NMR Control Porting

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1 Progress

Over the course of the semester, we were able to plan out and begin implementing a port of the Igor NMR Control software (written by Prof. Gordon Jones) to Python. We started out by attempting to replicate the interface from Igor as accurately as possible using PyQt5 and QtDesigner. We were able to fully reproduce the full control panel set up from Igor with minimal modifications. There are two different files associated with this UI. The first is the QtDesigner nmr_control.ui file which can be used to easily edit the interface using QtDesigner. The second is the nmr_ui.py file which is the Python file generated via QtDesigner. Both of these could be used to launch the UI, but it is currently set up to run from the .ui file.

Once the interface was sorted out, we begun to work on the low-level communication between Python and the various instruments. This ended up being more difficult than expected, partially due to the lack of physical access to the equipment due to COVID-19. However, we were able to work through some of the basic input and outputs for the various instruments. Examples of how to do the various types of write and read instructions for analog and digital channels are included in io_examples.py.

2 Packages Used

2.1 PyVisa

PyVisa is a tool that allows Python to interface with various different instruments. Specifically, this was useful for communicating with the GPIB whenever called for in the code. The syntax is fairly straightforward and the documentation is decent.

2.2 NI-DAQmx Python

NI-DAQmx Python is the Python version of the NI-DAQmx framework and allows Python to communicate with NI instruments, specifically useful when communicating with the NI board. The syntax, while arguably simpler than it is in Igor, is somewhat hard to understand and the reference documentation leaves much to be desired.

2.3 Numpy

Numpy is an incredibly useful package for storing and manipulating arrays of data. Useful for storing waveforms and data that has been read and manipulating it.

2.4 Matplotlib

Matplotlib is a plotting library for Python that copies the functionalities of MATLAB. This could be useful for the plotting and fitting components of the NMR software.

2.5 PyQt5

PyQt5 is an architecture for easily creating application interfaces using Python. It is relatively easy to learn and there are many resources available online for help. Additionally, in my experience, it is compatible with many different operating systems.

2.6 QtDesigner

QtDesigner is a graphical editor for user interfaces (UIs) built with PyQt5. It allows the user to easily drag and drop buttons and fields without having to manually align them via code. Once the user is happy with the layout of the interface, it can be exported to either a .ui file or a .py file for use in code. I would recommend not adding your own code to this file as it will be remade any time you edit the interface, and you will lose any changes.

3 Next Steps

As the semester was coming to an end, we had begun connecting the UI buttons and fields to actual functionality at the low level. The obvious next step would be to continue doing this, following along with the Igor code as closely as possible. While many of the technical hurdles have been overcome, this is quite a large program, and translating all of the code over will likely take some time. Other hurdles that we did not have sufficient time to address were refining the timing of when the various instrument reads and writes are triggered, and plotting the various graphs associated with the scans. For the former, it may be necessary to dig into the triggering details of NI-DAQmx. For the latter, a good path would potentially be using Matplotlib, which has extensive plotting capabilities, to plot and then fit the data.

4 Package Documentation

NI-DAQmx Python Documentation
https://nidaqmx-python.readthedocs.io/en/latest/index.html
PyVisa Documentation
https://pyvisa.readthedocs.io/en/latest/api/index.html
PyQt5
https://doc.bccnsoft.com/docs/PyQt5/
Numpy
https://docs.scipy.org/doc/
Matplotlib
https://matplotlib.org/3.2.1/index.html