Practicalities of Muon Data Analysis

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ISIS Muon Training Course
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Outline of Talk

Computing infrastructure at ISIS

• Network organisation
• Front-end and data analysis machines
• Instrument control programs
• Data formats and data access
2002 Configuration of ISIS Computing

Currently a gradual migration to PC-based instrument computers
Current ISIS $\mu$SR Computing Layout

Muon Instruments

- MUSR
  - Windows
  - FEM

- EMU
  - Windows
  - FEM

- HiFi
  - Windows
  - FEM

- ARGUS
  - Windows/Linux
  - FEM

Samba (files)
Exceed (xterm)

Remote access (ssh, scp)

Data Archive (ISISA)

VMS Cluster

Analysis PC

Analysis PC

Analysis PC
Using the ISIS Computers

- Individual PCs
  - User:
  - Password:

- VMS alpha cluster
  
  Login to ISISA from an x-terminal window, use the account details available at each instrument

ISIS Computing Support can be contacted by emailing
support@isise.rl.ac.uk or ISISsupport@rl.ac.uk
or by phoning extension 1763
Using Personal Laptops at ISIS

Connecting Laptops at ISIS

Visitors to ISIS are welcome to connect their laptop to our network in Ridgeway House/R70 hostel as well as the R55 experimental hall and R3 Offices. The ISIS internet connection is behind the RAL site firewall, which allows most connections going out, but connections coming in are restricted.

Physical Connections

Network sockets are available in all instrument cabins and public areas. Wireless access is also available in many parts of the R55 experimental hall.

IP address

IP addresses are allocated automatically using DHCP. Please set your network settings to use DHCP and reboot (if you have fixed settings for your home institution it may be worth recording their values).

Mail

Receiving mail should work immediately. Sending SMTP mail needs to go out through outbox.rl.ac.uk. Access to web based email will work once a proxy server has been configured.

Web

Web access off site needs to go through a proxy server. Set your browser to use the automatic configuration script http://wwwcache.rl.ac.uk/proxy.pac

Printers

Access to certain printers is enabled. Please ask your local contact for information on connecting to your nearest printer.
Using Personal Laptops at ISIS

For connecting to network resources at ISIS from a personal laptop use the isis\muontc account

e.g. to connect to the emu instrument data

*click Start\Run → enter \emu\data*

(then provide isis\muontc details when prompted)
Remote Access

• All external access is via ISISA (isisa.rl.ac.uk)
  (use ssh for terminal login
  and scp for file copying)

• Data from PC controlled instruments (i.e. all current
  ISIS muon instruments) can be downloaded via the
  web interface to the data portal:

  http://data.isis.rl.ac.uk
Data Acquisition Control Systems

Currently we have two different systems:

**MACS/EXP**  Windows/Linux system (ARGUS)

**SECI**  Windows system (MUSR, EMU, HiFi)
Hybrid Linux/Windows system used on ARGUS
SECI (MUSR and EMU)
Data Formats for Muon Data

- SECI NeXus-1: hierarchical, extendable format
- MACS MACS binary (also option for new NeXus-2)

Typical run file is 200-600 kb in size
Data compression reduces the size by up to a factor of 7
(bzip2 is the most efficient zip algorithm for muon data)
NeXus

The NeXus hierarchical data format has three components:

A set of subroutines
to make it easy to read and write NeXus files

A set of design principles
to help people understand what is in them

A set of instrument definitions
to allow the development of more portable analysis software

Example part of data structure:

NeXus webpage: www.nexus.anl.gov
ISIS muons NeXus webpage: www.isis.rl.ac.uk/muons/data analysis/nexus/intro.htm
μSR Data Formats in Use Worldwide

- PSI (Switzerland)
  - .dat (VMS binary)
  - .bin (standard binary)
  - .nxs (Nexus-2, eventually)

- TRIUMF (Canada)
  - .tri (VMS binary)
  - .mud (hierarchical)

- KEK/JPARC (Japan)
  - .kek (VMS binary)
# Finding the Muon Data

<table>
<thead>
<tr>
<th>Instrument</th>
<th>ISIS Network Path</th>
<th>ISISA Path</th>
</tr>
</thead>
<tbody>
<tr>
<td>ARGUS</td>
<td><code>\bhuna\macs\argus0005634.ral</code></td>
<td>not available</td>
</tr>
<tr>
<td>EMU</td>
<td><code>\emu\data\emu00010000.nxs</code></td>
<td><code>emu$disk0:[data.emu]emu00010000.nxs</code></td>
</tr>
<tr>
<td>MUSR</td>
<td><code>\musr\data\musr00001025.nxs</code></td>
<td><code>musr$disk0:[data.musr]musr00001025.nxs</code></td>
</tr>
</tbody>
</table>
Temperature Logs

- Usually stored in a tlog subdirectory within the data directory.
  
  Same name as the data file but with extension .tlog

- NeXus files store the tlog data internally
Taking Data Away

• Copy to own laptop
• Burn CD using PC in instrument cabin
• Send to remote system back home – pushing is easier than pulling!
• Fetch using remote login from home
Muon Data Analysis Software
Used at ISIS

UDA (VMS, General Purpose)

RUMDA (VMS, General Purpose)

MESA (VMS, Maximum Entropy for TF Studies)

WiMDA (Windows, General Purpose)

Many user groups have also developed their own programs over the years
Muon Data Analysis Software Used at ISIS

WiMDA will be used for the practical sessions

WiMDA website from which the software can be downloaded:

http://www.isis.rl.ac.uk/muons/data_analysis/wimda/
Main Stages in Muon Data Analysis

1. Preparing the data to be analysed, ‘setting up’

2. Fitting the measured asymmetry to a chosen relaxation function; ‘analysing’

3. Assessing the fitted relaxation parameters, which may involve a further stage of fitting these parameters to an appropriate model; ‘modelling’

4. Preparing plots of the results of analysing and modelling the data, ‘plotting’
1. Setting Up the Data

a) Checking the time origin $t_0$ and the time of the first and last good data points

b) Defining the detector grouping

c) Correction for counting loss due to counter deadtime

d) Correction for steady background count rate

e) Choice of binning
1. Setting Up the Data

a) Checking the time origin $t_0$ and the time of the first and last good data points

![Graph showing bin number vs. counts with $t_0$ and $t_{good}$ marked]
1. Setting Up the Data

b) Defining the detector grouping

e.g.

for LF/ZF:
- Forward group: 1-16
- Backward group: 17-32

for TF:
- Group 1: 1-4, 17-20
- Group 2: 5-8, 21-24
- Group 3: 9-12, 25-28
- Group 4: 13-16, 29-32

Notes:

ARGUS has 192 detectors (usually pregrouped to 32 histograms in the data analysis software)

MUSR has 64 detectors (usually pregrouped to 32 histograms in the data analysis software)

EMU has 32 detectors and no pregrouping is required
Note that a dephasing effect will reduce the asymmetry of TF data if not enough groups are used:

\[ \text{Dephasing factor} = \frac{\sin(\pi/N)}{\pi/N} \]

<table>
<thead>
<tr>
<th>TF Groups</th>
<th>Dephasing Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>99 %</td>
</tr>
<tr>
<td>8</td>
<td>98 %</td>
</tr>
<tr>
<td>4</td>
<td>90 %</td>
</tr>
<tr>
<td>2</td>
<td>64 %</td>
</tr>
</tbody>
</table>

i.e. 8 TF groups are sufficient for most purposes
c) Correction for counting loss due to counter deadtime

characterised by a deadtime $\tau$ for each detector channel, typically $\tau \sim 10$ ns

deadtimes for particular instruments are obtained from high statistics calibration runs using Ag data rate correction to the observed rate $r_{ob}$ is applied to give the true rate $r$

the simplest form of correction is $r = r_{ob} / (1 - r_{ob}\tau)$
d) Correction for steady background count rate

can be included as part of the fitting procedure
e) Choice of binning:

The standard raw time bin for ISIS data is 16 ns. It is often useful to choose to increase the bin size for data analysis.

**bin width:** tradeoff between number of points and fitting speed

allows separate focus on fast and slow parts of the relaxation

**fixed/variable:** variable binning compensates for the deteriorating signal-to-noise at longer times

best to keep to fixed binning for weakly damped oscillations, e.g. TF studies
2. Analysing the Relaxation

- Try fitting to possible alternative relaxation functions
- Look for systematic deviations of the fit from the data – are additional relaxation components needed?
- Use the reduced chi-squared $\chi_r^2$ to judge the quality of the fit and appropriateness of the model

$$\chi_r^2 = \sum_{i=1}^{N} \left( \frac{y_i - Y(x_i; p_1, p_2, ..., p_m)}{\sigma_i} \right)^2 / (N - m)$$

$N-m = \nu$ is the number of degrees of freedom
Expected standard error of $\chi_r^2$ is $(2/\nu)^{1/2}$
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** Too good fit! 

** High $\nu**

** Low $\nu**
Expected standard error of $\chi_r^2$ is $(2/\nu)^{1/2}$
3. Modelling Fitted Parameter Sets

- A further stage of fitting involves modelling the fitted parameters for a related set of runs:
  - e.g. following the temperature dependence of a precession frequency within a magnetic phase
  - or fitting the field dependence of a relaxation rate to an appropriate model

- Online analysis and modelling allows feedback to the experimental data taking process
  - helps in getting more efficient and complete data sets
4. Plotting the Results

Close integration with the fitting process is desirable for rapid feedback on:

- the data quality
- the state of the analysis
- the progress of the experiment

GLE (Graphics Layout Engine)

Graphics scripting system closely integrated with WiMDA and used in the data analysis workshop for making plots

http://www.gle-graphics.org/
Analysis of Complex Rotation Spectra

1. Fourier and All Poles transforms
2. Maximum Entropy spectral analysis
3. Time domain analysis versus frequency domain analysis
Fourier and All-Poles Transforms

**FFT (Fast Fourier Transform)** is the standard way to convert from time domain to frequency domain.

FFT assumes frequency spectrum is well represented by array of evenly spaced points, which works well for spectra containing broad spectral features.

However, if the spectrum contains very narrow features, other types of frequency transform can work better.

The **All-Poles (maxent)** method is one such method, which makes an expansion of the data in terms of a series of sharp frequencies.

See Press et al, Numerical Recipes, CUP for further details of the All-Poles transform.

**All transform methods assume that the data error is independent of time, which is clearly not the case for μSR data.**

**Data filtering (apodization) is essential before transforming.**
Fourier and All-Poles Transforms

Optimal filtering time constant for a single undamped test frequency

Single undamped frequency; 10 MEv test data

FFT

Spectral Intensity

Frequency (MHz)

All-poles Maxent

Spectral Intensity

Frequency (MHz)
Fourier and All-Poles Transforms

A close pair of undamped test frequencies

Pair of undamped frequencies 0.95/1.05 MHz; 10 MeV test data
The Maximum Entropy Method

Avoids the noise problem and need for filtering; takes data errors fully into account

Iterative procedure for constructing the frequency spectrum with the minimum structure (i.e. maximum entropy) that is consistent with the measured data

Entropy here is determined from the frequency spectrum $p_k$

$$S = -\sum_k \frac{p_k}{b} \log \frac{p_k}{b}$$

The procedure involves maximising $S - \lambda \chi^2$, where $\lambda$ is a Lagrange multiplier

See Rainford and Daniell, Hyperfine Interactions 87, 1129 (1994) for a detailed discussion of using Maximum Entropy in $\mu$SR

for a general reference see:

The Maximum Entropy Method

Demonstration using the test data for the transforms

Single frequency test

Pair frequency test
Organic Superconductor Example

Maximum Entropy Spectra

Characteristic field distribution due to vortex lattice
Melting of the Vortex Lattice
# Time Domain Analysis versus Frequency Domain Analysis

## Single Frequency

<table>
<thead>
<tr>
<th></th>
<th>Freq (MHz)</th>
<th>Width (MHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test Data</td>
<td>1.0000</td>
<td>0.000</td>
</tr>
<tr>
<td>Time domain fit</td>
<td>0.9998(1)</td>
<td>0.001(1)</td>
</tr>
<tr>
<td>Maximum Entropy</td>
<td>1.006</td>
<td>0.003</td>
</tr>
</tbody>
</table>

## Pair of Frequencies

<table>
<thead>
<tr>
<th></th>
<th>Freq (MHz)</th>
<th>Width (MHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test Data</td>
<td>0.9500, 1.0500</td>
<td>0.000, 0.000</td>
</tr>
<tr>
<td>Time domain fit</td>
<td>0.9493(1), 1.0499(3)</td>
<td>0.003(3), 0.004(3)</td>
</tr>
<tr>
<td>Maximum Entropy</td>
<td>0.956, 1.054</td>
<td>0.002, 0.005</td>
</tr>
</tbody>
</table>
Time Domain Analysis versus Frequency Domain Analysis

**Summary**

Transforms are good for determining a qualitative picture of data:
- **FFT** best for spectra containing relatively **broad** features
- **All-poles transform** best for spectra composed of **sharp** features

**Maximum Entropy** gives an ‘unbiased’ view of the data but **Time Domain Fitting** gives best ultimate accuracy, provided the correct model is being used.

Combination of **Frequency Domain** and **Time Domain** analysis works best.
Tomorrow:

Practical Data Analysis Workshop