Current Status of Microcontroller-Based Earth-Field NMR Project

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Abstract

In this document, I outline the current condition of the project to construct a microcontroller-based apparatus to perform nuclear magnetic resonance (NMR) using the earth's magnetic field, as outlined by *Michal* [2]. The basic theory of NMR is reviewed, and the implementation of the device is explained. The project is well underway, and schematics have been created using National Instrument's Multisim software that yield SPICE simulation results in agreement with literature values. In particular, the transmitter and receiver components of the device perform in simulations as expected. I recently finished a rough draft of a printable circuit board (PCB) to hold the electrical components. Next steps include finishing the PCB design and moving on to programming the microcontroller driving the device.

Introduction

Nuclear magnetic resonance (NMR) is a useful technique for studying a variety of properties of many materials. Traditional NMR spectrometers, such as those used in medical-grade MRI's and many research settings, make use of immensely powerful superconducting magnets and operate at fields in the 1-10 T range. While operating with such large magnetic fields produces great results due to increasing the magnetization of the sample and decreasing the impact of external field inhomogeneities, these superconductors are often very expensive and for many applications the costs outweigh the benefits. We present as an alternative an NMR apparatus that uses an Arduino microcontroller and several simple circuits to drive and process NMR signals. *Michal* [2].

Michal's microcontroller apparatus has both pros and cons when compared to traditional NMR methods. First and foremost, the cost of *Michal's* entire apparatus is around $200, while a medical-grade MRI can cost in the range from $100,000 -$1,000,000. Due to few materials required, *Michal's* NMR can be constructed easily and is portable, making it ideal for use in the field. A traditional NMR that uses superconducting magnets is huge, and cannot be removed from the lab. The main downside is that using such a weak magnetic field leads to relatively low sample magnetization, and the strength of the signals produced by the relatively small spin excess cannot match that of traditional setups. This can be addressed by exposing the sample to a strong pre-polarizing field before measurements are taken. Assuming our sample is large enough and access to a pre-polarizing field is available, the benefits of *Michal's* device more than outweigh the sacrifices for many routine applications.

Theory

Much of the theory outlined below was taken from Magritek's teaching series on the principles of NMR [1]. Consider a sample containing many hydrogen nuclei in thermal and magnetic equilibrium at room temperature in the presence of an external magnetic field, B_0. Hydrogen nuclei can take on two quantum states: spin-up or spin-down, with spin-up corresponding to the high-energy state anti-parallel to B_0 and spin-down corresponding to the low-energy state parallel to B_0. At room temperature, the number of nuclei in each state is nearly equal, as thermal energy promoting entropy is much greater than magnetic energy promoting the low-energy state. But the difference in energies between the two states will lead to a slight excess of nuclei in the spin-down state, and all spins except those in excess will cancel. We can increase the proportion in the lower energy state by decreasing the temperature or by increasing the strength of B_0.

In the presence of B_0, each nucleus will precess, with each its angular momentum vector tracing a cone surrounding the field lines. The frequency of this precession is called the Larmor frequency, and is given by

$$\omega = \gamma B_0, \tag{1}$$

where γ is a property of the material known as the gyromagnetic ratio. Because for a given magnetic field strength, the Larmor frequency is fixed, the visibility of this precession for a given sample in a static magnetic field depends on the angle between its angular momentum vector and the magnetic field lines. If the angle is 0, then the precession won't be visible because rotation around the azimuthal angle won't change the direction of the angular momentum vector. If the angle is near 90°, then the precession will be at a maximum and the cone traced by the angular momentum vector will approach a perfect circle.

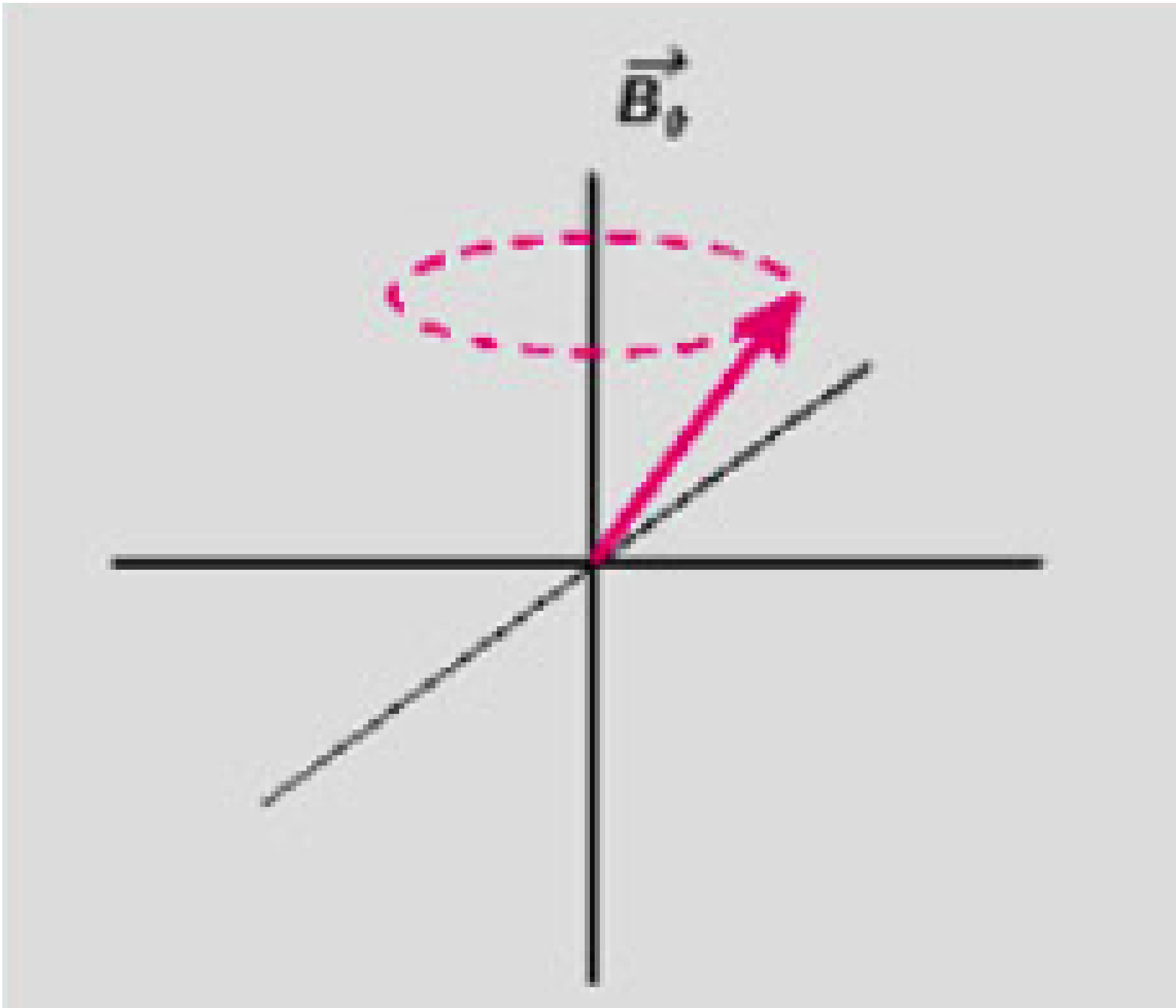

Figure 1: The radius of the circle outline by the angular momentum vector depends on its angle relative to the magnetic field.

For NMR to be effective, we want to maximize the strength of this precession. One way to do this is by increasing the magnetization of the sample by using a stronger stabilizing magnetic field, which increases the spin excess. In the case of earth-field NMR, the earth's weak magnetic field is provides only a minimal spin excess, and if the earth's magnetic field alone were used to create magnetization, the resulting signal would be very weak. To improve upon this, the sample is to be exposed to a pre-polarizing magnetic field several orders of magnitude stronger than that of the earth before each measurement for several seconds to increase magnetization.

The other technique used to increase the visibility of the precession involves keeping the angular momentum vectors of the nuclei in the sample perpendicular to the external magnetic field. This can be done by applying a second magnetic field, denoted B_1, that oscillates at the sample's Larmor frequency in the plane transverse to that of the external field. B_1 will cause those nuclei in spin excess to oscillate in the plane perpendicular to B_0, and will maximize the visibility of their precession. When B_1 is removed, the angular momentum vectors will gradually realign with B_0 through a process called relaxation.

By Faraday's Law, if we surround these oscillating nuclei with a coil of wire, the changing magnetic flux caused by the nuclei's angular momentum vectors constantly changing direction will induce an electromotive force in the coil. By measuring this voltage over time with a free induction diagram, we can get a grasp on the quantity of Hydrogen nuclei in the sample. This same coil can also be used as the source for B_1, as by running a current through it we can create a magnetic field transverse to B_0. Because the same coil can be used for both transmission and receiving, I will refer to it as the Transmission-Receiving (T/R) coil for the remainder of the paper.

So, in a single NMR measurement, we first run a large, steady current through an external coil to produce the strong pre-polarizing field. We then run a sinusoidal current through the coil to produce B_1 and align the the angular momentum vectors in the plane perpendicular to B_0, the magnetic field of the earth. Lastly, we shut off the current through the coils in order to detect any voltage induced by the sample's precession. The strength of the signal will rapidly decrease due to relaxation, so the time between transmission and receiving is essential, although switching between transmitting and receiving too fast makes the coils susceptible to self-resonance.

Sample Calculations

To put numbers to the variables being used, we will calculate the Larmor frequency of Hydrogen first in a 2T field which is a reasonable estimate for medical-grade MRI machine, and in the earth's magnetic field. The gyromagnetic ratio, γ, for Hydrogen is 42.58 MHz/T. For the 2T field,

$$\omega_{MRI} \approx (42.58 \text{ MHz/T})(2 \text{ T}) \approx 85 \text{ MHz}. \tag{2}$$

The strength of the earth's magnetic field is approximately 50 μT. So,

$$\omega_{Earth} \approx (42.58 \text{ MHz/T})(50 \times 10^{-6} \text{ T}) \approx 2129 \text{ Hz}. \tag{3}$$

First, note that the Larmor frequency for a traditional MRI is roughly five orders of magnitude greater than that of the earth. It is this low frequency that allows an earth-field NMR to be implemented by a microcontroller as simple as the Arduino, whose 16 MHz crystal oscillator is far too imprecise to drive measurements at the Larmor frequency at 2T, but is more than precise enough for the earth's.

Device

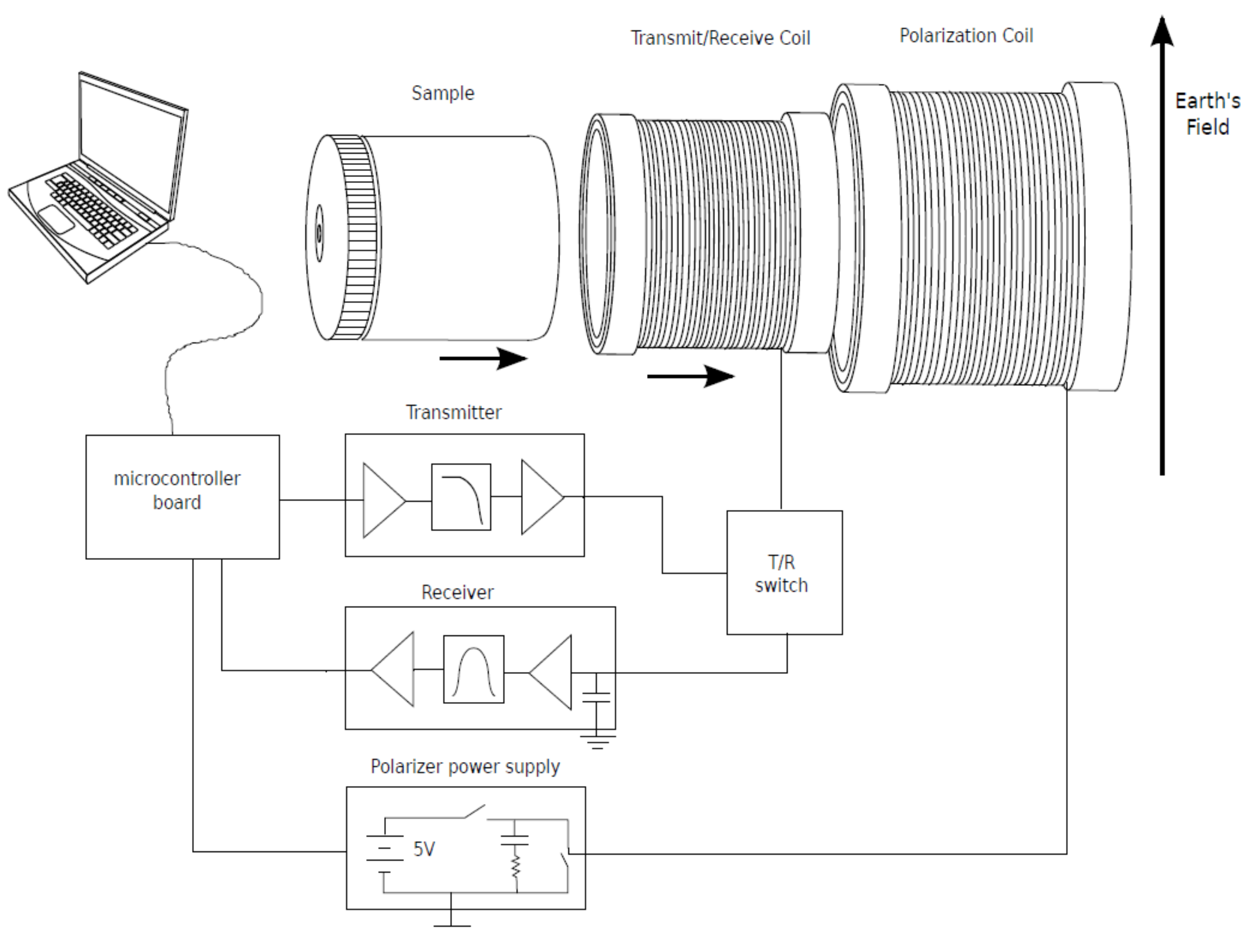

Figure 2: Approximate layout of earth-field NMR device

We are in the process of building an Arduino microcontroller-based NMR device as described by *Michal*. The device can be broken into three main components: the transmitter, the receiver, and the polarizer's power supply. I produced schematics for the transmitter and receiver, and am in the process of placing them on a PCB.

Transmitter

The transmitter's main function is to convert a +/- 5V DC signal from the Arduino to a sinusoidal signal between roughly -6 and 6 V. It accomplishes this with the use of several operational amplifiers. Because the Arduino's digital outputs only have a range between 0 and 5 V, but a 10 V range is needed, the transmitter has two digital inputs, each of which provides the DC source for one end of the waveform. The first op-amp is a subtractor, which converts the difference of these two digital inputs to a single signal. The subtractor gives us the full -5 to 5 V range required. The second op-amp is a low-pass filter, which has the effect of smoothing the DC waveform to a more analog, sinusoidal shape. The third op-amp is an amplifier, which converts the signal to the range desired to produce the proper amount of current through the T/R coils.

Receiver

The receiver's main function is to convert the voltage signal induced by NMR, which is on the order of mV, to a filtered and amplified output to be processed by the Arduino. The receiver consists of several operational amplifiers to accomplish this. The first op-amp is a band-pass filter tuned to exhibit resonance near the sample's Larmor frequency. This band-pass filter helps isolate the small NMR signal from ambient noise. The second op-amp used is an amplifier, which applies a gain of roughly 50,000 to the signal. The third op-amp is provides a DC offset of 2.5V, which places the resulting signal in the most reliable part of the Arduino's 0-5 V range, and helps the microcontroller effectively process the signal.

Other components

A set of diodes and switches connected to the Arduino's digital outputs help ensure that the device switches from outputting a voltage and driving NMR to receiving the small signal induced in the T/R without being susceptible to self-resonance. If we simply switched from powering the transmitter to powering the receiver without allowing a delay, the relatively huge magnetic fields produced by the coil during transmission would create its own signal that would be picked up by the same coils, and would significantly weaken the signal actually produced by NMR. Thus, a delay of about 10 ms is added to allow most of the transient current to decay before we start measurements. Making this delay too long, however, can lead to its own problems as the voltage induced due to the Larmor precession decays rapidly as the nuclei's angular momentum vectors realign with the earth's magnetic field. According to Michal, 10 ms is a reasonable amount of time to allow transients to decay without missing the majority of the signal.

Software Used

This project is still in its initial stages, and so far all efforts have been centered around implementing the electronics that run it. I initially used the open-source software, KiCad, to design the schematics due to KiCad's being free and accessible on any PC. After spending about a month learning how to use KiCad and drawing preliminary schematics, we discovered that not only did KiCad not provide SPICE models or PCB footprints for several of the operational amplifiers needed, but the results from SPICE simulations for even simple op-amp circuits were wildly unpredictable.

This conclusion led me to instead use National Instruments' Multisim software, which by nature of being commercial software is much more robust and has models for every component needed. I copied the schematics from *Michal* and ran simulations to test the behavior of the transmitter and receiver circuits.

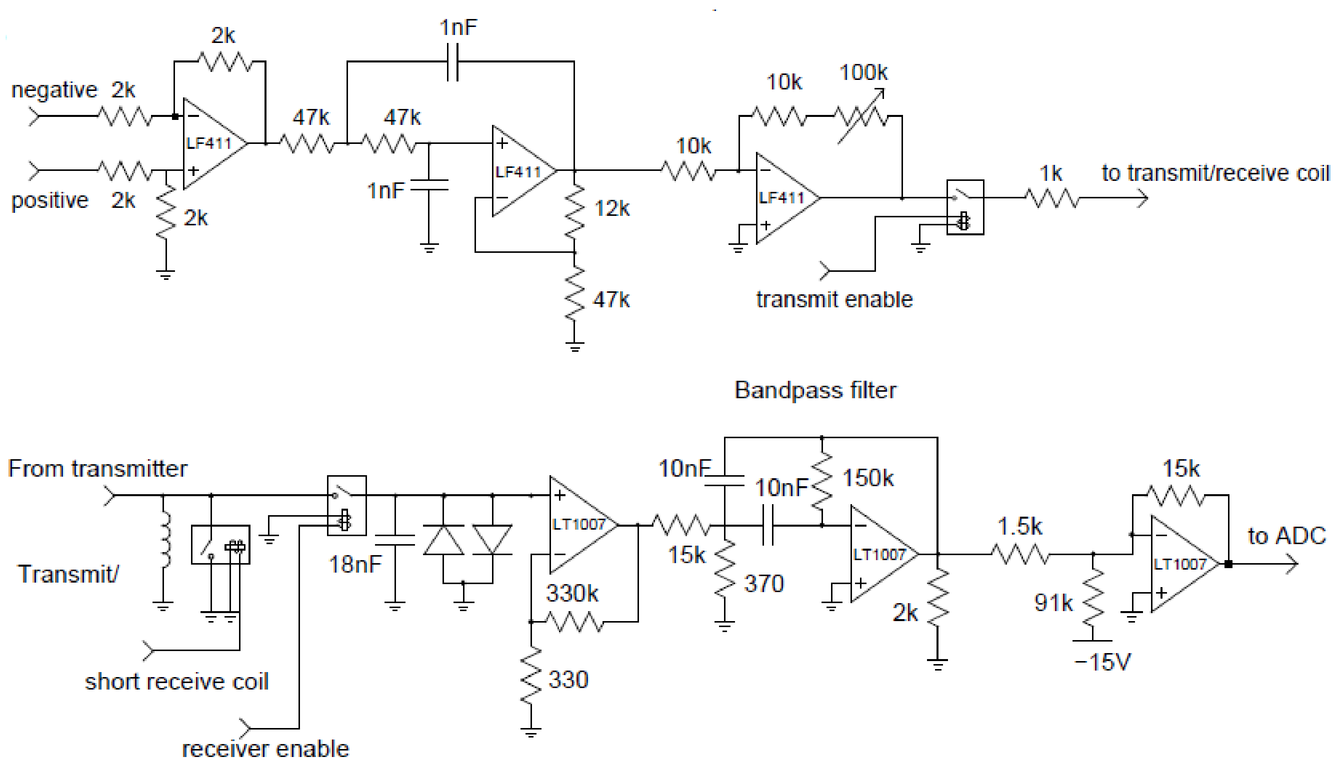

Figure 3: Schematics as taken from *Michal*. Top: Transmitter. Bottom: Receiver

National Instruments also provides software called UltiBoard, which I am currently using to design a printable circuit board implementation of the schematics.

Results

Transmitter

Figure 4 shows the schematic that I created using Multisim.

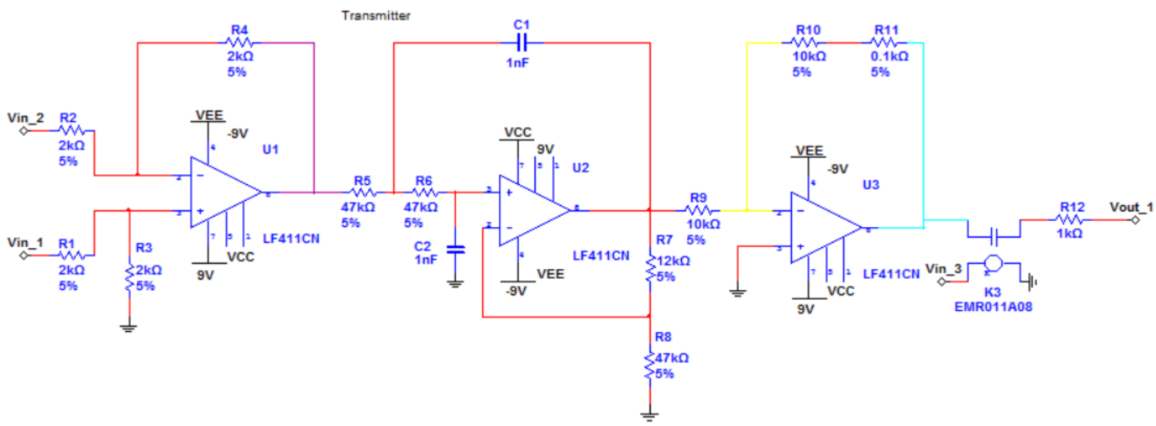

Figure 4: Schematic for transmitter created in Multisim

I tested this schematic by wiring a variable voltage generator directly to the low-pass filter and giving it a DC signal of +/- 5 V oscillating at 2 kHz (near the Larmor frequency we calculated for the earth's magnetic field). The wiring is shown in Figure 5.

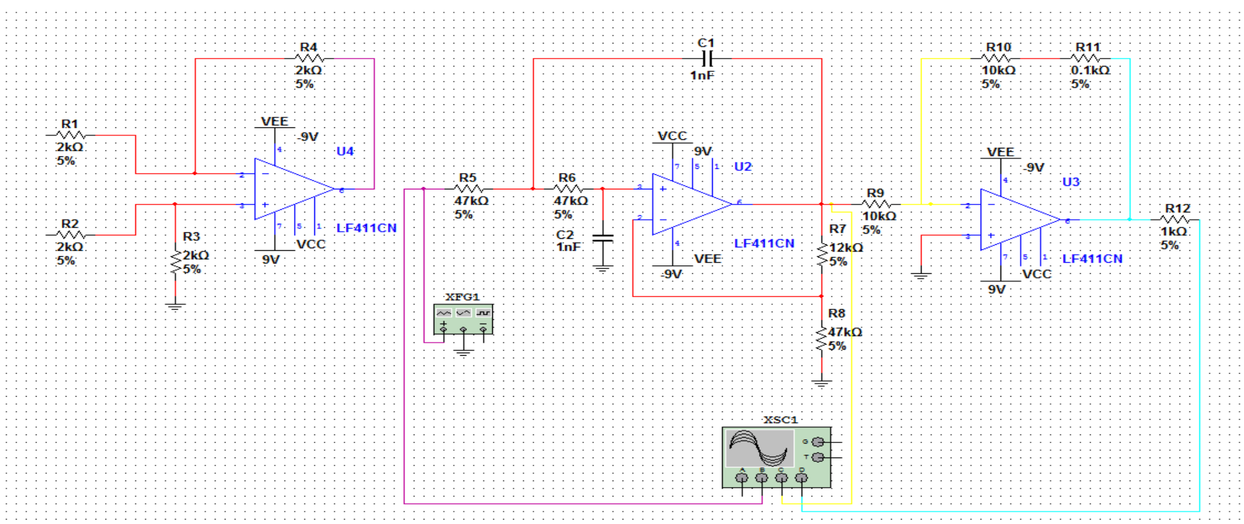

Figure 5: Transmitter wired with +/- 5 V DC waveform with voltages read with an oscilloscope

The results from this trial are shown below.

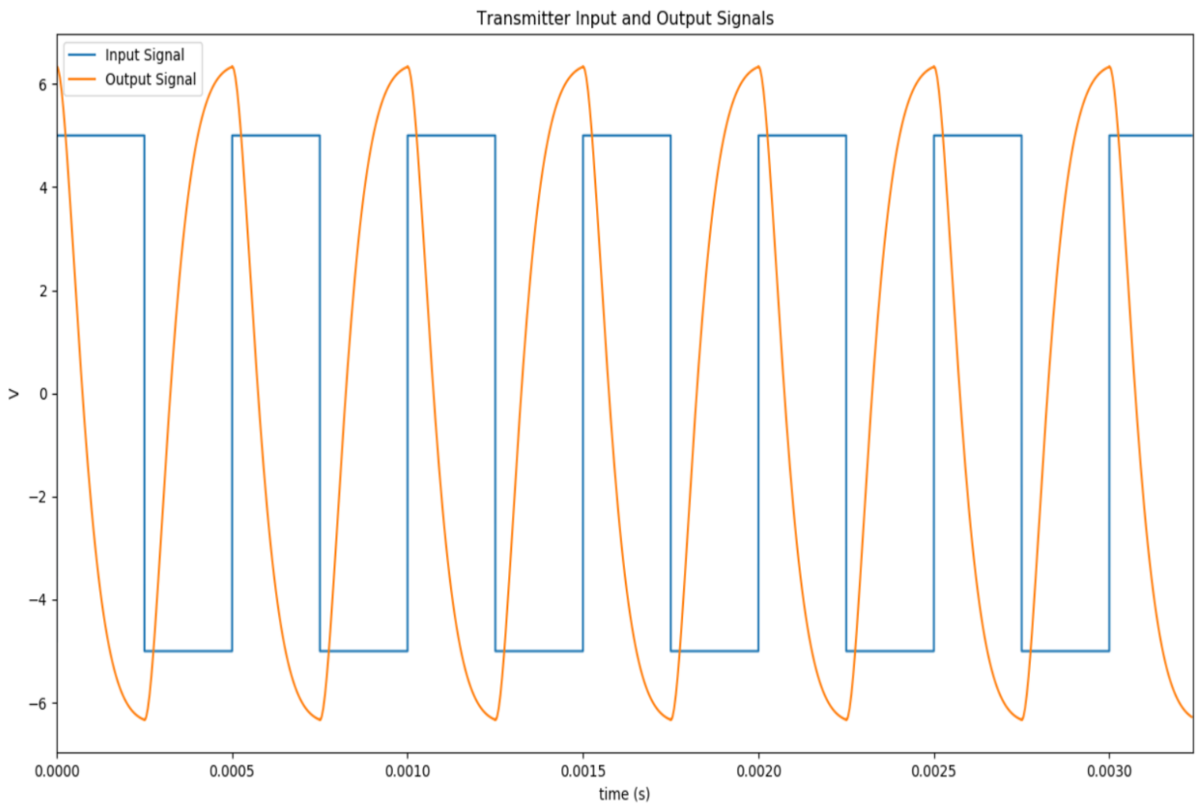

Figure 6: Input and output voltages for the transmitter

As expected, the DC signal given to the transmitter is amplified, ranging from +/- 6 V rather than the input's +/- 5 V. Also, the waveform is much more smooth, and it nearly sinusoidal. While there is a slight difference in phase, the frequency of the output signal is identical to that of the input. While the waveform is not perfectly sinusoidal, running a current through the coils of this pattern will induce a magnetic field B_1 more than capable of exciting the Hydrogen nuclei. The other group working on this project produced an output signal of the same shape.

Receiver

Figure 7 shows that schematic for the receiver created with Multisim.

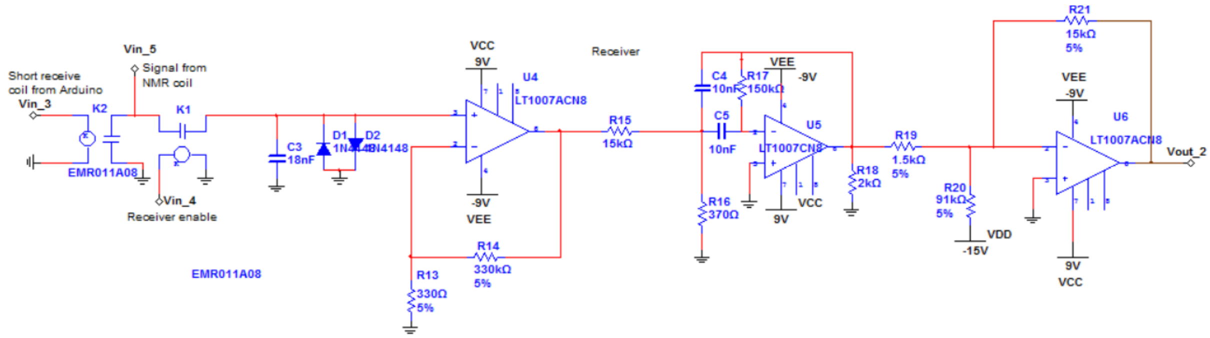

Figure 7: Schematic for receiver created with Multisim

To test the receiver, I wired a variable voltage generator to the input, and measured the voltage at several points using an oscilloscope. I also added a bode plotter to measure the gain between the input and output over the entire frequency spectrum. The wiring is shown in Figure 8.

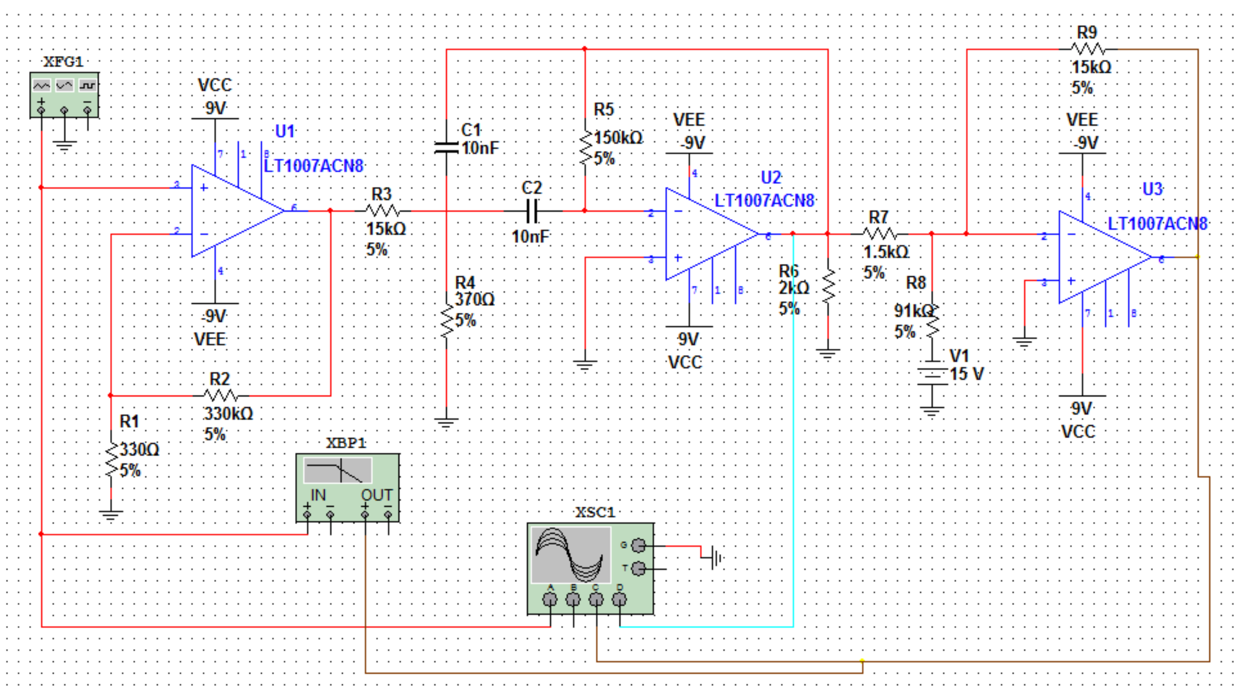

Figure 8: Wiring for SPICE simulation of receiver

The receiver is designed to take voltages in the mV range oscillating at the sample's Larmor frequency, and output an amplified, offset, and attenuated signal to be read by the Arduino. I tested the receiver's frequency response from 0.5-2.5 kHz with the hopes of detecting a resonance peak at the Larmor frequency, calculated earlier as slightly greater than 2 kHz. The bode plot is shown in Figure 9.

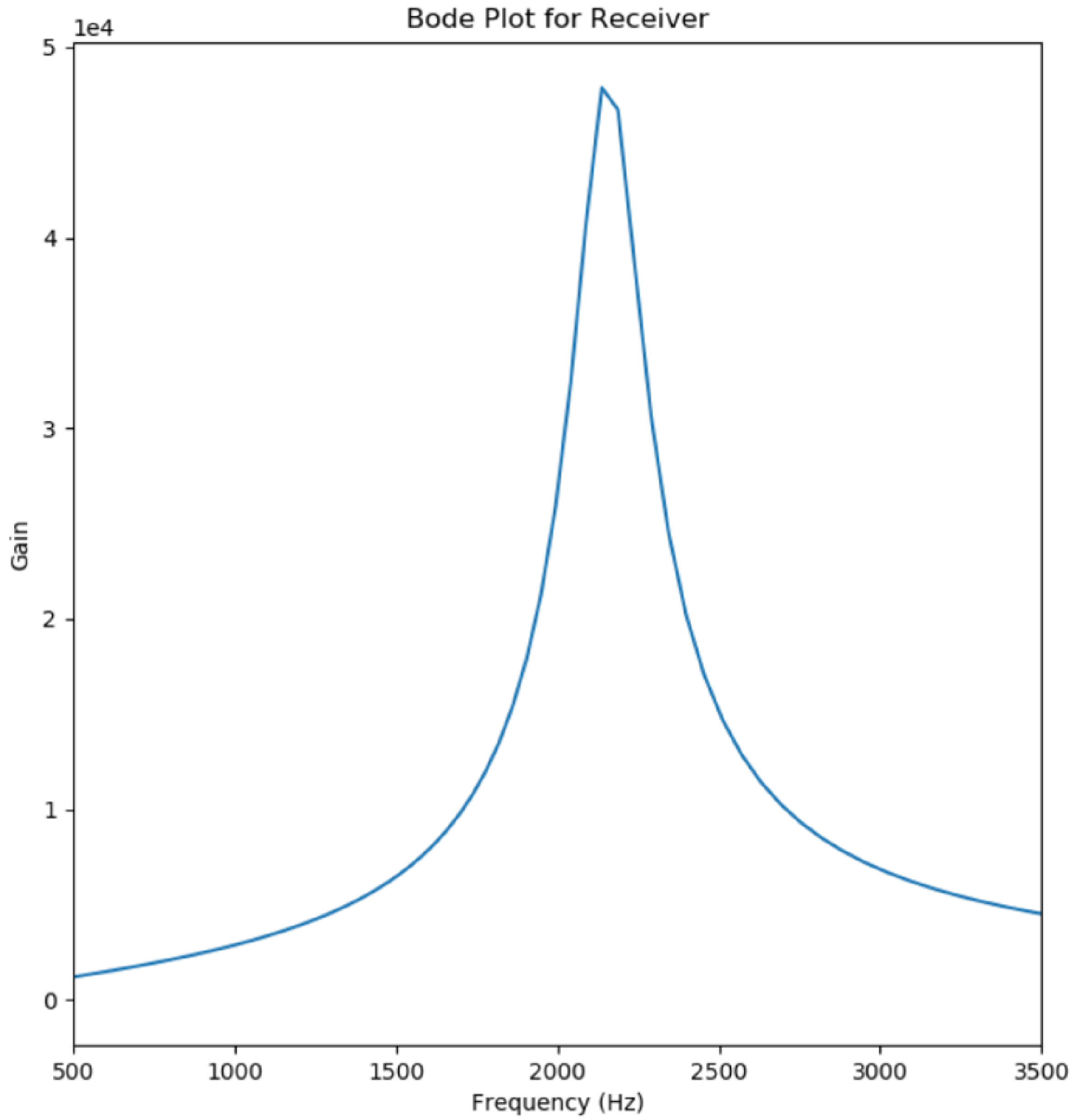

Figure 9: Plot of gain as a function of input voltage frequency

The maximum gain was found at a frequency of 2.138 KHz, and this maximum was 47,840. These results match our expectations perfectly, as the Larmor frequency calculated of 2.129 kHz is well within the resonance peak. *Michal* predicted a maximum gain of roughly 50,000, which is near our calculated value. My values also agree with those from the other group working on the project.

PCB

After completing schematics for the transmitter and receiver, I exported the results to Ultiboard and produced a rough draft of a final PCB. The wiring diagram is shown below.

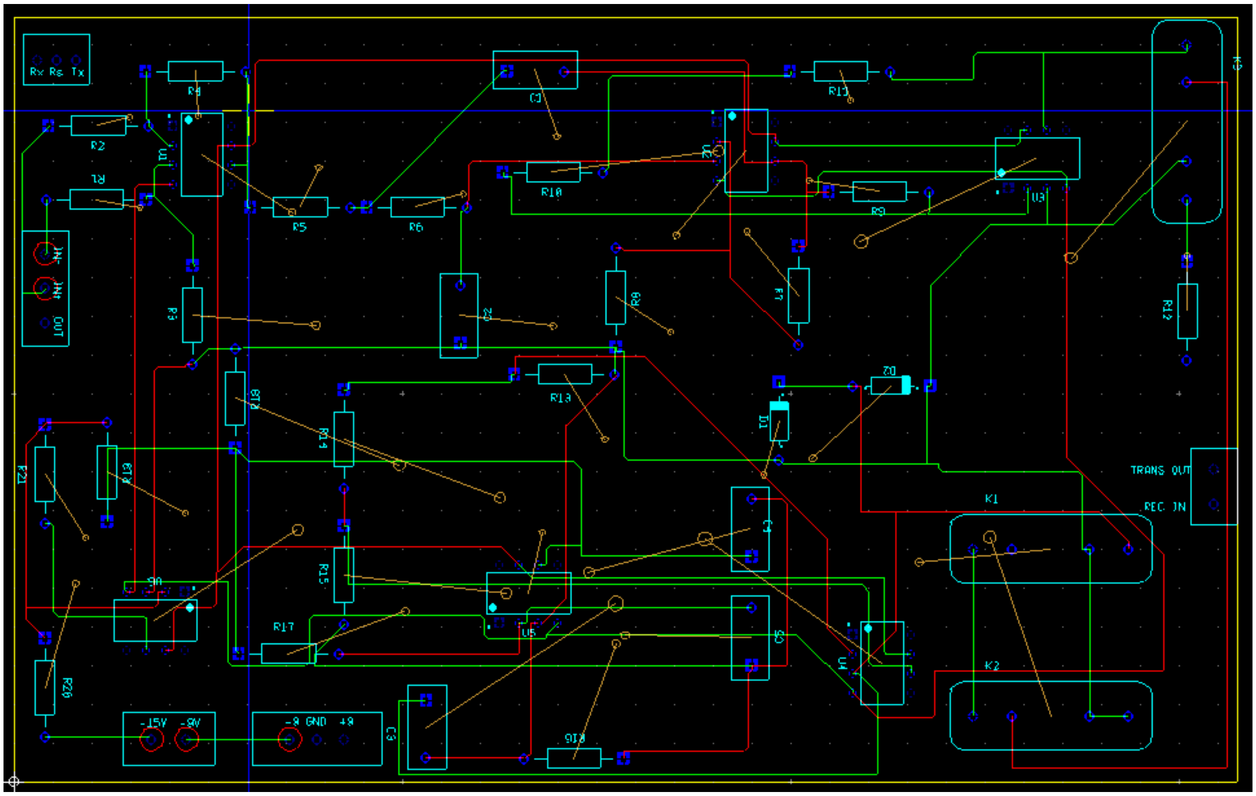

Figure 10: PCB layout created with Ultiboard

This wiring corresponds to the following 3D rendering:

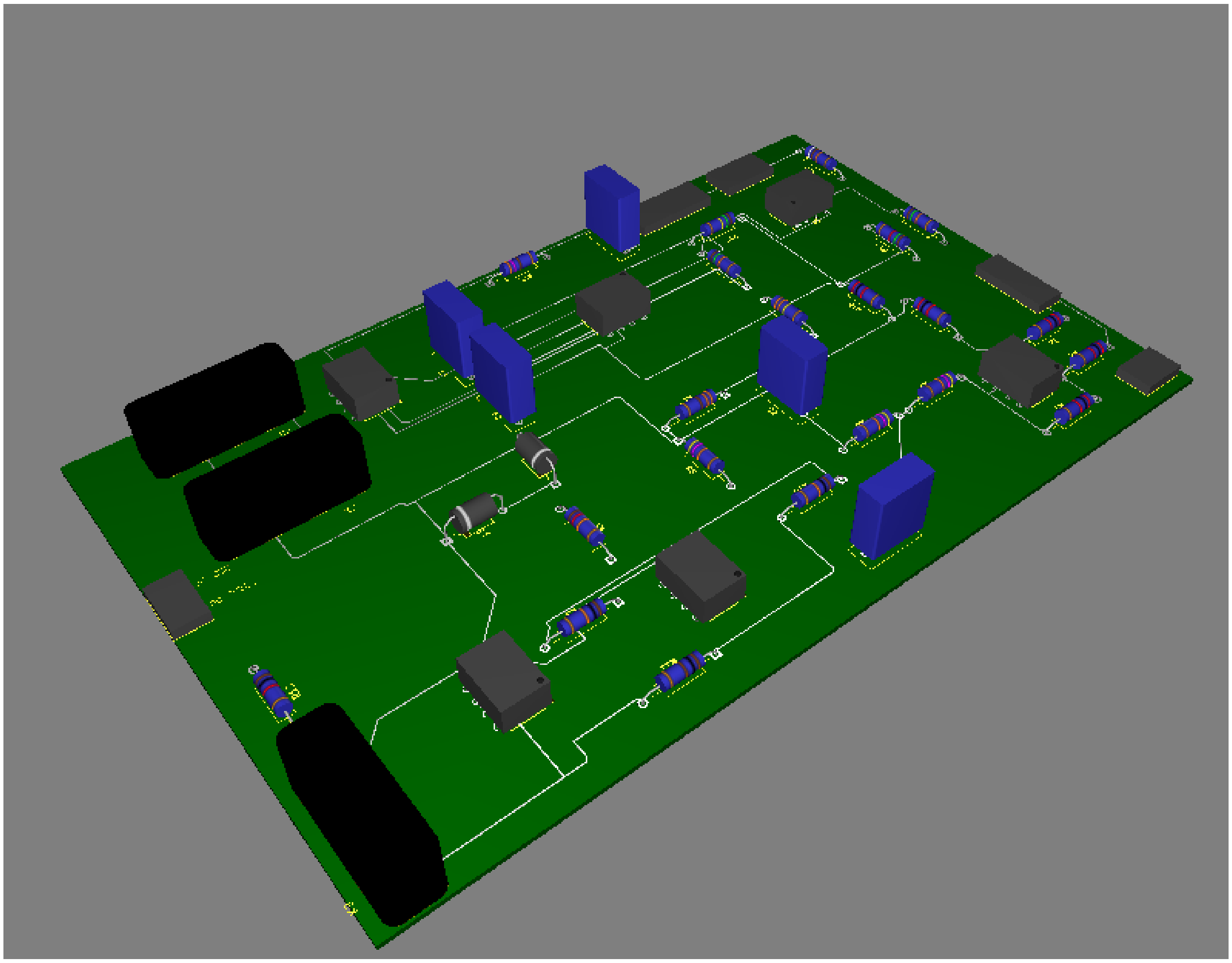

Figure 11: 3D rendering of PCB produced with Ultiboard

The PCB design is not yet complete, and although all electrical components are connected, connections need to be added for a common ground, and for transmit and receive signals from the Arduino.

Next Steps

The earth-field NMR project is well underway and will soon be ready for the next stages of microcontroller programming and physical construction. The schematics produced with Multisim agree with the expectations and with the results from the other group. I hope to finish the PCB within the first few weeks of the next semester, so that I can order the board printed and move onto the next stages soon.

In the meantime, more testing needs to be done with the current PCB design to ensure that all connections are in the desired positions, that no lines are too close or parallel to the power line in order to avoid electrical interference from power line harmonics, and and that all op-amps are wired with the correct pin layouts.

References

[1] Paul Callaghan. Principles of NMR and MRI [online]. 2009. URL: http://www.magritek.com/products/terranova/videos/.

[2] Carl A. Michal. A low-cost spectrometer for nmr measurements in the earth's magnetic field. *Department of Physics Astronomy, The University of British Columbia*, Aug 2010.