Simulation of μSR data analysis

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October 2023

The ambition of this project relies on what can be achieved in terms of the understanding of a system (using the muSR technique) when the simulation is tuned to fit the experimental data. Here, WiMDA is combined with MuSpin-Sim in constant communication via sockets using the atomic variables of the simulation as fitting parameters. As a result, our simulated system is optimized to represent our experimental system with the great advantage that the physical variables are recovered by the fitting process. This translates to possessing a more complete set of information and understanding of the system probed by the muon.

1 Backgroound

To fully appreciate the interaction between simulation and experimental analysis it is crucial to understand both systems, their limitation, and their mathematical description. μSR experiment makes use of the decay of the muon planted in a system and the Larmor procession that this particle experiences in the presence of a magnetic field (originated internally or externally in the system). It is important to note that the emission of the positron on the decay of the muon is asymmetric presenting a preferentially aligning with the spin of the muon.

In terms of measurements let's consider two detectors forward and backward expressing their position relative to the sample. The is a difference between the positron counts on the forward and backward detectors due to the asymmetry figure 1.

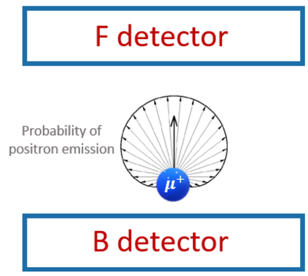

Figure 1: μSR set up representing the forward and backward detector and the asymmetry of the positron on the muon decay

Subsequent to the clarification above it is necessary to formally engage in this physical system. The asymmetry can be defined as the quotient of the difference between forward and backward counts and their sum expressed in equation 1.

$$A(t) = \frac{F - \alpha B}{F + \alpha B} \tag{1}$$

This same quantity is also described as the product between a constant and the polarization function as described in 2. The polarization function is the evolution of the average muon spin projected along an axis α which is formally defined as the trace of the product of the density function and the Pauli Matrix on a specific axis α demonstrated on the first equation of the set 3).

$$A(t) = a_0 P_z(t) \tag{2}$$

$$\begin{cases} P_a = Tr(\rho(t)\sigma^a) \\ \rho(t) = \hat{u}(t)\rho(0)\hat{u}^{\dagger}(t) \\ \hat{u}(t) = e^{-\frac{i\hat{H}t}{\hbar}} \end{cases} \tag{3}$$

Let's take into account the set of equations 3 where the density function is defined using Schrodinger's picture and the unitary operator expressing. This serves the purpose to enhance that once the Hamiltonian is characterized mathematically we can retrieve the asymmetry $A(t)$.

The simulation is described using the Hamiltonian and the asymmetry data provided by the simulation is calculated from it. The experimental data on the other hand is retrieved by directly measuring the asymmetry. It is this very conclusion at the heart of our ambition to use simulation to further understand the system being probed by the muon.

2 Method

For the method, it was very important to conserve established scripts and work with them as closely as possible. In WiMDA the 'Analyse' script received new functions to read and interpret the simulation data. To the 'Oscillation' parameters 'MuSpinSim' was added associated with a button that launches the GUI represented in figure ??. The server is activated and the client confirms the connection. Independently, the simulation can run and the experimental data loaded as usual according to the user instructions. With the sockets communication, the stream is constantly available to read or send any messages. The flowchart below figure ?? showcases the architecture used in the implementation of the process described above. The intended usage of the software starts with the user, who launches WiMDA and loads the experiential data with a good understanding of the system then sets the initial parameters of the MuSpinSim, and selects the ones to be fitted against.

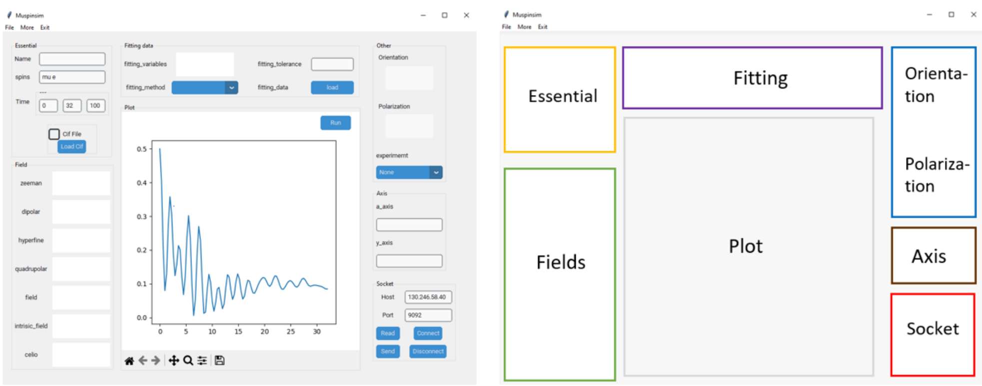

Figure 2: Muspinsim GUI supporting cif files and moderating the sever on the socket communication. The same GUI in the right where the design encompasses the possible category of variables in MuSpinSim including a plot section to visualize the output data after running the simulation.

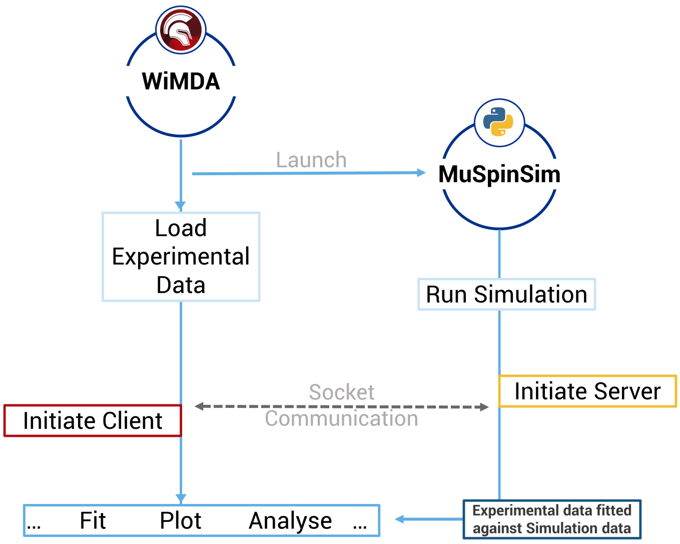

Figure 3: Flowchart of the code structure emphasizing the system's encompassing the interaction between the experimental data analysed in WiMDA and the Simulation data generated on MuSpinSim. Note that MuSpinSim is launched from WiMDA, however, the communication between the programs are made by socket communication.

3 Progress

As this project is ongoing and the aim described before is still to be archived, instead of results or future the progress will be discussed. The server-client communication between MuSpinSim and WiMDA has been established and with this, the simulation data has been plotted and fitted against the experimental one in WiMDA 4.

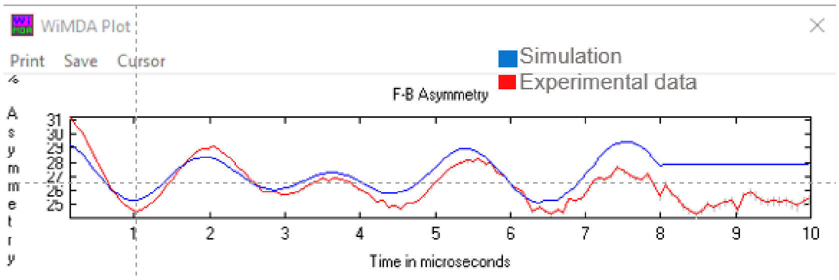

Figure 4: Simulation and experimental data plotted (and fitted) in WiMDA. Experimental data obtained from MuSR probing CaF2

The next step is to fit using any of the simulation variables as fitting parameters to obtain a simulation variable that minimizes the square difference between the two data sets (simulation and experimental). With this in mind, the dipolar interaction will be varied and fitted. This will consist of varying only one axis (for example) and it will be necessary to automate the fitting and varying of them between two different softwares. The challenges faced here are numerous the structure of the code already established and working around it, the limited time, and the ways it can escape my scope of competency.

The immediate next stages of the project addressed the structure of the fitting parameters in WiMDA. Automation of the varying parameters and regenerating simulation data accordingly.

References

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[5] J. M. Wilkinson and S. J. Blundell *Information and Decoherence in a Muon-Fluorine Coupled System* DOI: 10.1103/PhysRevLett.125.087201