Philipp MALIN

Graphical User Interface and Data Handling in for a Nuclear Quadrupole Resonance Software Defined Radio Spectrometer

Bachelor's Thesis
to achieve the university degree of
Bachelor of Science
Bachelors's degree programme: Biomedical Engineering

submitted to

Graz University of Technology

Supervisor
Hermann Scharfetter Ao.Univ.-Prof. Dipl.-Ing. Dr. techn.

Institute of Biomedical Imaging
Head: Martin Uecker Univ.-Prof. Dipl.-Phys. Dr. rer. nat.

Graz, March 2022

Affidavit

I declare that I have authored this thesis independently, that I have not used other than the declared sources/resources, and that I have explicitly indicated all material which has been quoted either literally or by content from the sources used. The text document uploaded to TUGRAZonline is identical to the present bachelor's thesis.

Date	Signature

Eidesstattliche Erklärung

Ich erkläre an Eides statt, dass ich die vorliegende Arbeit selbstständig verfasst, andere als die angegebenen Quellen/Hilfsmittel nicht benutzt, und die den benutzten Quellen wörtlich und inhaltlich entnommenen Stellen als solche kenntlich gemacht habe. Das in TUGRAZonline hochgeladene Textdokument ist mit der vorliegenden Bachelorarbeit identisch.

Datum	Unterschrift

Abstract

Running a Software Defined Radio (SDR), which is used for the Nuclear Quadrupole Resonance (NQR) spectroscopy an intuitive gaphical user interface (GUI) and a automatic data handling system is essential for a efficient testing and measuring. A automated structured overview minimises the risk of experiment errors an the loss of important acquired data. Additionally a Sequence generator was implemented with the ability to dynamic select, from one pulse up to ten pulses. The GUI is able to be used to set the represented Phases from $\varphi_{min} = 0$ up till $\varphi_{max} = 2\pi$ for every pulse and all the hardware specific parameters.
As one of the requirement was that the Software will be used for a lab exercise with students, it should include warning statements if destructive settings are saved to be run on the SDR. On the other hand for experienced user it has the ability to load standardised .cfg files from the system.

Contents

List of Figures

1 Introduction

Nuclear Quadrupole Resonance (NQR) is a technique to analyse samples in solid state with absence of a external magnetic field like in nuclear magnetic resonance (NMR). With a radio frequency pulse the samples gets excited. For this setup a software defined radio (SDR) [4] is used to generate the pulses. If the sample gets excited at its resonance frequency a gaugeable signal gets back induced into the coil. Based on an SDR based NMR system, leading developments and publications were made by Doll [1]. The system was further adopted by Kaltenleiter[2] in the institute of Biomedical Imaging at the TU Graz for NQR spectroscopy.

Single frequency measurements and broadband measurements are made in the very high frequency (VHF) range. [3]

The task of the this thesis was to implement an intuitive GUI for this existing setup with the SDR in object oriented python script. Extending, also a sequence generator was implemented for a fast and easy setting of the sequence parameters. All Parameters for a standard sequences are predefined, additionally for extended options, there is the option to set the own sequence in the GUI. In the background data handling with the SDR is done. Results are immediately presented in the main window. Rounding the system off, a file handler for structured saving of all data acquisition is implemented.

2 Methods

All the software is available on the Git repository, additionally there is also the description of the complete software in the wiki section. The GUI was written is Python 3.9.7 with the module Tkinter
The software is developed to run on a Linux machine, but a limited number of features also run on a windows system. This can be used, for example, to generate sequence files in advance or reload measurement data for reevaluation.

2.1 Download links

Repository:
http://www.github.com/OE9NAT/bacharbeit

Wiki:
http://www.github.com/OE9NAT/bacharbeit/wiki

3 Results

3.1 What it can do

The Software was designed to handle user input on a structured designed graphical user interface. A set of standard sequences are pre-configured and can be selected from the main window, but there is also the option to generate one for itself. It will update the set sequence as an info in the main window. From the main window after selecting the data, if the resonant circuit is tuned, the measurement can be started with the specific sample.

As the LimeSDR is a duplex capable software defined radio, starting with the sequence the signal logging will start.However, boundary conditions must be set beforehand so that the recorded signal is cut to a desired size. The cut should be chosen sow that the re-induced signal will be completely enfold in the recording. This information will be plotted and saved in the predefined file structure for further analyses.

3.2 What can it do not sow well

Repetitive tuning and matching is done manually for measuring ever frequency. As this is very tedious task and can manually only be done to a certain accuracy in a given time an automatic system needs to be developed. As this feature is foreseen, arrangements have been made to easily implement this in the future.
On the other hand after the acquire, the information from the last run is shown in the plotter on the main window. The basic plotter should give a short overview, but for an additional analyses cornerstone have bin set to developed a more detailed plotter.
For broad band frequency measurements safety precaution have to be made. Now for a new measurement for the ascending frequency the old result will not be overwritten but will be appended. This type of acquire is special as this will fill in the plot from the starting frequency to the end frequency.
Error handling is only checked for plausibility. It is mainly done throw structured logical entry of the Parameters. Before saving all not pre-set values will be checked if they are in the right format.

3.3 What can it not do

Fly to the moon.
It has the Potent ial to be more intuitive from setting the Parameters. While doing the experiment it can be more obvious to put some settings and Parameters in different locations.
Error handling can be implemented for more cases. Parameters are not check for hardware specific limitations. Additional it could also be an option to do an automatic correction of Parameters witch are set incorrect.

3.4 System evaluation

The test sequence was an FID with an offset 3000 samples, pulse length of 3 µsec, start acquisition 22.5 µs, stop acquisition 22.5 µs. The result are shown in the plot in the main window.

4 Conclusion and Future Work

4.1 Main Window

In the main window all relevant data for the experiment will be presented and set. The initial start of the system will also be run from there.

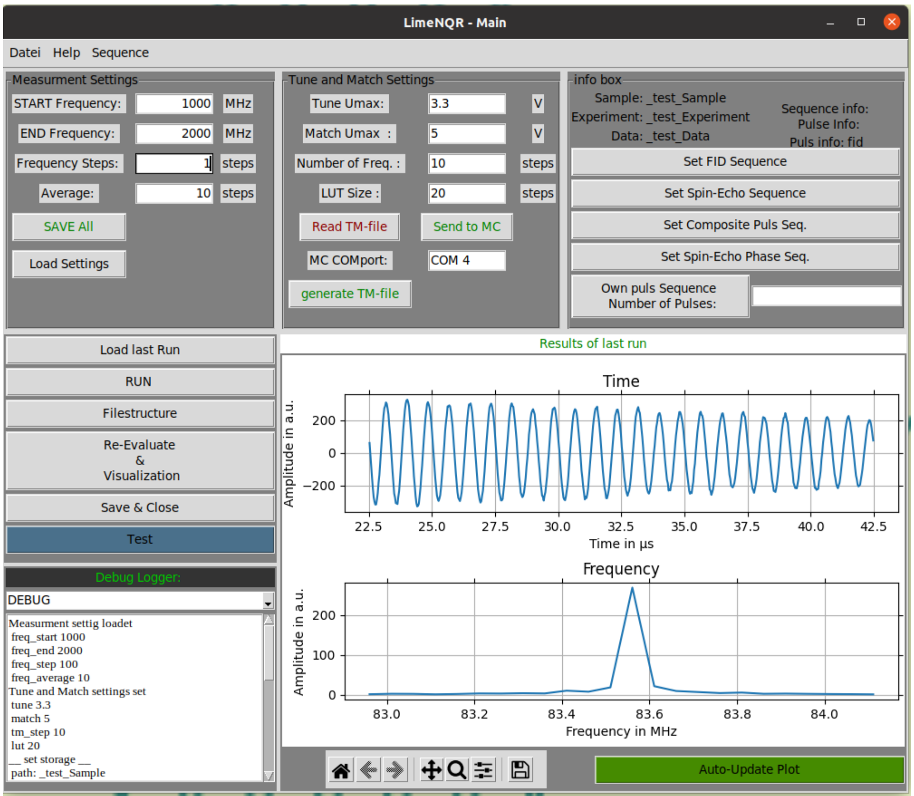

Figure 4.1: Main window, where all controls flow together

4.2 File Handle

All relevant file handling parameters can be initially set and also be changed in a later state. In this additional window at the beginning and end of every experiment comments can be added which will be logged to a .txt file.
For now it is hard-coded to save all measurement data in the folder named

Storage_vault but this can be changed very easily sow that it can also be automatically to a decentralised file handling server.

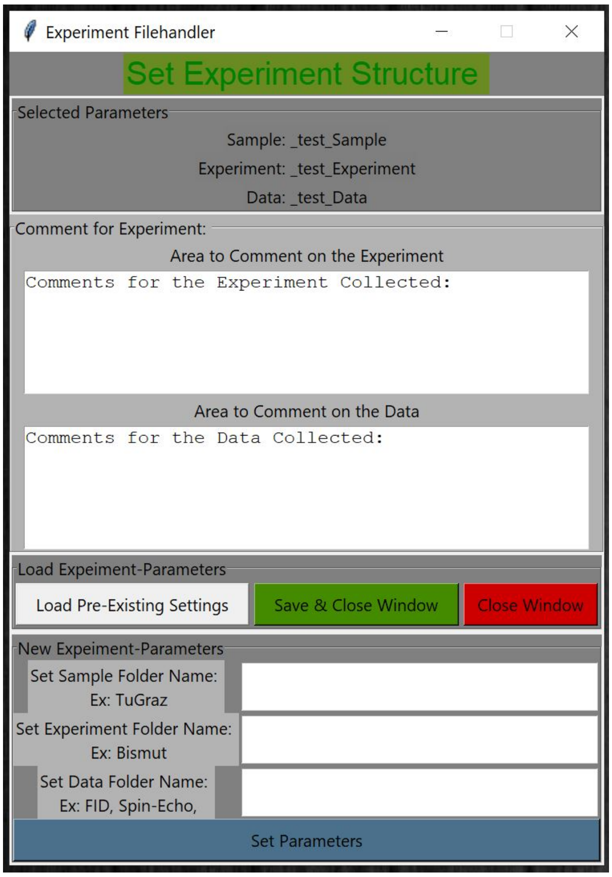

Figure 4.2: File handler window, used for editing the structure of storage

4.3 Sequence generator

All Standard sequences can be directly called from the main window. It includes the the free induction decay (FID) sequence, the Spin-Echo sequence, the Composite Pulse sequence, the Spin-Echo phase sequence and an own to be defined sequence. With the own sequence an arbitrary sequence can be generated with up to ten pulses and their respective offsets.

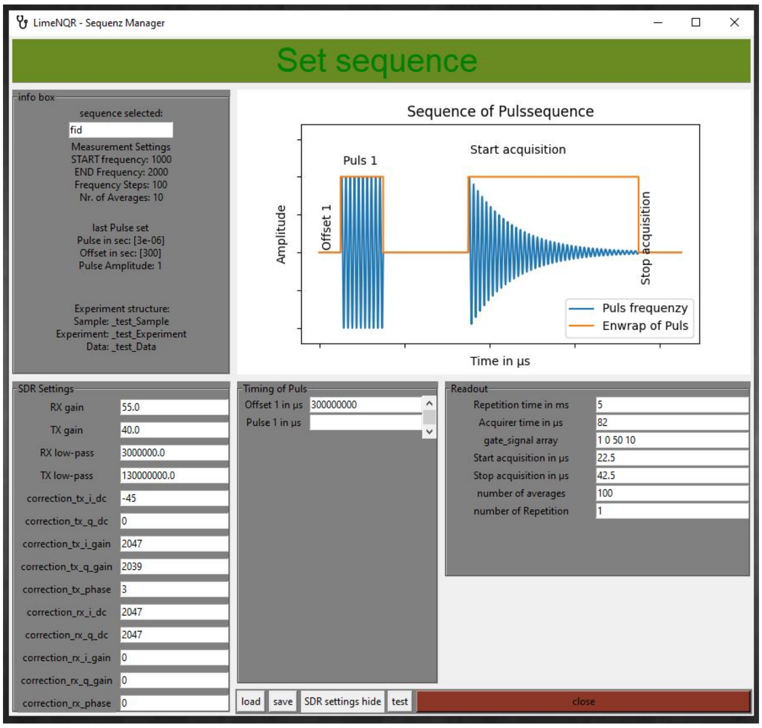

Figure 4.3: Sequence manager window, specific prepared for the FID

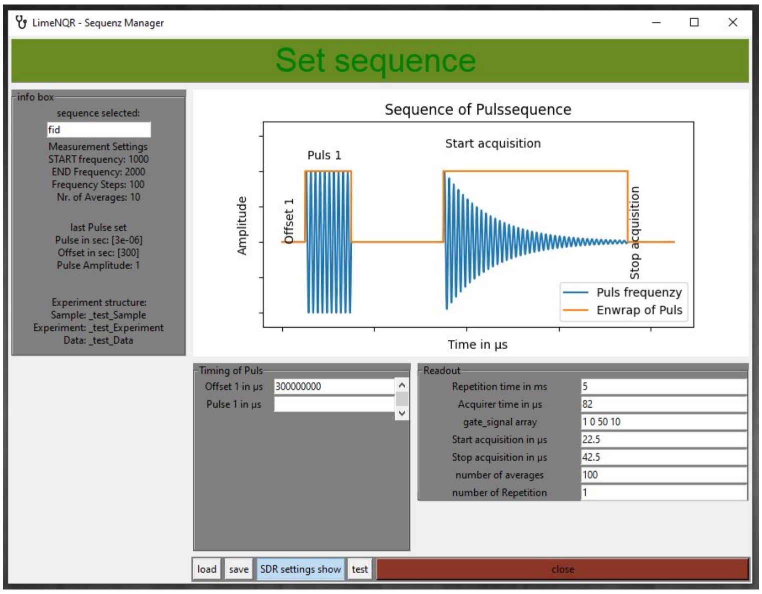

Figure 4.4: Sequence manager window, specific prepared for the FID with the addition of the hidden SDR Settings for a better overview

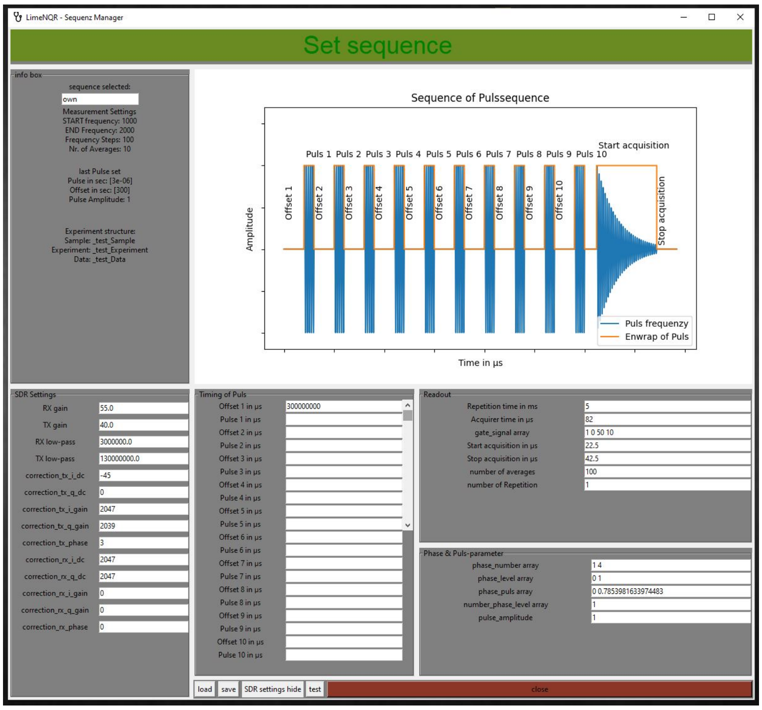

Figure 4.5: Sequence manager window, displaying the maximum number of 10 pulses and all possible set Parameter

4.4 Future

Options for expansion are numerous, as this interface is only the start of the Project of using an SDR for NQR analysis. Initially it was only a proof of concept and starting now onward with multiple improvements it will develop into a stable robust stand alone system.

Shortly after, the development on a automatic tuning and matching system, started. Manual tuning and matching is very time consuming and to set up a broad band measurement it is essential to have a certain accuracy.

A great potential lies in evaluating and comparing recorded measurements afterwards. This could look like, recorded files will be selected and loaded together into the same plot. Such options are prepared to be implemented in a later state.

The ability for a better design is always possible. For a modern design this can be done with coloring and shaping of button and ares of entry. Moreover there is also great potential in the back end handling of variables an measuring data.

4.4.1 Puls shaping

The foundation for shaped pulses were made but more implementations need to be made.

4.4.2 Re-Evaluate Plotting

This was prepared for reading saved .h5 files. When calling the window you are prompted with a file selector. This fill read in the file and plot its data. Further development needs to be made .

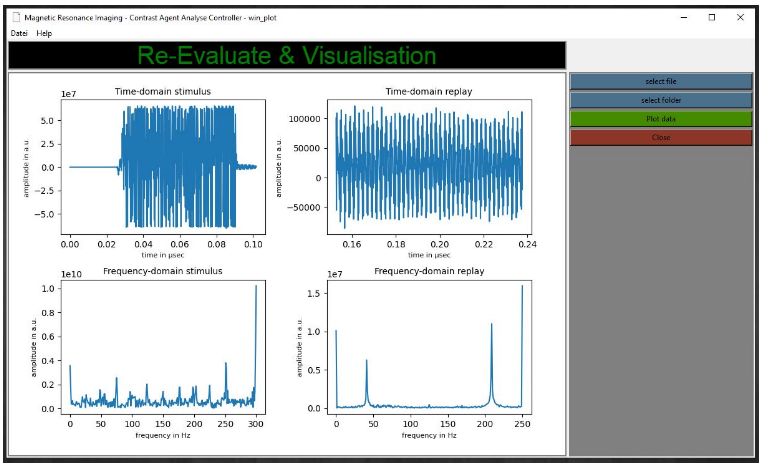

Figure 4.6: Re-Evaluate and Visualisation window, this has the potential to be developed into a visualisation and rework station for saved data. Further development is compulsory.

Bibliography

[1] Andrin Doll. Pulsed and continuous-wave magnetic resonance spectroscopy using a low-cost software-defined radio. *AIP Advances*, 2019.

[2] Lukas Kaltenleitner. Software defined radio based nuclear quadrupole resonance spectrometer. *TU Graz*, 1(1):1–155, feb 2022.

[3] Hermann Scharfetter. An electronically tuned wideband probehead for NQR spectroscopy in the VHF range. *Journal of Magnetic Resonance*, 271:90–98, oct 2016.

[4] Wikipedia. Software defined radio.