraction polarisation analysis.

This is the user manual for the first step of the OSIRIS project, which means that phase 2 is now almost finished, ie we have a high resolution large d-spacing diffractometer, but the incident beam polarisation is as of yet only used for tests. You can find more information on the Osiris web-pages at `<http://www.isis.rl.ac.uk/crystalanalysers/OSIRIS/osiris.htm>`. This document is also available in an html version at that address.

This document is divided into five different parts. First, this short introduction, then what you need to think about before your arrive at ISIS, thereafter, the different parts of the instrument are described, together with some examples of sample environments. Fourthly, the actual running of an experiment is dealt with, and you should read this carefully. When you understand how to write a command file to run the experiment you are ready to go. Finally, the the data reduction programmes available on OSIRIS are described. Reading the short part about syntax will save you a lot of trouble. Good luck!

2 Before the experiment

2.1 Some things, to think about before the experiment

As with all other experiments you need to have a good plan of action before you arrive. Most of this will be in your application for beam time already, but even though you have done neutron diffraction experiments before, some things are particular to OSIRIS. Since we do not measure the whole diffractogramme in one measurement but normally a range of 2Å (in d-spacing) at a time see table 2, you can choose if you want better statistics in one particular range. The standard ranges are found in table 2. If you want to use other ranges please contact you local contact *before* the experiment. It helps if you have thought through how small errors you want to achieve when deciding how long to measure on each d-range setting.

There are only detectors in backscattering position, so if you want to measure out to very long d-spacing you will be using very long wave-length neutrons. You will have very good resolution but if the sample is highly absorbing the long wave-lengths will mean that you have very high absorption. If you want us to supply you with the sample can, please let us know in advance how many and what size of can you need.

2.2 Admin

When you arrive at ISIS you should:

- Register with the University Liaison Secretariat, UG3 R3
- Register with the ISIS Main Control Room (MCR) in R55 and get a film badge and the swipe card which is necessary for you to be able to enter the ISIS experimental hall.
- Get your sample record sheet. It is normally in the Data Acquisition Central (DAC). The sheet contains a safety assessment of your sample and should be on display at your beam line during the whole time of the experiment.
- If you have not seen the safety video, you should do this, either in the photo copier room on the top floor in R3, or in the coffee lounge in R55.

Find your local contact and discuss if there are any particular hazards associated with your sample and the instrument. Finally, do not forget that you are obliged to, within three month, after the experiment, complete an Experimental Report, a so called A3 report.

3 The instrument

3.1 Principle of operation

Here[1] follows a very sort and by no means complete introduction to how the instrument is working. The reason for neutron diffraction to be a useful tool in material science is the fact that the wavelength of thermal neutrons coincide with inter atomic distances in condensed matter. This and the fact that the scattering cross-section does not depend on the atomic number, as it does for X-rays, makes neutrons particularly valuable when you need to find the position of light atoms, ie atoms with low atomic number. Furthermore

[1]This part is only available in the LaTeXversion

since the neutron interacts very weakly with matter it penetrates deep in to the substance under study, whereby you are sure to measure bulk properties and not only surface properties.

The de Broglie relation

$$p = mv = \hbar k = h/\lambda, \tag{1}$$

and the fact that the neutron, as opposed to the photon, can be treated as a classical particle, makes it possible to write down the energy of the neutron as

$$E = \frac{mv^2}{2} = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m} \cdot \frac{1}{\lambda^2}, \tag{2}$$

where m is the mass of the neutron and all other symbols take their usual meaning. The kinetic energy is related to the temperature via $E = k_B T$ where k_B is the Boltzmann factor, and as is common practice, a factor of $\frac{3}{2}$, has been left out. The average wavelength of a neutron moderated at 20°C is then

$$\lambda = h/\sqrt{2mE} = h/\sqrt{2mk_BT} = 1.8\text{Å}, \tag{3}$$

which is as mentioned before comparable to inter atomic distances in condensed matter. OSIRIS is actually looking at a moderator at 22K so the wavelength distribution has its maximum at some what lower wavelengths.

As soon as the neutrons are created we start our timer and since the neutron can be treated classically the time of flight t for the neutron is:

$$t = L/v = L/(h/m\lambda) = \frac{h}{m} L\lambda = c_1 L\lambda, \tag{4}$$

with the flight path [L]=m, wavelength [λ]=Å, time of flight [t]=μs and c_1=252.78. This now allows us rewrite Braggs law:

$$\lambda_{hkl} = 2d_{hkl}\sin(\theta) \tag{5}$$

$$t_{hkl} = c_1 L 2d_{hkl}\sin(\theta). \tag{6}$$

We know L, that is the distance from the moderator to sample, plus the distance from the sample to the detectors, and Θ the angle at which the detector is placed. This means that by measuring the time of flight we can calculate the d values, which is our goal.

We cannot resolve infinitely sharp peaks because of the finite resolution of the instrument. The resolution depend on several factors. The size of the moderator is finite, so not all neutrons are going to be produced at exactly the same time and place, and are not moderated in the same way. There are also some small flight length and angular uncertainties. All this will limit our resolution. Assuming that the uncertainties are uncorrelated, they will add in quadrature

$$\frac{\Delta d}{d} = \left\{ (\frac{\Delta t}{t})^2 + (\cot\theta\Delta\theta)^2 + \frac{\Delta L}{L})^2 \right\}^{1/2}. \tag{7}$$

At low angle the $(\cot\theta\Delta\theta)^2$ is dominating. At high angles this term is minimised, as is the case on OSIRIS, and the the dominant broadening comes form the moderator. The other two terms are then minimised by making the flight path of the instrument longer. With $L = 35$m for OSIRIS we achieve in backscattering a resolution of $\frac{\Delta d}{d} = 2.5 \cdot 10^{-3}$.

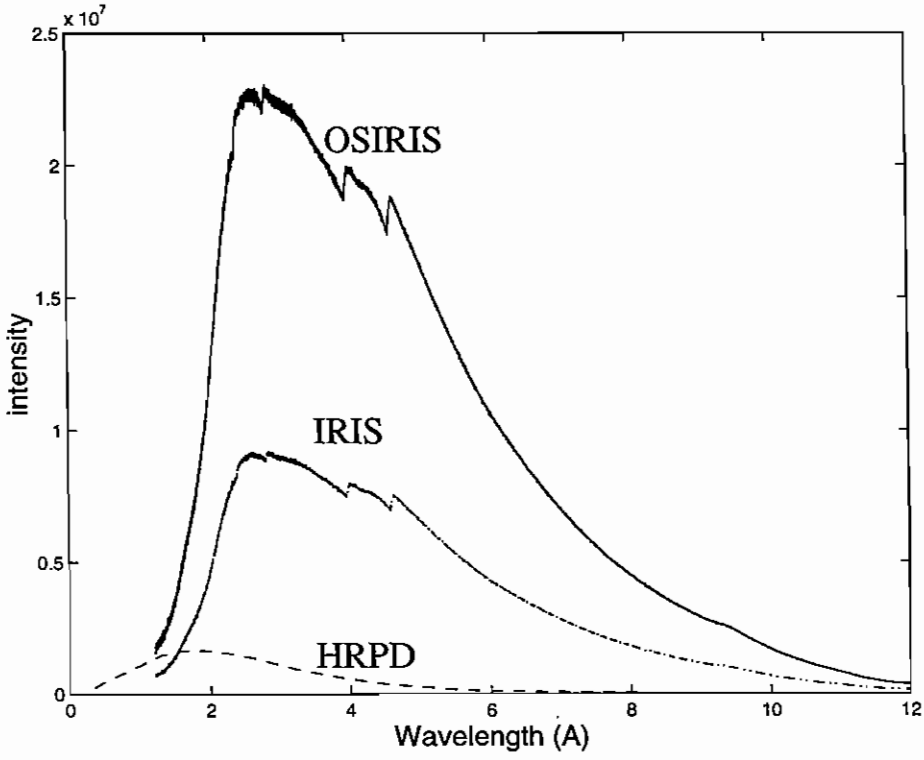

Figure 1: Flux comparison between OSIRIS, IRIS and HRPD.

3.2 From moderator to detector

3.2.1 Moderator

ISIS is not a continuous source of neutrons, as is a nuclear reactor. Neutrons are produced in pulses by letting a burst of protons hit a target (at present tantalum) where by neutrons are produced by spallation. At ISIS, neutrons are produced every 20000μs (ie with a frequency of 50Hz). The neutrons released are however far to fast/hot and have to be slowed/cooled down. This is done in a moderator. Around the target there are different moderators at different temperatures. The OSIRIS guide is directed towards the H_2 moderator at 22K. This means that the Maxwellian distributions of velocities/wavelengths has its maximum around 6Å. The actual maximum is slightly lower, since there also exists a wing from the high energy (low wave-length) epithermal neutrons which moves the maximum to lower wave lengths, see fig.1.

In fig. 1 we compare the neutron flux at OSIRIS, IRIS and HRPD. Expect from the fact that the flux is much higher at OSIRIS there is now big difference between it and IRIS. The flux on HRPD though much lower extends to much shorter wavelength. This diffractometer is directed towards the hotter CH_2 moderator at 100K, which gives a maximum around 2.5Å.

3.2.2 Guide and Choppers

Another difference between the two instruments regarding incident neutrons is that OSIRIS has a curved super-mirror guide, that will not transmit neutrons below ca 1Å, whereas this is not the case for HRPD. The curved guide decreases the background from high energy neutrons but limits the lower d-spacing range

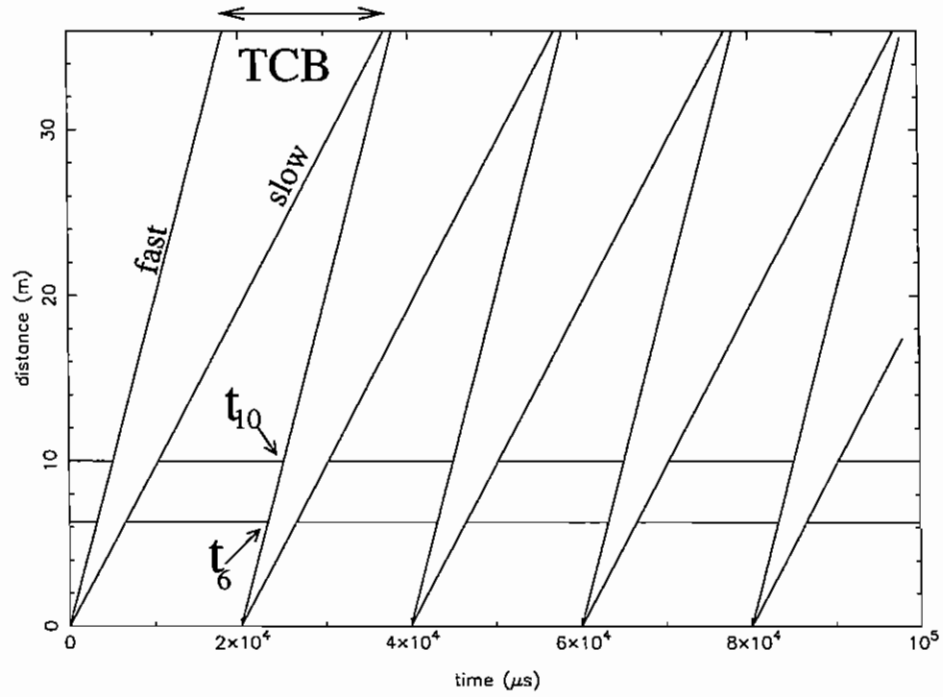

Figure 2: Time distance plot of 5 neutron pulses at OSIRIS. The choppers are running at 50Hz and are set for 2Å as the lowest wavelength. The fast neutrons are marked fast and the slow slow. On the second pulse the opening times of the 6.3 and 10 meter choppers are marked.

attainable at OSIRIS to ca 0.7Å. As you understand from fig.1, OSIRIS is focused on the long wavelength part of the diffractogramme.

Both OSIRIS and IRIS, the instrument next to OSIRIS, have the same main shutter (N6) and look at the same moderator. OSIRIS, however has a curved super-mirror guide made of NiTi it is 65×43 mm, though just before the sample, there is a piece of converging guide and after that part the beam is 44×22 mm.

If we were to let all the neutrons in one pulse hit the sample, some of the slowest neutrons of pulse 1 would not reach the detectors before the fastest neutrons of pulse 2 did, and we would have no way of telling them apart. We need to pick out a small wavelength band of neutrons. On OSIRIS we use two choppers to "cut" a slice, of the full wavelength distribution, such that the time spread when they arrive at the detectors is no larger than that of one pulse, ie 20000μs, it is possible to run the choppers at an integral fraction of the ISIS (50Hz) and thereby create a longer window for counting the neutrons.

In fig.2 a time distance plot of 5 ISIS neutron pulses are shown, one pulse every 20000μs. The choppers are marked by the two horizontal lines, on at 6.3 (opening angle 60 deg) and one at 10m (opening angle 100 deg). This gives a bandwidth of about 2Å at 50Hz and 4Å at 25Hz. The choppers are opened where the line is broken. The opening times for the 6m chopper t_6 and the 10m one t_{10} are shown for the second pulse. The line marking the fastest neutrons (shortest wavelength) let through is marked fast and the corresponding one for the slowest neutrons (longest wavelength) is marked slow.

You note how, when the neutrons reach the detectors at 35 meters, they have spread out in time, but they do not overlap with the next pulse. The times at which the fastest and slowest neutrons reach the detectors define the boundaries between which the computer should count one frame, these times then define the Time Channel Boundaries (TCB). If we were to measure slight faster neutrons the TCB's in fig. 2 would shift to

Wavelength	Chopper	TCB
2-6Å	3180,5056	13000-53000
4-8Å	6370,10100	28000-68000
6-10.4Å	9555, 15150	45500-85500
8-12Å	12740,20200	63200-103200
10-14Å	15900,25250	80000-120000
12-16Å	19100,31750	100800-140800
14-18Å	22250,36700	117800-157800
16-20Å	25450,1790	136000-176000
18-22Å	28665,6845	152000-192000
20-24Å	31850,11900	170000-210000
22-26Å	35035,16955	186000-226000

Table 1: The current chopper settings and the matching TCB values.

the right. For every chopper setting there is a corresponding set of TCB's.

There are already a set of wavelength ranges and their corresponding TCB's calculated for OSIRIS, so here we just go through a simplified way of how to calculate the phases and TCB's. To decide the phase of the choppers we start by deciding the shortest wavelength to pass the first chopper. These are the first neutrons we want to pass, all the rest have longer wave lengths and are therefore slower. The first chopper is opened when these neutrons reach the chopper. To calculate the time at which these neutrons reach the chopper, we use the simple formula:

$$t = c_1 L \lambda, \tag{8}$$

where c_1=252.78, the time $[t] = \mu$s, the wavelength of the neutrons $[\lambda]$=Å and the distance from the moderator to the chopper $[L]$=m.

Assume we want to look at a d-spacing larger than 10Å. We decide to use the highest resolution, the highest scattering angle, almost 180 degrees (actually 171). This means with

$$2d\sin(\Theta/2) = n\lambda, \tag{9}$$

that we want $\lambda = 2d = 2\times10$=20Å neutrons. The 6.3m chopper should then open at t=$c_1\times6.3\times20$=31850.8 The uncertainty in the chopper phase is about 40 so we set t_6=30850. We set the second chopper to open at the same wavelength t=$c_1\times10\times20$=50556 and we set t_{10}=50570. These times are now the chopper phases.

The last thing we have to do is to tell the computer between what times after the neutron pulse it should count, ie calculate the TCB's. The first neutrons hit the detectors at 34+1 meters at t = $c_1\times35\times20$=176946=177000, from the opening angle of the choppers we can also calculate the slowest neutrons to arrive, see fig.2, and we could set this to be the high limit of the TCB but in practice, after making sure that we have no frame overlap, we set the width of the TCB to be one pulse long, ie 20000 μs.

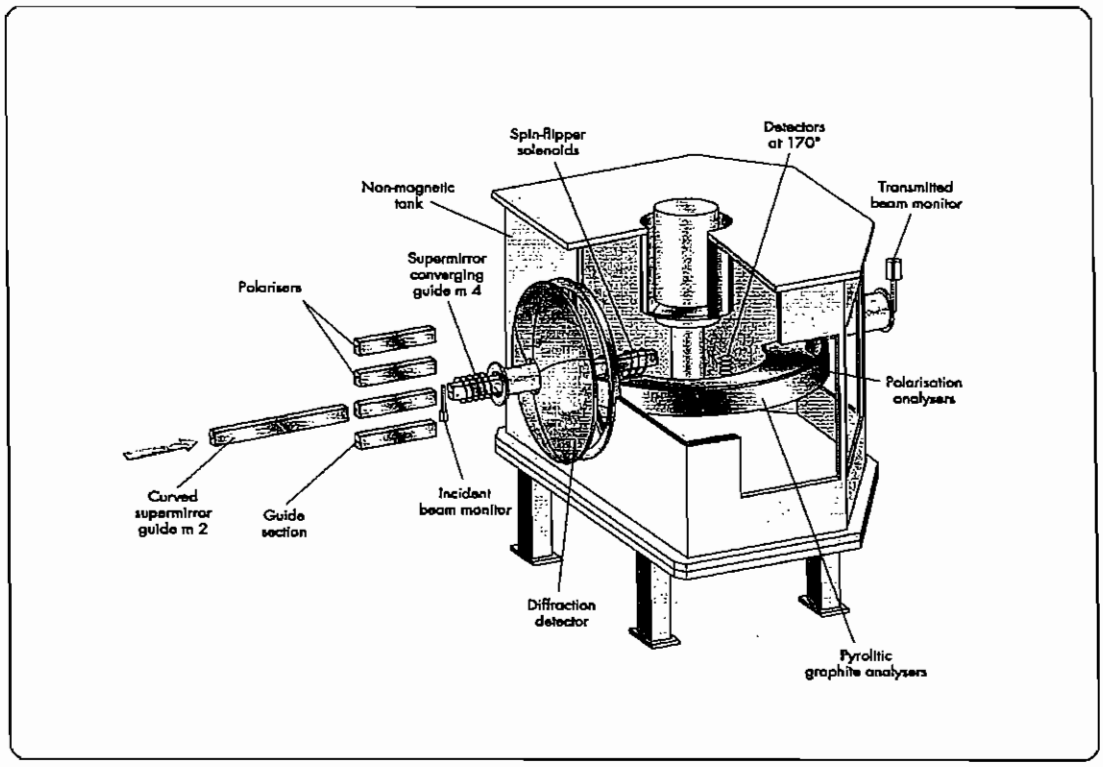

Figure 3: The artists view of the OSIRIS spectrometer. At present the operative part is the diffractometer, see text.

3.2.3 Detectors and Monitors

Monitors The monitors are glass bead monitors. There are five beads horizontally and 6 vertically. The active component is ^{6}Lithium. The calculated efficiency of the monitor is

$$e(\lambda) = 1/(1 - \exp(-0.2066 * \lambda)). \tag{10}$$

There is one incident monitor (spectra 1) and one transmitted beam monitor (spectra 2).

Detectors In fig.3 you see an artists view of OSIRIS. From the left: the curved super-mirror guide (the choppers are further left); polariser, only used for testing now; incident beam monitor; converging guide; and then the neutrons are backscattered from the sample into the diffraction detector bank.

The detectors are Scintilators and the full detector bank contain 8 modules, whereof 3 are at present operative, see fig.4. The further 5 modules are being put in place as they are delivered. Each module contains 120 scintilator elements, see fig.5. The first 20 are single detectors. Between 21 and 120 the even numbered detectors are still single ones but the odd numbered are physically composed of one detector above and one below the even ones, see fig.5. The detectors are numbered sequentially starting at number 3 (the first two spectra are the monitors). Module 1 is 3-122, module 2 is 123-242 and module 3 is 243 to 362. As a user you will most often not use these number but refer to the first 20 in all modules as "high" resolution and all detectors as "all".

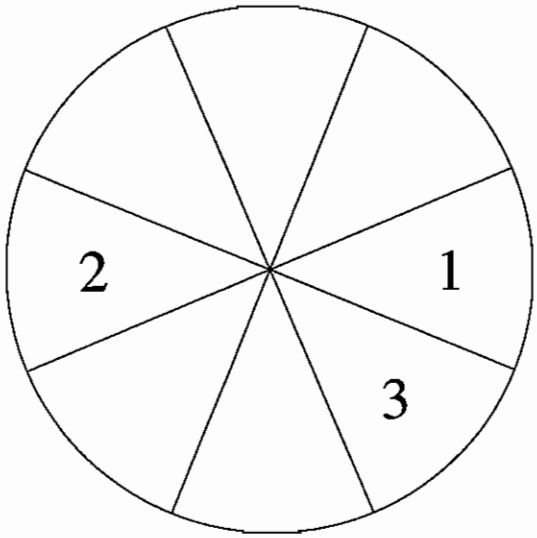

Figure 4: The layout of the OSIRIS diffraction detectors, view from the sample position. At present there are three modules of eight in place.

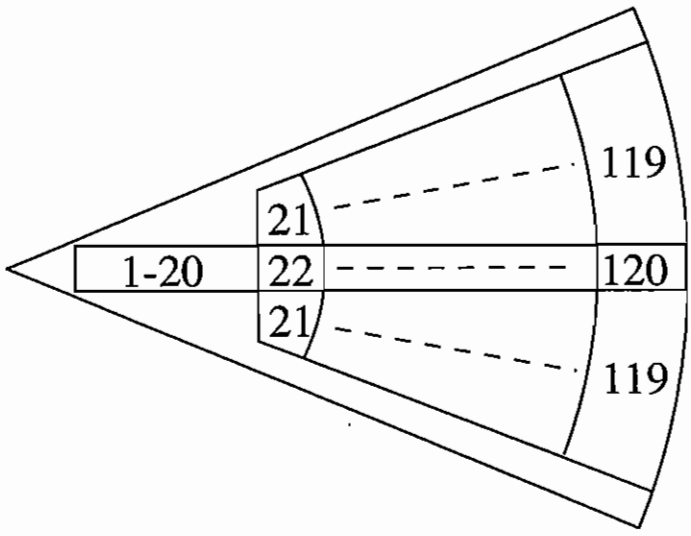

Figure 5: The layout of the one detector module (not to scale). The first twenty detectors are single detectors, there after the odd numbered detectors actually are composed of two couple detectors.

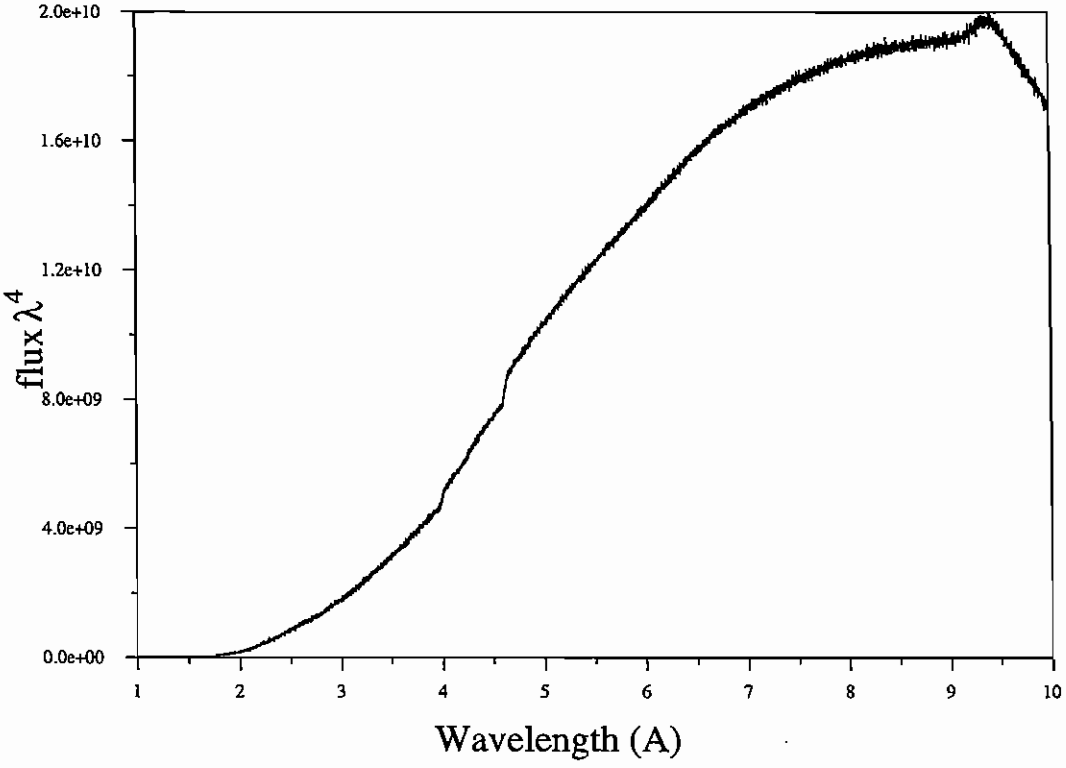

Figure 6: Flux times λ^4. Bragg scattering increase as λ^4, so the effective flux for diffraction is increasing long after the actual maximum in the neutron flux.

3.2.4 Counting rate and d,Q-range

As standard one measures from d=0.7Å up to about 10Å. The lower limit is fixed by the fact that there are no neutrons of low enough wavelength to be diffracted. The higher limit is not a real limit however. Wavelenths up to 50Å corresponding to d-spacings up to 30Å have been measured. It is appreciated if the user makes clear before the experiment if he wants to measure d-spacings large than 10Å. To choose the adequate measuring time one has to take into account that as the incoming intensity decreases for higher wavelength the scattering increases as λ^4, see fig.6, but the absorption also increases with λ, which you have to take into account if your sample is highly absorbing.

3.3 Sample environment equipment

This is a short summary of some of the sample equipment that has been used on OSIRIS, for a full description of the equipment mentioned here and much more see the SE-miniguide on the web page of the SE-group <http://www.isis.rl.ac.uk/UserSuport/isisusg.htm>.

Ambient This is of course the simplest experiment to do your sample is screwed on to a center stick, put in the sample tank, which is then evacuated.

orange/blue cryostat There are two cryostats normally used on OSIRIS, the older orange/ILL and the newer blue/Oxford Instruments one. They are both helium cryostats and can reach down to 1.5K when

pumped on. There is a choice between 100 and 50 mm bore for the orange one (the blue is 50) and Vanadium or Aluminium windows (blue has Aluminium).

(cryo)-furnace The RAL furnaces can reach a temperature of 1200 degrees and they come with sample space between 32 and 65 mm. There is also a cryo furnace which can reach temperatures from 1.5 to 600K.

cryo magnet The cry-magnet can achieve fields up to 7.5 T and temperatures from 2 to 300K.

pressure Various pressure cells can be used depending on what pressure you want to reach, see the SE-miniguide for further info.

4 The Experiment

4.1 First

All the sample equipment you applied for will be at the instrument around 10am on the day you begin. It is your responsibility to get the sample record sheet from the DAC (Data Acquisition Central) and put it in the box on the side of the instrument. If there is something wrong on the sample sheet you must inform your local contact. First, the sample has to be placed in the beam. All equipment has a note saying how far down the center of the beam is, to make it easy for you to put your sample at the right height.

4.2 Safety

The safety system is composed of an electrical and a mechanical system. Your local contact will go through the safety system with you.

4.3 Computer introduction

The OSIRIS computer is a Digital Alpha workstation running OpenVMS. There are four desktops on the computer: data monitor is used to monitor the experiment and run all the command files; osimgr is reserved for the instrument responsible; Analysis for analysis; and User is for the user to do with what ever he wants.

Since VMS might not be familiar to all users, we start with some VMS commands. To find out where your are your can type either `where` or `show def` and then to change your directory simply type `set def directory`. Directories are always written within square brackets, you either type the full name or if you want to go down to dir1 you need only type `[.dir1]` and if you want to go up one step you can use `[-]`. You create a new directory by writing create/directory [.name]

If you open a new window you will be in the [osiris] area. If your name is Smith and you want to change directory to your directory you would type

```
set def [.users.smith]
```

to get down to your directory (the first dot is needed) and if you want to get up again you type either directly

```
set def [osiris]
```

	1	2	3	4	5	6	7	8	9	10
(Å)	0.9-2.8	1.9-3.8	3.0-4.8	4.0-5.8	5.1-6.8	6.2-7.8	7.3-8.8	8.3-9.8	9.3-10.8	10.3-11.8

Table 2: The standard d-ranges at 25Hz .

or

```
set def [-.-]
```

meaning you want to go upwards two steps One file not in the osiris area that you might be interested in is `[osimgr.data]journal.txt`. This contains run number, username, title, time the run ended and number of microamps of each run.

If you want to print a postscript file, this is most easily done by using one of the `plaser` scripts. The printer in the DAC is number 2 and if you want to print to it just type `plaser2 fil.ps`. The printer on the 3rd floor in R3 (photo copier room) is number 1.

4.3.1 organisation

The area you work in on osiris is `osiris$disk0:[osiris]`. Programmes being developed are in `[.alpha]`, and other programmes are in `[.programmes]`. In `[osimgr.tcb]` are all the files with the Time Channel Boundaries. They contain tcb files which should not be changed by the user. These files should only be edited by the `ochange` command.

OSIRIS data that is directly accessible are in the areas `OSIRIS$DISK1:[OSIMGR.DATA]` and `OSIRIS$DISK0:[OSIMGR.DATA]`. You access these areas via the logical name `osiris_data`. OpenGenie is configured to automatically search these directories.

4.3.2 your files

Users should only keep files in the [osiris.users] directory and on scratch$disk:[osiris]. The files in [osiris.users] will be saved for the current cycle but if the disk space is needed they will be deleted during the next cycle. When you have finished you experiment, copy the files you want to save to your own account on user$disk. If you have not got an account the computer support will help you get one.

4.4 Setting up to run

Running the experiment and most of the sample environment is controlled by the computer.

4.4.1 d-spacing

To begin with you need to decide what d-spacing range you want to measure. You can choose from the values in table 2

The choppers are set up with the command

```
drange range
```

where range corresponds to the numbers in table 2. drange is a command file which for range 1 does the following:

```
$ cset c_ph6 3180
$ cset c_ph10 5056
$ load [osimgr.tcb]l2.tcb
```

First the phase of the 6.2 meter chopper is set to 3180 μs and then the 10 meter one is set to 5056 μs. At last the right TCB values are loaded. The name l2 stems from lamda=2Å, which is the lowest wavelength for that setting.

4.4.2 Sample environment

There is usually one temperature sensor on the sample, and another in the cryostat/furnace. They are connected to the EuroTherm in the cabin. The right side of it (temp) is used for controlling the cryostat and the left side (temp1) for controlling a furnace.

All CAMAC (Computer Aided Measurement And Control) parameters are checked and changed with the two commands cshow and cset

Depending on your sample environment, there are different values that you want to set, see section 3.3. The temperature is controlled by setting either heater or temp depending on what equipment you use. For the cryo-magnet he magnetic field is set with the command file magset value where values is the field in Tesla.

When you eg use the orange cryostat or furnace, to set the temperature, you typically type

```
$ cset temp/value=50/range=10/control
```

where 50 is the temperature in Celsius for the furnaces and in Kelvin for the cryostats, range means that data is collected as long as the temperature is within plus minus 5 degrees of the value you did set. This is not fully correct since if you type nocontrol instead of control, data is collected irrespective of what temperature you are at. Every sensor is identified by a device number. To change device (something your local contact will do) you type,

```
$ cset temp/devspec=number
```

The heating power is set in percentage of the maximum voltages, (which is set by hand on the physical heater, also done by your local contact), with the parameter max_power. To see what power is presently used cshow power/enq. Note that if you are controlling on temp1 and not temp you just replace temp1 for temp

4.5 Collecting data

The current status of your experiment can be read on the dashboard. If there is no dashboard on your screen you can start one with the command stat on and conversely you turn it of with on replaced by off. There is a "windowed" version of the dashboard, which is started with the command dash if you prefer that.

If e.g. temp is not display in the dashboard you can "turn it on" by

```
cset temp/disp.
```

The run is started by typing `begin` ended by `end` paused by `pause` resumed by `resume` and aborted by `abort`.

4.6 Command files (VMS)

You are now ready to write down your whole experiment in a command file. A command file would typically look like this:

```
$ Set Verify
$
$ cset max_power 10
$ cset temp/value=200/range=10/control
$ cset temp1/value=200/range=10/control
$
$ drange 1
$ change title """new title"""
$ begin
$ waitfor 30 uAmps
$ end
$
$ drange 2
$ change title """new title"""
$ begin
$ waitfor 30 uAmps
$ end
$
$ cset max_power 30
$ cset temp/value=500/range=10/control
$ cset temp1/value=500/range=10/control
$
$ drange 1
$ change title """new title"""
$ begin
$ waitfor 30 uAmps
$ end
```

The first line `set verify` is for the command file to echo the commands it is performing. The maximal power of the heater is then set to 10%. Temperature is set to 200 degrees and with `range=10` we are not going to collect data if the temperature is plus minus 5 degrees from what was set. If we would have typed `nocontrol` instead of `control` this vetoing of out of range data would have been overridden. The range to measure is then set to range number 1, by the `drange` command. Each run needs it own title and this is set by the `change title` command. Note that you really need three quotation marks. The `waitfor` command will here make the computer wait till ISIS has delivered 30μamps, and then the run is ended. The new range is set, and so on.

level	action
>10μSv/hour	Phone ISIS duty officer leave sample within interlocked area.
>0.1μSv/hour	Store sample in osiris active sample cupboard with sample record sheet. The sample may NOT be removed from its container. For removal from ISIS contact the duty officer
<0.1μSv/hour	The sample is not radioactive. For removal from ISIS contact the duty officer

Table 3: Treating a radioactive sample, (ISIS duty officer x6789) .

4.7 Finally

When you have finished your experiment the sample needs to be taken out of the beam. As soon as you have taken it out you should measure the induced radioactivity and act according to table 3

If the sample needs to be stored in the active sample cupboard you must mark you sample and fill in the sample cupboard log book. THE ACTIVE SAMPLE CUPBOARD LOG-BOOK MUST BE COMPLETED FOR ALL SAMPLES WHEN STORED IN OR REMOVED FROM THIS CUPBOARD. Do not forget do leave your e-mail address, so that we can contact you when the sample is safe for you to bring back.

5 Data Reduction and Visualisation

5.1 OpenGenie (OG)

5.1.1 read me first!

setting up To set up the OSIRIS programmes to run with OG on your account you should put the following lines in your login.com file

```
osiris:== @osiris$disk0:[osiris]user_set_up.com.
```

When you type `osiris` you will then among other things define the logical genie_gcl_init, and OG will find the right genieinit.gcl file to use. Definitions needed to find the raw-data files are also performed

remote access You login to an Alpha station, e.g. ISISA. When you login from a remote computer, and want to use graphics, you have to set the display with

```
set display/create/node=ip.ip.ip.ip/transport=tcpip
```

where you replace `ip.ip.ip.ip` with your own ip address/number. You can define a symbol in your login.com if you need to type this often,

```
remote == "set display/create/node=ip.ip.ip.ip/transport=tcpip"
```

so that when you type `remote` the display is set up.

You probably have to set some sort of protection on your own computer, if it is a unix machine typically `xhost ip.ip.ip.ip.`, where you type the ip number of the machine you want to allow to open a window on your local computer. This way you set the security level varies between operating systems.

gcl It is strongly recommended that you write your analysis in the form of command/gcl files. To start inspecting the data the interactive approach is much easier but when you have decided what to do, use a command file!! The use is twofold, if you want to redo your analysis it is easy and you have a very good log of what you actually did with your data. It is not necessary to give the files the extension .gcl but it does help you to keep track of your files. They are very easy to write as these short examples show:

```
PROCEDURE test1
RESULT run
LOCAL run1 run2
run1=focus_norm_bank(1,"high","raw")
run2=focus_norm_bank(2,"high","raw")
run=merge_diffractogram(run1,run2)
ENDPROCEDURE

PROCEDURE test2
PARAMETER NAME=String
RESULT run
LOCAL run1 run2 fil
fil=NAME&"in3"
sum_raw 1 2 0.05 0.1
run=focus_norm(1,5,122,"raa")
put/new run file=fil
ENDPROCEDURE
```

To run these you first have to load them `load "filename"` and then run them with the commands `result=test1()` and `result=test2(saved)` or just `test2 saved` if you just want to save the result to the file `saved.in3`.

Syntax In what follows [ ] always means qualifiers that not need to be used. Also remember that in OG all strings have to be enclosed with quotation marks. In all examples that follows, when you see quotation marks, they should be typed. Every procedure that returns a result needs to written with parentheses, even if there are no 'in' parameters. You can type:

```
procedure(a)
```

but you have to type

```
work_space=procedure(a)
```

(cf. focus_norm) to save the result of the procedure in a workspace. If however the procedure writes to a file it is alright just to write (cf. sum_raw):

```
procedure a
```

Note that `work_space=procedure a` is always WRONG, whereas `procedure(a)` can be right. In OG as opposed to old Genie you can give your workspaces any name and not just w1, w2... as in Genie.

5.1.2 Some OG commands

Read log files(SC) Help is often available with the /help qualifier. toggle/info To get the long title: get("titl") and to see a list of all parameters in the raw file list "file_name" or just list/in to list the current in file rebin:log(bound1,step1,bound2) rebin(w,w2.x)

5.1.3 aliases (alias.gcl)

There are some non-standard aliases defined in the file `alias.gcl` that you can use. They are:

alias	function
d	display
p	plot
fnb	focus norm bank
md	merge diffractogram
a/b	alter/binning

5.1.4 local extensions (local.gcl)

ASCII To export an x,y,e array of your workspace use the routine "ascii_export", it takes two parameters:

```
ascii_export work_space "file name"
```

where "work space" is the work space you want to export and "file name" is the name you want to give to your exported data. There is no default value for "file name" and if you do not give a name with a full stop the computer will still put a full stop at the end of the file name. To import an ascii file (three columns or the "genie" ascii) use the

```
work_space=ascii_import("file name","type")
```

where type can be plain or genie. (not written yet)

in3 To save a work space to an intermediate genie, in3, file you type

```
put/new work_space file="name.in3"
```

you can then continue adding blocks by the same command, just remember not type new. When you later want to read in your saved workspaces you type

```
work_space=get(3,"name.in3")
```

to get block 3 from file name.in3

graphics You can change the colour of your next plot by the commands `red green blue` and `white`. A small plot window can be opened with the command `fonster`.

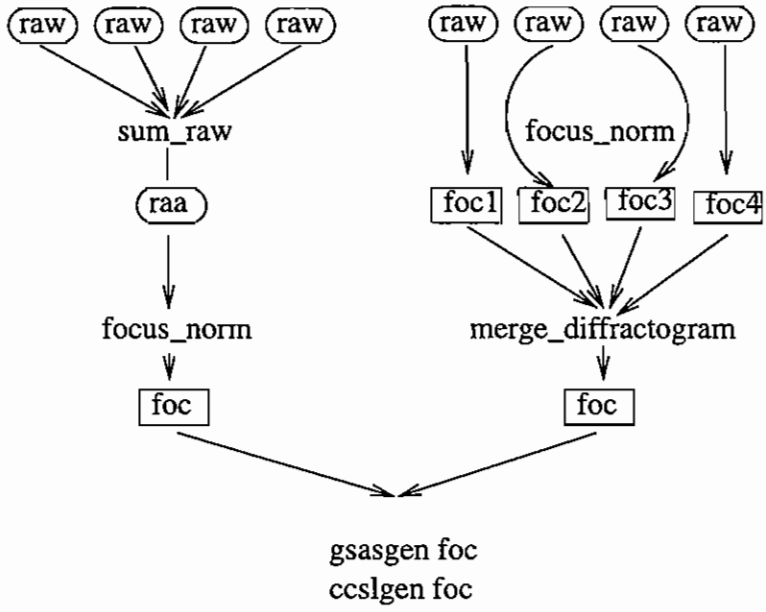

Figure 7: Different ways of analysing data, see text.

dae To display the dae you type `assign "dae"` where you have to type the quotation marks since `dae` is a string. You can, however type only `assign` and the default value is to set your input to the dae

correctL You can correct old runs with wrong angle and flight path with this command. Either you have a detector.dat file you want to use to replace both angle and flight-path. It is also possible to have a genie intermediate file that hold shift of each detector. The output file will have the extension caw instead of raw and the commands should look like:

```
correctL/all run_number "detector.dat"
correctL run_number "dL.in3"
```

5.2 Diffraction

5.2.1 OSIRIS routines (osd.gcl)

There are to different ways of doing reduction for the diffraction data.

sum_raw The program takes at least two parameters

```
sum_raw first_run_number last_run_number [%low %high]
```

The runs are summed where they overlap, otherwise they are just appended together into one file with the same run number as the first file but the extension "raw" replaced with "raa" and the run_no is changed to the range summed. The monitor is "unwrapped" before the summation and only data points where both monitor and detector data (in wavelength) are available are saved. The numbers %low and %high (type 10% as 0.1) gives you the possibility to skip the first %low and last %high part of each spectra. Something you would want to do to be sure that opening and closing of the choppers are not influencing your data.

The routine unwrap is used to unwrap the monitor. This is done by searching for the minimum value in the spectra and then moving everything from the right of that point to the left side of the spectra.

focus_norm This routine reads "raw", "sav" or "raa" files. The units are changed to wavelength the monitor is corrected for efficiency (see 3.2.3) and, detector efficiency corrections are performed Units are changed to d-spacing and the spectra are focused and normalised with the monitor. The spectra are focused in d-space. This routine takes three parameters.

```
work_space=focus_norm(run_number,first_detector,last_detector,"ext")
```

The default value for ext is raa, and as standard we use all detectors.

focus_norm_bank (fnb) Same as `focus_norm` but takes slightly different parameters

```
work_space=focus_norm_bank(run_number,"bank","ext")
```

where bank is either all or high, and high means high resolution. Default values are `bank=all` and `ext=raw` so to focus all detectors from a `raw` file you need only to type

```
work_space=fnb(run_number)
```

merge_diffractogram If you run focus_norm on your raw files you will have to merge the the workspaces into which you have focused your raw data.

```
work_space=merge_diffractogram(f1,f2,f3...)
```

Here f1, f2, f3... are the workspaces you want to merge, the maximum is 10 at a time. They should be typed in order of increasing d-spacing. You will see a plot of the overlapping regions of f1 and f2 to start with and you have to decide where you want to cut your data.

ccslgen A workspace can be exported to ccsl format (three columns x,y,e) with the command

```
ccslgen work_space
```

and then you follow instructions.

5.2.2 ISIS routines

gsasgen A workspace can be exported to gsas format with the command

```
gsasgen work_space
```

and then you follow the instructions. If you have any problem try rebinning your data before exporting. Background subtraction should be done before you generate gsas format.

You should choose bank 1 for `"all"` detectors and bank 2 for the `"high"` resolution option.

A Appendices

A.1 food and drink

On <http://admin-www.rl.ac.uk/admin/services/ral_restaurant/> you can find todays menu.

A.2 phone numbers

name	ext	
Ken Andersen	6731	0777-5533909
David Martin	6157	
OSIRIS	6896	
Main Control Room	6789	
emergency	2222	
User Liaison Office	5592	