User Manual for OPENGENIE muon data analysis suite

Contents

Introduction

This document aims to explain how to reduce/analysis uSR data using the OPENGENIE routines.

Installation

1. Install OpenGENIE from ISIS website (http://www.isis.rl.ac.uk/OpenGENIE)
2. Download and unpack muon openGENIE files
3. Edit opengenie_startup.gcl and replace <your_install_dir> with the directory you unpack the muon openGENIE files
4. type load "<your_install_dir>/opengenie_startup.gcl". You need to type this every time you start OpenGENIE.

Data reduction

Setting the data directory:

Type at the OPENGENIE command prompt:

```
Datadir="<data directory>"
```

Getting the Run information:

At the opengenie prompt type

```
Headers
```

This will create a text file called "headers.txt" and open a text editor.

Optaining Alpha:

To obtain Alpha, type

T20fitg (for a Gaussian envelope)

Or

T20fitl (for a lorentzian envelope)

Alpha will be given at the end.

Converting NeXus files to ascii:

To convert data into xye format and fit using the opengenie fit routines then

```
Convert_ascii2
```

The defaults are read from the first Nexus data file. Typing zero will read the current run (if data directory is the MuSR disk).
For Opengenie analysis use the rumda output option. This will write files to the working directory called "r<runnumber>".dat (rumbda option) or "musr<run number>.dat" for general output.

Data visualisation

Viewing data:

To view the data

```
V
```

The data will be shored in a workspace called dataw. This can be manipulated with the usual Opengenie commands, such as:

Adjusting the xmin, xmax, ymin and ymax

```
d/m dataw 0 16 0 0.3
```

Adjusting the data binning

```
a/b <bin size>
```

To view the short time data then after typing v typing short will view the data from 0 to 3 μs with a data binning of 1.

Viewing multiple runs:

To view multiple runs if the runs are in a sequence (i.e. every run or every n runs)

```
Mulp
```

If not then use

```
MuPlot (not fully implanted yet)
```

Which asks for the run numbers to plot.

Viewing data and fit:

To view the data

```
Vf
```

The data will be shored in a workspace called dataw and the fit will be stored in fitw. This can be manipulated with the usual Opengenie commands, such as:

Adjusting the xmin, xmax, ymin and ymax

```
d/m dataw 0 16 0 0.3
p/l fitw
```

Adjusting the data binning

```
a/b <bin size>
```

To view the short time data and fit then after typing v typing shortf will view the data and fit from 0 to 3 μs with a data binning of 1.

Viewing multiple runs:

To view multiple runs if the runs are in a sequence (i.e. every run or every n runs)

```
Mulpf
```

If not then use

```
MuPlotf (not fully implanted yet)
```

Which asks for the run numbers to plot.

Colour of plot:

In order to change the colour of the plot; type any of the following:

```
Blue
Red
Yellow
Green
Purple
Black
```

Viewing the logs in the data file:

To view the logs stored in the data file type

```
Plotlog
```

Exporting data, fits and plots

Rebinning data

To rebin the data ready to be written to a statistically group data set ready for importing into another plotting package then

```
              Rebin/lin dataw <xmin> <xmax> <bin size (μs)>
Or      newwksp= Rebin:lin(dataw,<xmin>,<xmax>,<bin size (μs)>)
```

Dataw can of course be replaced by fitw.

Writing data to files

Workspaces (such as dataw and fitw) can be written to disk using

```
Writexye dataw "filename.dat"
Writexy fitw "filename.fit"
```

The data will of course all ready exist in the ungrouped from after converting to acsii and then fitting.

Printing plots

Select print from the plot window.

Fitting data

Fitting data from convert_ascii output:

To fit data type

```
fit_new2
```

This will use the least squares fitting routine within OpenGenie. It will ask you for start time, stop time, number of variables, initial starting parameters, whether to vary the parameters and the function to be fitted. This will create a .fit and .par file. If you wish to fit using an old .par file then

```
fit_new2/fo
```

Or if you wish to fit your data using a par file which is the results from another data file then

```
fit_new2/f
```

Preloaded Functions

There are some preloaded functions installed (listed below):

Lor $G_z(t) = A_0 \exp(-\lambda t) + C$

Parameter 1 = A_0

Parameter 2 = λ

Parameter 3 = C

Slo $G_z(t) = A_0 \exp\left(-(\lambda t)^{\beta}\right) + C$

Parameter 1 = A_0

Parameter 2 = λ

Parameter 3 = β

Parameter 4 = C

Gkt $G_z(t) = A_0\left(\frac{1}{3} + \frac{2}{3}\left(1-\sigma^2 t^2\right)\exp\left(-\frac{\sigma^2 t^2}{2}\right)\right) + C$

Parameter 1 = A_0

Parameter 2 = σ

Parameter 3 = C

Lkt $G_z(t) = A_0\left(\frac{1}{3} + \frac{2}{3}\left(1-\lambda t\right)\exp\left(-\frac{\lambda t}{2}\right)\right) + C$

Parameter 1 = A_0

Parameter 2 = λ

Parameter 3 = C

Gktlor $G_z(t) = A_0\left(\frac{1}{3} + \frac{2}{3}\left(1-\sigma^2 t^2\right)\exp\left(-\frac{\sigma^2 t^2}{2}\right)\right)\exp(-\lambda t) + C$

Parameter 1 = A_0

Parameter 2 = σ

Parameter 3 = λ

Parameter 4 = C

Gktslo $G_z(t) = A_0\left(\frac{1}{3} + \frac{2}{3}\left(1 - \sigma^2 t^2\right)\exp\left(-\frac{\sigma^2 t^2}{2}\right)\right)\exp\left(-(\lambda t)^\beta\right) + C$

Parameter 1 = A_0
Parameter 2 = σ
Parameter 3 = λ
Parameter 4 = β
Parameter 5 = C

Gaussosc $G_z(t) = A_0 \cos(\omega t + \varphi)\exp\left(-\sigma^2 t^2\right) + C$

Parameter 1 = A_0
Parameter 2 = ω
Parameter 3 = φ
Parameter 4 = σ
Parameter 5 = C

Lorosc $G_z(t) = A_0 \cos(\omega t + \varphi)\exp\left(-\lambda t\right) + C$

Parameter 1 = A_0
Parameter 2 = ω
Parameter 3 = φ
Parameter 4 = λ
Parameter 5 = C

Additional functions

Additional function can be added by

Comfunc

This can auto generate the function for you, but requires Compaq visual fortran. This creates .so files which can be loaded into Opengenie. The Comfunc script will auto load the .so file created.

Loaded additional functions

To load function module to fit your data with

Module/load <funcname.so>

Batch fitting

In order to batch fit a set of data then type

```
Fitit
```

The first run must have been already fitted.

Plotting fit results parameters

Firstly a file must be created with two columns: First run number, second x-axis parameter (e.g. Temperature or Field). Then use the Opengenie script

```
Plotpara2
```

This will plot all the variables as a function of the second column in the dependent parameter file (see above). These plots can be made larger by clicking on the plot. Crtl-x will exit this script.

After viewing the data these results can be written to a file using

```
Writeres
```

This will write the results to a file called "results.dat"

Extra Scripts:

Maximum Entropy analysis

The maximum entropy analysis is available. However, in the current working directory there must be

1) a stdgrp file, called stdgrp.par, which contains detector groupings
2) a deadtime file, called taud.dat, which contains the deadtimes for each group.
3) a phase file, called phase.dat, which contains the phase of each detector group.

Examples of these files are given in Appendix A. Running the maxent will generate a file called <runnumber>.max.

Simulations

There are several simulation programs that have been written and can be ran within OpenGenie.

Static dipole fields

This program simulates longitudinal μSR data with a field distribution for static nuclear dipole. The command is

```
Zsimsgkt
```

The results can be viewed/analysed as if the data was real, i.e. use the v or fit_new2 commands.

Static dilute atomic moments

This program simulates longitudinal μSR data with a field distribution for static dilute atomic moments. The command is

```
Zsimslkt
```

The results can be viewed/analysed as if the data was real, i.e. use the v or fit_new2 commands.

Static dipole fields with a hopping muon

This program simulates longitudinal μSR data with a field distribution for static nuclear dipole with a hopping muon. The command is

```
Zsimdgkt
```

The results can be viewed/analysed as if the data was real, i.e. use the v or fit_new2 commands.

Static dilute atomic moments with a hopping muon

This program simulates longitudinal μSR data with a field distribution for static dilute atomic moments with a hopping muon. The command is

```
Zsimdlkt
```

The results can be viewed/analysed as if the data was real, i.e. use the v or fit_new2 commands.

Static dipole fields from a crystal structure

This program simulates longitudinal μSR data with a field distribution for static dipole fields from a crystal structure. The command is

```
Zsimxtal
```

The results can be viewed/analysed as if the data was real, i.e. use the v or fit_new2 commands.

The program will ask for an atom file which should be in the format of

```
LattA  LattB LattC
NumofAtom
Atomxpos Atomypos Atonzpos
```

Appendix A

Example files for maxent.

Transverse groupings:

Stdgrp.par

```
64 GROUPED IN 8
 NO. OF HISTOS 1X,I2  NO. OF GROUPS 1X,I2
 64 08
 GROUPING OF HISTOS : HISTO NO. 1X,I2  GROUP NO. 1X,I2
 GROUP ZERO MEANS IGNORE HISTO
 01 01
 02 01
 03 02
 04 02
 05 03
 06 03
 07 04
 08 04
 09 05
 10 05
 11 06
 12 06
 13 07
 14 07
 15 08
 16 08
 17 07
 18 07
 19 06
 20 06
 21 05
 22 05
 23 04
 24 04
 25 03
 26 03
 27 02
 28 02
 29 01
 30 01
 31 08
 32 08
 33 01
 34 01
 35 02
 36 02
 37 03
 38 03
 39 04
 40 04
 41 05
 42 05
 43 06
 44 06
 45 07
 46 07
 47 08
 48 08
 49 07
 50 07
 51 06
 52 06
 53 05
 54 05
 55 04
 56 04
 57 03
 58 03
 59 02
 60 02
 61 01
 62 01
 63 08
 64 08
```

taud.dat

```
 2.5023159E-03
  8.8687800E-03
  2.5076472E-04
  1.4882313E-02
  6.1632111E-03
  5.7040760E-03
  4.6056886E-03
  1.1012390E-04
```

phase.dat

```
59.9817
62.5343
45.6286
-101.088
-112.891
-108.478
-83.3170
```

```
34.0910
```

Longitudinal grouping

```
64 GROUPED IN 2
 NO. OF HISTOS 1X,I2  NO. OF GROUPS 1X,I2
 64 02
 GROUPING OF HISTOS : HISTO NO. 1X,I2  GROUP NO. 1X,I2
 GROUP ZERO MEANS IGNORE HISTO
 01 02
 02 02
 03 02
 04 02
 05 02
 06 02
 07 02
 08 02
 09 02
 10 02
 11 02
 12 02
 13 02
 14 02
 15 02
 16 02
 17 02
 18 02
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 34 01
 35 01
 36 01
 37 01
 38 01
 39 01
 40 01
 41 01
 42 01
 43 01
 44 01
 45 01
 46 01
 47 01
 48 01
 49 01
 50 01
 51 01
 52 01
 53 01
 54 01
 55 01
 56 01
 57 01
 58 01
 59 01
 60 01
 61 01
 62 01
 63 01
 64 01
```

taud.dat

```
0.00250232
0.00886878
```

phase.dat

```
-78.1690
117.215
```