musrfit: a free platform-independent framework for μSR data analysis

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Abstract

A free data-analysis framework for μSR has been developed. musrfit is fully written in C++, is running under GNU/Linux, Mac OS X, as well as Microsoft Windows, and is distributed under the terms of the GNU GPL. It is based on the CERN ROOT framework and is utilizing the Minuit2 optimization routines for fitting. It consists of a set of programmes allowing the user to analyze and visualize the data. The fitting process is controlled by an ASCII-input file with an extended syntax. A dedicated text editor is helping the user to create and handle these files in an efficient way, execute the fitting, show the data, get online help, and so on. A versatile tool for the generation of new input files and the extraction of fit parameters is provided as well. musrfit facilitates a plugin mechanism allowing to invoke user-defined functions. Hence, the functionality of the framework can be extended with a minimal amount of overhead for the user. Currently, musrfit can read the following facility raw-data files: PSI-BIN, MDU (PSI), ROOT (LEM/PSI), WKM (outdated ASCII format), MUD (TRIUMF), NeXus (ISIS).

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1. Introduction

Currently, various data-analysis tools for analyzing muon-spin-rotation (μSR) data are available, however, the situation is unsatisfactory for different reasons. Most of these programmes are limited to a single platform, e.g. Microsoft Windows, others are not maintained anymore, and some of them are not free software. Another problem arising from this situation is that more elaborate modelling is almost impossible from within the current frameworks and hence, the users are forced to write their own code. This was especially true for low-energy μSR (LE-μSR) where often the μ+ stopping distribution has to be taken into account in the analysis. Therefore, we started to develop a free data-analysis framework for μSR, called musrfit, which should overcome the problems described.

From the points raised, the design criteria were: (i) musrfit has to be free software according to the GNU licenses [1], and hence available to everyone. (ii) It should be transparent and user-friendly, e.g. a clear and complete online documentation should be available. (iii) Extensions to the basic framework should be possible on the user level. (iv) musrfit should be able to read all currently used μSR-data-file formats directly. (v) Data-visualization and fit-parameter tools should be available. (vi) The maintainability should be warranted.

In order to fulfil all these requirements we decided to build up on the ROOT framework [2] developed and maintained at CERN and heavily used in particle physics as well as other fields of physics and engineering. The ROOT
framework is a collection of C++ libraries together with a C++ macro interpreter. It provides graphical-user-interface tools and contains the Minuit/Minuit2 optimization routines [3]. For us it is a "natural" choice since the ROOT framework is already part of the μSR-data-acquisition systems at PSI. musrfit consists of a collection of C++ classes [4] which can be used either directly using the ROOT macro capabilities, or—probably simpler for most of the users—can be accessed via some user-friendly programmes, provided within the musrfit suite described in the next section.

2. The musrfit suite

The analysis of μSR data using the musrfit suite is controlled by text files with the extension m sr ("m sr files"). These human-readable files contain all information needed to fit a model function to the μSR data: the fit parameters, the definition of the model, some details on the relevant μSR data files, and the fitting routines to be used. Moreover, information used for the graphical presentation of the data and fits, such as plot ranges and parameters for Fourier transforms are stored in the m sr files as well. These m sr files are also used as a protocol of the fit results. A detailed explanation of the structure and syntax of the m sr files can be found in Ref. [5]. In the following, only a basic overview of the different programmes shall be given.

2.1. musrfit—fitting a model

After musrfit is called to fit a model it analyzes the respective m sr file and reads in all specified data files. Successively, the fit is performed and the resulting parameters are written to a m log file which also complies with the m sr file structure. Additionally, the covariance matrix and the correlation coefficients of the free fit parameters as determined by Minuit2 are saved as ASCII and binary ROOT files. In a final step, the m sr and m log files are swapped so that the m sr file contains the updated parameter values while the m log file holds a copy of the parameter set used as input to musrfit. This procedure is summarized in Fig. 1. Currently, musrfit supports χ² minimization and log-likelihood maximization.

![Figure 1: General file flow during a fit using musrfit.](image)

2.2. musrvie w—graphical presentation

The analyzed data and the model functions can be visualized using the programme musrvie w. Like the actions of musrfit also the initial plotting frame of musrvie w is controlled by the m sr file. For example, it can be specified which data should be drawn in which range; if more than one set of data should be drawn it can be chosen if they should appear in a single canvas or in separate ones, and so on. Since the plotting routines are based on ROOT as well, the initially drawn graphs can be easily modified using conventional ROOT editing features—e. g. labels or arrows could be added, colours could be changed, and so on. musrvie w also offers the possibility to calculate and show the Fourier transforms of μSR time spectra. As an example, Fig. 2 depicts the time spectrum and the corresponding field distribution of a selected μSR measurement plotted by musrvie w. Despite not being shown in Fig. 2, also the difference between the analyzed data and a given model can be plotted. Furthermore, a set of keyboard shortcuts has been implemented to make the navigation more easy, e. g. pressing ‘f’ toggles between the data presentation in the
time and frequency domains, ‘d’ changes the view to the difference plot. Finally, there also exists the possibility to save the shown data and model curves in an ASCII file which facilitates the further use of these data in the user’s favourite programme.

$$\text{In-37 B} = 48.04 \text{(G)/1.49 (A)}, \text{T} = 2.83 \text{(K)}, \text{Tr} = 15.02 \text{(kV)}, \text{Sa} = -0.01 \text{(kV)}, \text{En} = 14.13 \text{(keV)}, \text{RAL-RAR} = 0.01 \text{(kV)}, \text{RAT-RAB} = 0.04 \text{(kV)}$$

Figure 2: Left panel: Time spectrum of selected $\mu$SR data plotted using musrview. Right panel: Corresponding magnetic-field distribution. In both cases, the solid lines represent the fitted model. Both graphs contain information on the fit parameters (upper right box), the model function (lower right box), the fit statistics as well as the plotted data (bottom box).

### 2.3. msr2data—advanced msr-file handling

The musrfit suite also hosts a tool called msr2data. Its main purpose is to process multiple msr files with the same parameters and to summarize the fit parameters contained in the msr files either in a TRIUMF DB file [6] or a column ASCII file. Moreover, msr2data can be used to generate from a template new msr files and even a “global” msr file for various runs sharing a subset of common parameters; for details on the “global” msr-file handling refer to Ref. [5].

Figure 3(a) shows schematically the parameter extraction from different msr files. msr2data is provided with a list of runs to be processed; optionally, external parameters which should be included in the resulting parameter file can
be specified for each of the runs. Also optionally, parameters potentially stored in the \( \mu \text{SR} \) data files (temperature, applied magnetic field, and so on) can be asked to be included. \texttt{msr2data} then reads the \texttt{msr} files for all given runs and adds all the parameter information to a parameter file. Figure 3(b) illustrates the \texttt{msr}-file generation using a template—essentially, new \texttt{msr} files are created by substituting the run number in the template.

It is possible as well to combine the above described actions: a template can be used to create new \texttt{msr} files for a list of runs, these files in turn are processed by \texttt{musrfit}, and finally the parameters of each of the files are summarized automatically in a parameter file. A detailed description of all possible options can be found in Ref. [5].

2.4. \texttt{musredit/musrgui}—editing \texttt{msr} files

Even though the \texttt{msr} files can naturally be edited with any text editor and the various programmes of the \texttt{musrfit} suite can be called from the command line, with \texttt{musredit/musrgui} dedicated text editors which also serve as frontends for the \texttt{musrfit} framework are provided. These are specifically intended to help the user handle \texttt{msr} files. Principally, \texttt{musredit} and \texttt{musrgui} have the same capabilities, however, they are based on different versions of Qt [7]: \texttt{musrgui}—Qt 3, \texttt{musredit}—Qt 4.6 or newer. Both programmes feature basic editor functions as well as interfaces to \texttt{musrfit} and are documented in Ref. [5]. A screenshot of \texttt{musredit} indicating the most important \texttt{musrfit} features accessible through the editor is shown in Fig. 4.

![Screenshot of a musredit window. The most important musrfit features are highlighted.](image_url)

2.5. User-defined functions

Additionally to providing a set of pre-defined muon-spin-polarization functions, the \texttt{musrfit} suite facilitates a plug-in mechanism allowing it to invoke user-defined functions implemented in C++ classes [5]. Hence, the functionality of the programmes can be extended with a minimal amount of overhead for the user. For example, for the analysis of LE-\( \mu \text{SR} \) data it is sometimes desirable to take into account the muon stopping distribution in the calculation of the depolarization function—the plug-in mechanism offers a possibility to do so. A couple of such add-on modules are already available together with \texttt{musrfit}, e.g. for modelling data obtained from superconductors which exhibit local [8] or nonlocal [9] Meissner screening of an applied magnetic field below their surfaces. It should be noted as well, that the so-defined plug-in classes are of course not limited to the use within \texttt{musrfit}; for instance, one could think about reusing them in other programmes or \textsc{ROOT} macros.
2.6. any2many—a “universal” μSR-data-file converter

The musrfit suite reads the currently available μSR data files without any conversion necessary. However, users might favour their own analysis software but have difficulties with all the different μSR facility data-file formats. Hence, the small helper programme any2many is included in the musrfit suite which allows virtually all possible conversions from one format into another, including ASCII output.

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