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Data formats and analysis codes – new software for μSR

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Abstract

Originally investigated as a candidate common data format, NeXus was an easy choice when ISIS developed the present PC-based acquisition system. After over ten years of use there was a clear need to revisit the original instrument definition to improve utility, and this work is discussed in the paper. Using NeXus has opened up the possibility of accessing analysis codes developed by the wider scientific community. The application of Mantid for analysingmuon data is particularly interesting, as this offers the muon community access to an analysis framework that is attracting broad international support. Recently, we have worked with the Mantid development team to program an interface for manipulatingmuon data that has confirmed the platform as an ideal tool for μSR analysis.

Keywords: μSR; data formats; data analysis; software;

1. Introduction

Data formats and analysis codes have long been a subject of debate amongst the muon community. A conference round table discussion lead by Risemanin 1999 [1] considered the advantages of the facilities moving to a common data format, while at the same meeting Pratt [2] introduced a new analysis program (WiMDA) with a key aim of directly reading the raw data files generated by each facility.Both had the same

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objective, enabling scientists to use a common (and well understood) analysis program across different facilities, although theintroduction of a common format might have been particularly beneficial in encouraging collaborative software development and the sharing of resources.However, a common data format has never emerged, and WiMDA remains as perhaps the closest the community has come to having a common analysis program.

During discussions [1], the NeXus data format[3] emerged as a candidate common format, and subsequent work at ISIS lead to the development of an Instrument Definition for muon instruments together with a set of tools for converting the existing ISIS binary data files [4].A subsequent move away from VMS to a Windows PC-based data acquisition system left ISIS muons needing a new data format and NeXus was an easy choice. To date, over 65000 NeXus fileshave been written using the original Instrument Definition published in [4]; however, it gradually become clear that a major revision was required and key aspects of this work are discussed in Section 2.

Despite ISIS being the only muon source currently using NeXus, the advantages of basing a data format on a recognized standard have become very apparent as the facility has been able to make use of NeXus or Hierarchical Data Format (HDF) [5] aware code developed by the wider community. BothHDFView [5] and OpenGenie [6] have come into regular use for inspecting and processing data, and there are many other programs that are able to read HDF files (e.g. MathWorksMatlab and WolframMathematica). More recently, however, the Mantid analysis framework [7] has gained widespread support in the neutron community, and work (discussed in Section 3) has demonstrated this to be an ideal platform for the analysis of muon data.

2. Developing the NeXus Instrument Definition

The need for a revision of the original Instrument Definition arosebothto provide a definition better able to adapt to the wide range of specialist muon experiments that now run at ISIS and also to better satisfy the requirements of the other muon sources. The proposed revision can be read at www.nexusformat.org/Muon_Time_Differential, and discussions are continuing with the NeXus International Advisory Committee regarding ratification. Key elements of the revised Definition include: better support for multi-period data for experiments involving pulsed stimuli; improved metadata; improved support for including diagnostic information and guidance for extending the definition.Data access routines can discover the version of the definition used to write the file and offer seamless access to the data.

Multi-period data acquisition is frequently used at ISIS while running experiments involving one or more pulsed stimulus(such as radio frequency, electric field, laser, etc). By interleaving acquisition periods with and without the stimulus a proper comparison can be made, with any drift associated with the experimental apparatus or muon beam removed. The Instrument Definition now specifies the data to be held as a rank 3 array with labels on the period axis properly describing the combination of stimuli applied during a particular acquisition period. In revising the definition the opportunity has been taken to define fields to include a comprehensive range of metadata. As an example, entries are defined to provide a complete description of the beamline elements, including geometric data and logged values of working currents and voltages. Sufficient information is included to allow simulation of the beam parameters using one of the standard beam transport programs such as TURTLE. The scope of the metadata extends to providing improved diagnostic information to help, retrospectively,with understanding the nature of faults and whether they affected data quality. Comprehensive sample environment logs and information as to the progress of data acquisition are examples of data typically included. Not all metadata will be appropriate to each experiment or facility, but by standardising the entry names read subroutines will easily be able to discover the information if it is available in the file. Finally, creating a Definition that encompasses all possible experiment scenarios at all facilities is probably impossible, and therefore the documentation includes guidelines as to how to extend the Definition to include new information – this is a key advantage of using the NeXus API that permits extensible data files that can be augmented by each facility without compromising general readability.

3. Data analysis using Mantid

The development of Mantid[7] offers the muon community access to an analysis framework that is attracting broad international support (including ISIS and ILL neutron facilities in Europe, and the SNS and HFIR facilities in the US), with both ISIS and the SNS committed to using it as the primary means of data reduction. The Mantid project aims to provide an open source cross-platform framework of core routines and visualisation tools on which the various scientific communities can build analysis software specific to their needs. Recently, we have worked with the Mantid development team to program an interface for analysingmuon data.

Figure 1(a) shows the muon interface running within the Mantid framework. Functionality for data access, detector grouping and data plotting is provided on a tabbed panel, together with an ability to setup preferences for interacting with the interface. Within Mantid raw and processed data is held in a number of Workspaces. The interface has been designed to hide these detailsfrom the new user, providing full functionality through the interface panel; however,the more experienced user can manipulate the Workspaces directly either using in-built algorithms or through the Python scripting language to develop more advanced data processing capabilities. As an example, the figure shows data previously read through the interface being analysed using the generic Mantidfitter, supported by a library of muon-specific fit functions that have recently been coded (compiled functions may easily be added by the user). The implementation of curve fitting within the muon interface is well advanced; however, this serves to illustrate the flexibility offered by the framework. The Mantidframework also offers functions to supportboth data analysis and instrument diagnostics, enabling the user to work entirely using a single software package. Mantid is intended to provide a complete solution for data analysis, replacing much of the functionality available in popular PC applications such as OriginLabs Origin. To this end, Figure 1(b) shows model fits of the Arrhenius equation applied to results obtained from previous curve fitting. Figure 1(c) demonstrates the capability for displaying diagnostic information by visualizing the EMU instrument detector array and the counts associated with each scintillating element. This interface is also useful for creating complex detector groupings for experiment analysis.

4. Conclusions

The development and application of NeXus as a raw data format has served ISIS muons well. The recent evolution of the Instrument Definition has been designed to enhance flexibility and improve standardization of metadata. Importantly, data access routines can adapt to provide seamless access to the data files. The decision to base the format on a recognized standard has provided immediate access to software developed beyond the muon community. This is ofincreasing benefit as the multitude of tools and algorithms available within the Mantid framework is accessed. The combination of a recognized underlying format and a self describing Definition benefits data archiving, giving confidence in future data readability and usability. While facilities may rightly prefer to continue writing raw data files in a convenient local format, the development of NeXus as a common exchange format would appearto offer significant benefits to the muon community.

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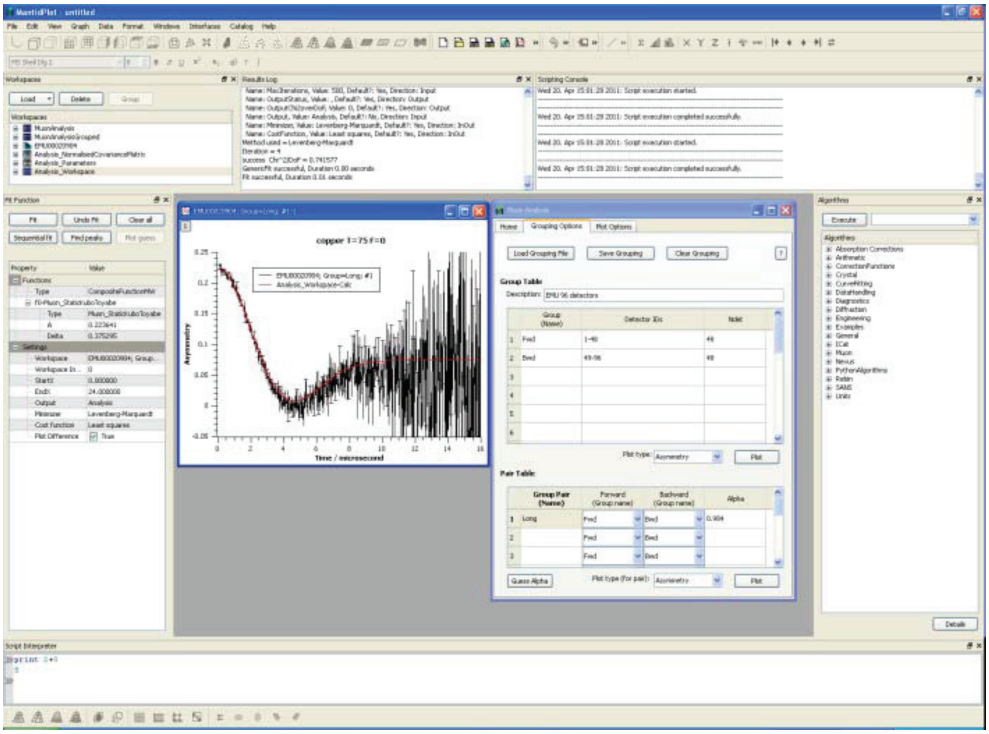
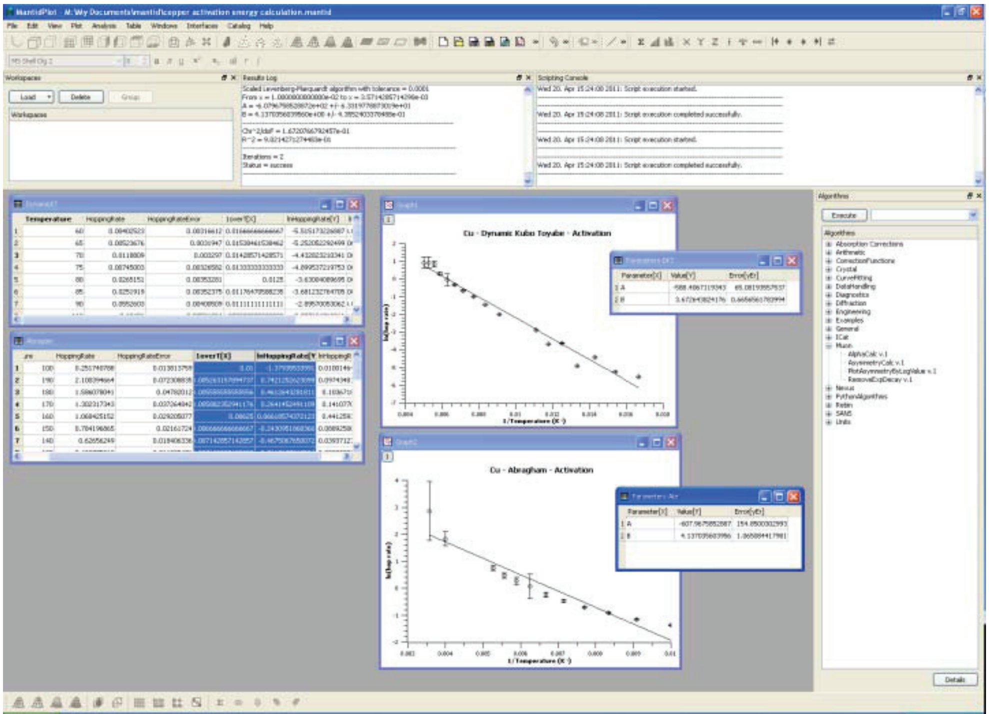
[7] See www.mantidproject.org

a)


MantidPlot - untitled
copper T=75 F=0
Time / microsecond
Asymmetry
Group Table
Pair Table

b)


Cu - Dynamic Kubo Toyabe - Activation
Cu - Abragham - Activation
1/Temperature (K⁻¹)

c)

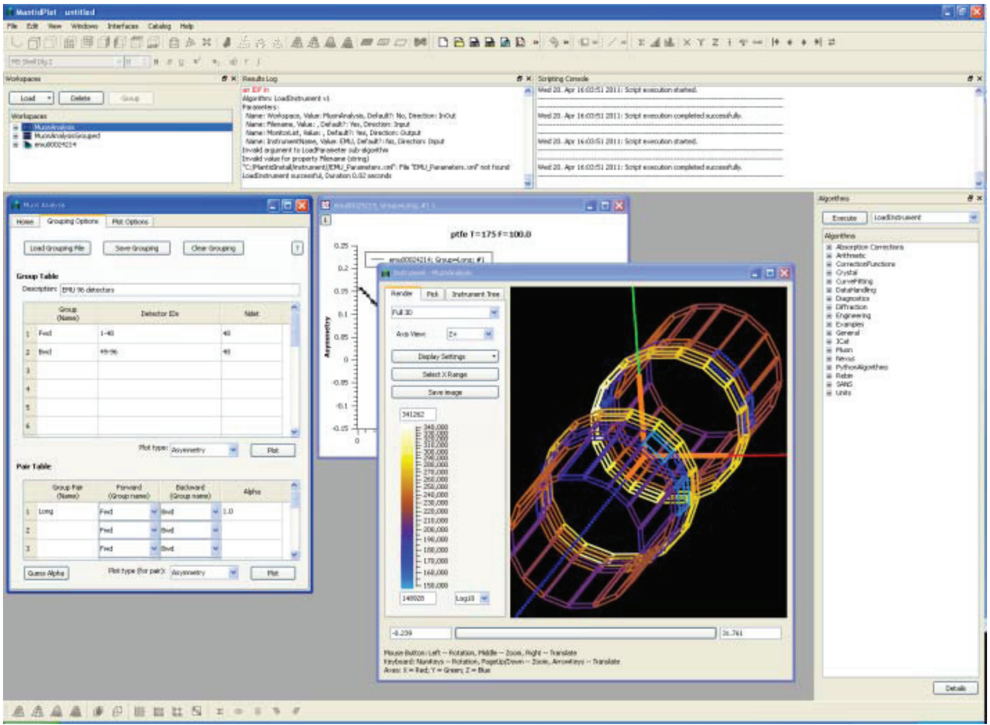


Figure 1: Screen shots of the Mantid analysis framework showing (a) data reduction and curve fitting, (b) data analysis and (c) instrument visualisation.