

musrfit: a free platform-independent framework for μ SR data analysis

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Abstract

A free data-analysis framework for μ SR 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 Currently, `musrfit` can read the following facility raw-data files: PSI-BIN, MDU (PSI), ROOT (LEM/PSI), WKM (outdated ASCII format), MUD (TRIUMF), NeXus (ISIS).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 (μ SR) 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 μ SR (LE- μ SR) 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 μ SR, 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 μ SR-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

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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 μ SR-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 μ SR data using the `musrfit` suite is controlled by text files with the extension `msr` (“`msr` files”). These human-readable files contain all information needed to fit a model function to the μ SR data: the fit parameters, the definition of the model, some details on the relevant μ SR 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 `msr` files as well. These `msr` files are also used as a protocol of the fit results. A detailed explanation of the structure and syntax of the `msr` 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 `msr` file and reads in all specified data files. Successively, the fit is performed and the resulting parameters are written to a `mlog` file which also complies with the `msr` 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 `msr` and `mlog` files are swapped so that the `msr` file contains the updated parameter values while the `mlog` file holds a copy of the parameter set used as input to `musrfit`. This procedure is summarized in Fig. 1. Currently, `musrfit` supports χ^2 minimization and log-likelihood maximization.

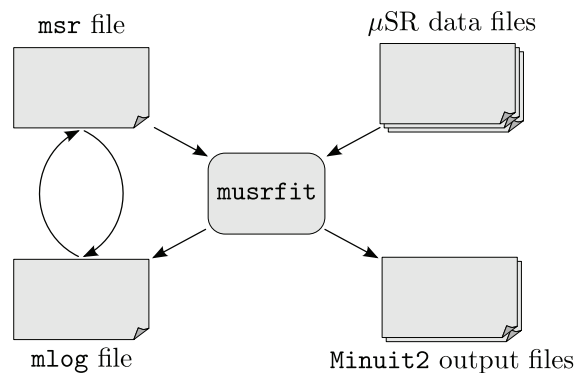


Figure 1: General file flow during a fit using `musrfit`.

2.2. `musrview`—graphical presentation

The analyzed data and the model functions can be visualized using the programme `musrview`. Like the actions of `musrfit` also the initial plotting frame of `musrview` is controlled by the `msr` 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. `musrview` also offers the possibility to calculate and show the Fourier transforms of μ SR time spectra. As an example, Fig. 2 depicts the time spectrum and the corresponding field distribution of a selected μ SR measurement plotted by `musrview`. 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.

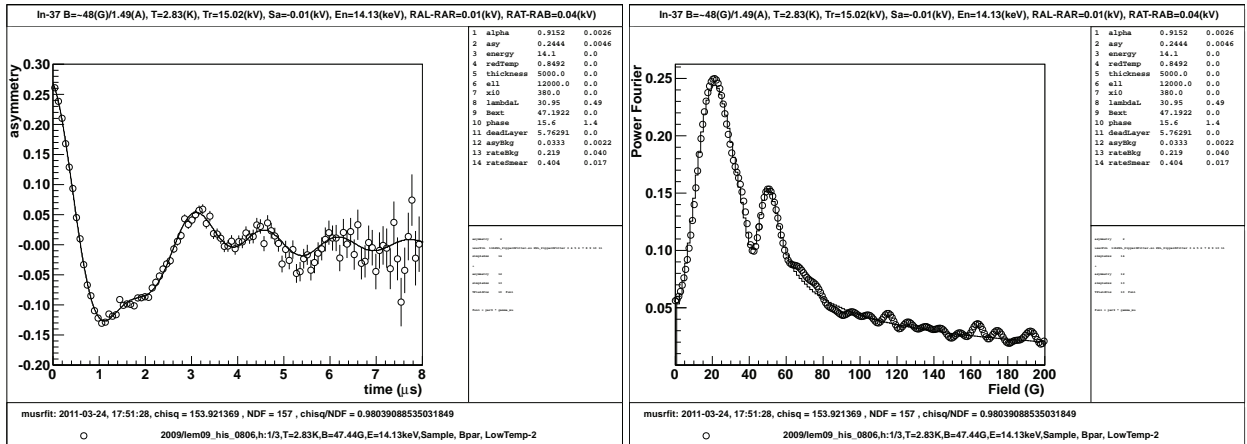


Figure 2: *Left panel:* Time spectrum of selected μ SR data plotted using *msrview*. *Right panel:* Corresponding magnetic-field distribution. In both cases, the solid lines represent the fitted model. Both graphs contain information on the fit parameters (upper right box), the model function (lower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

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

The *msrfit* 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].

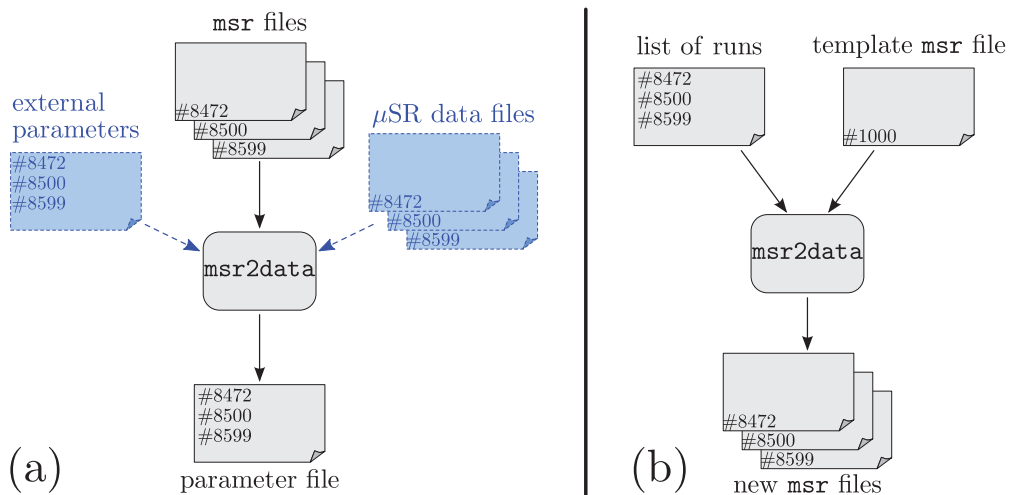


Figure 3: (a) *msr2data* used for extracting fit parameters from a list of *msr* files and summarizing them in a parameter file. The files sketched in blue with broken frames can be specified optionally. (b) *msr2data* used for generating new *msr* files from a template.

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 μ SR data files (temperature, applied magnetic field, and so on) can be asked to be included. `msr2data` then reads the `msr` files for all given runs and adds all the parameter information to a parameter file. Figure 3(b) illustrates the `msr`-file generation using a template—essentially, new `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 `msr` files for a list of runs, these files in turn are processed by `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. `musredit/musrgui`—editing `msr` files

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

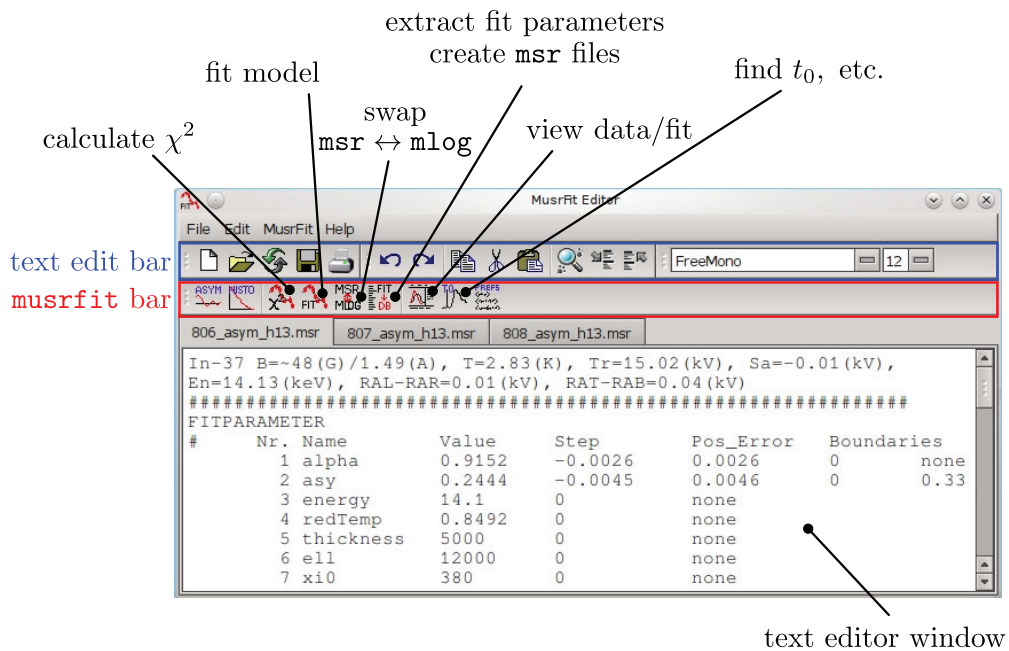


Figure 4: Screenshot of a `musredit` window. The most important `musrfit` features are highlighted.

2.5. User-defined functions

Additionally to providing a set of pre-defined muon-spin-polarization functions, the `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- μ 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 `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 `musrfit`; for instance, one could think about reusing them in other programmes or ROOT macros.

2.6. any2many—a “universal” μ SR-data-file converter

The `musrfit` suite reads the currently available μ SR data files without any conversion necessary. However, users might favour their own analysis software but have difficulties with all the different μ SR 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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