NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING

Building the Next Generation of NMR Software for Polarized Neutron Scattering Instruments

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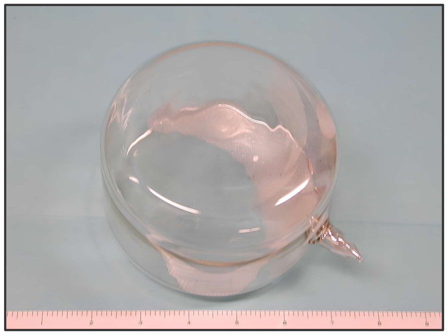
Introduction

Project Goal: Update NMR software in IGOR Pro programming language for ^{3}He spin filter characterization and control

Bonus: Reproduce and improve capabilities in python!

To do this we must understand:

- **Neutron scattering and ^{3}He Spin Filters**
- **High level procedures**
- **Hardware communication at NCNR**
- **Low level code and graphical user interfaces (GUIs)**



^{3}He Cell

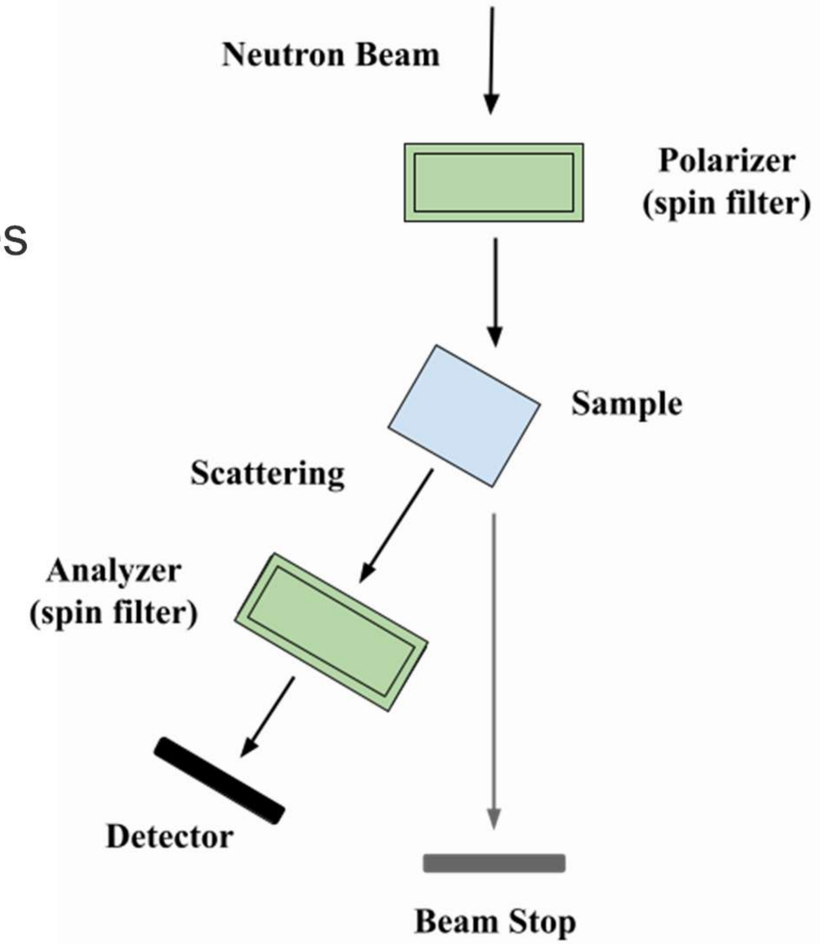
02

Physics Background

Neutron Scattering

Extract atomic and magnetic properties of sample or probe

- Neutron beam
- Polarizer (spin filter)
- Neutron interaction with a sample
- Analyzer (spin filter)



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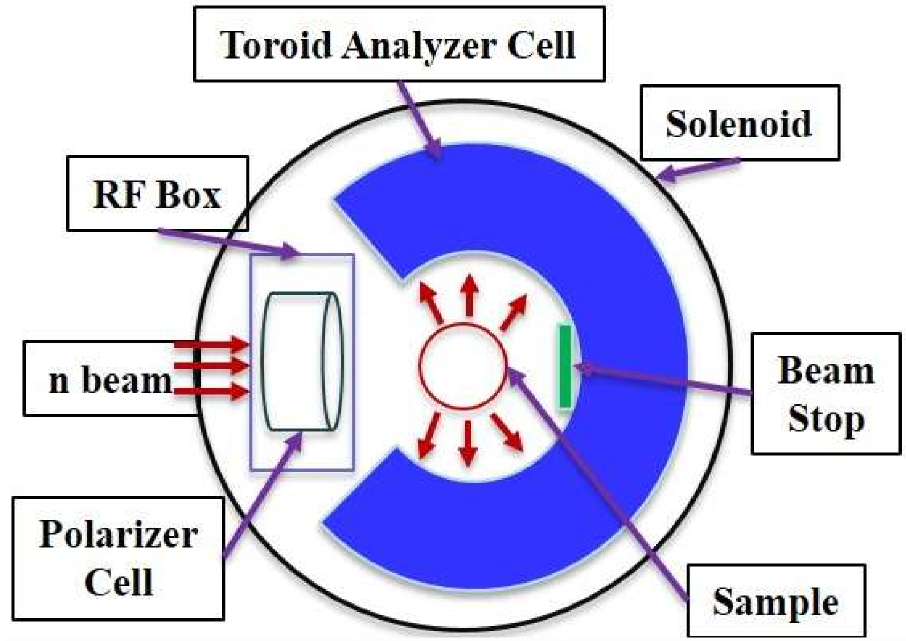
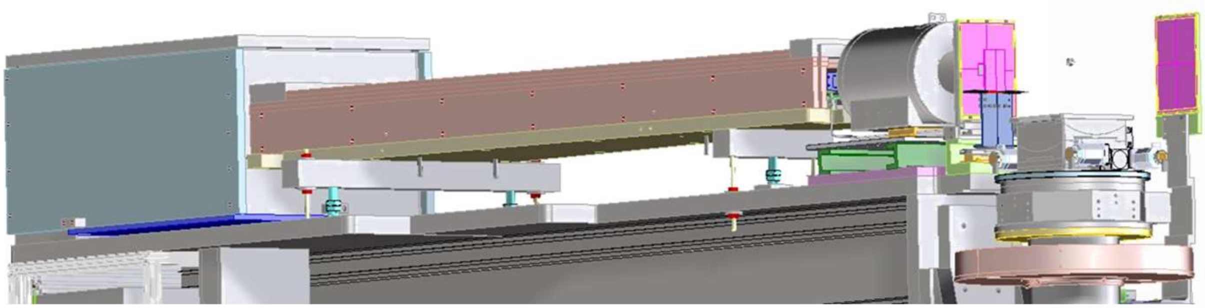
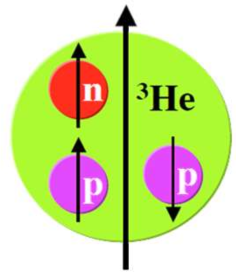


MACS



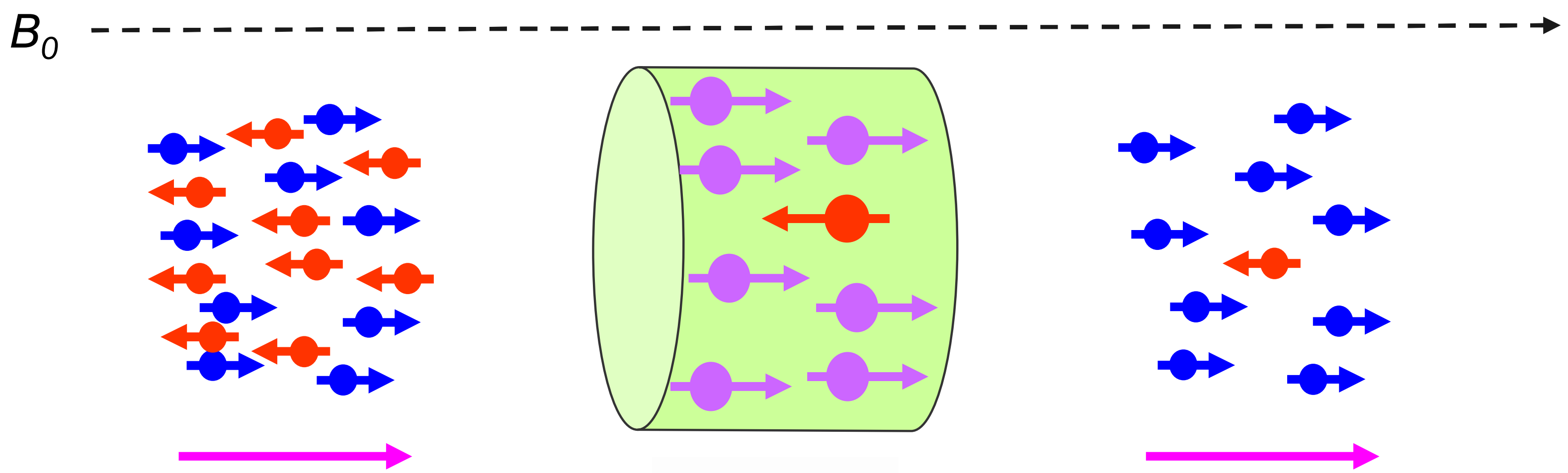
CANDOR

^{3}He Spin Filter



^{3}He nuclear spin carried mainly by neutron

$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} \qquad P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$



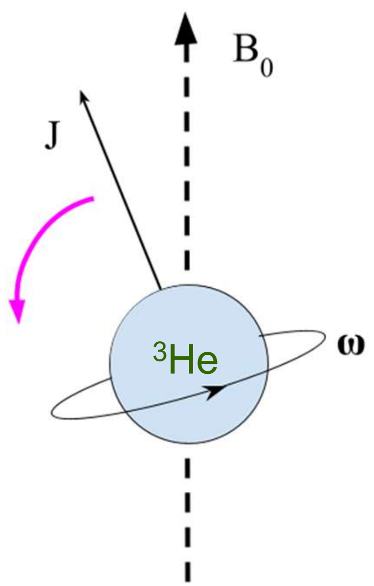
Unpolarized Neutrons

Polarized ^{3}He Cell

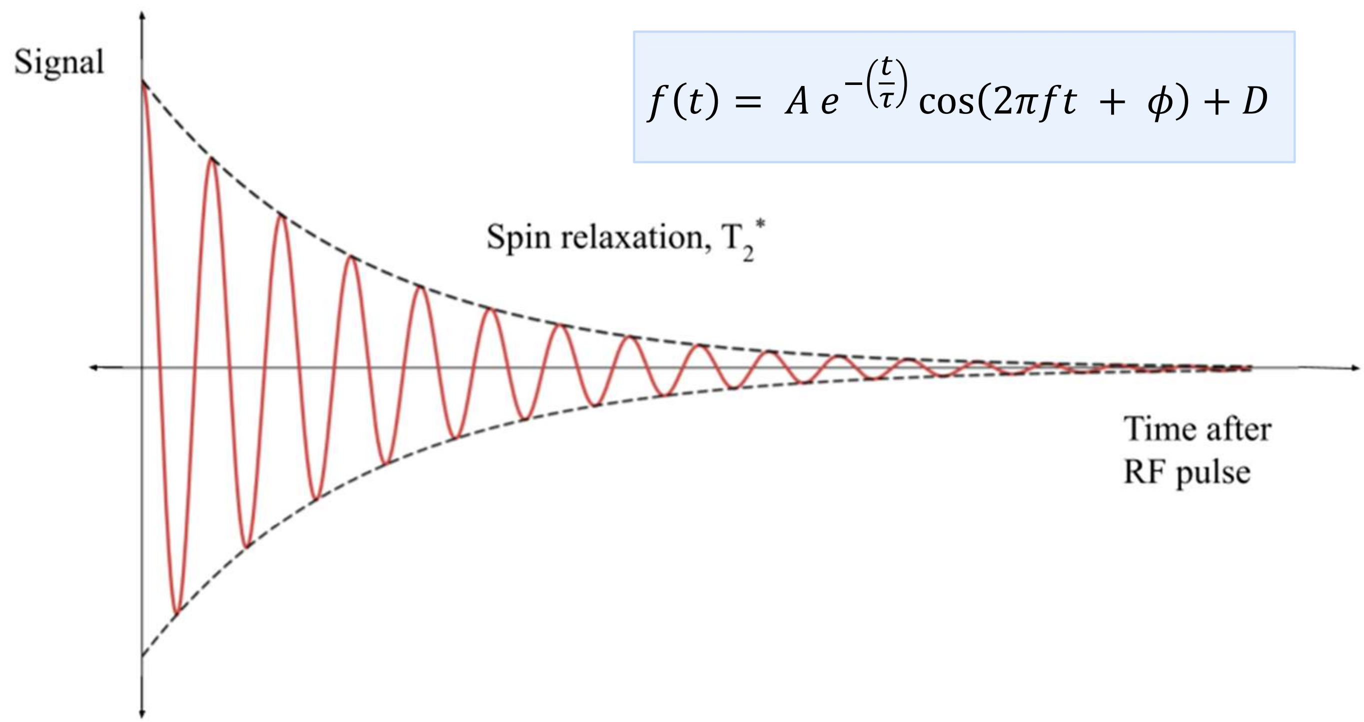
Polarized Neutrons

Free Induction Decay (FID)

Determine and track polarization of ^{3}He spin filter



$$f(t) = A\, e^{-\left(\frac{t}{\tau}\right)} \cos(2\pi f t + \phi) + D$$

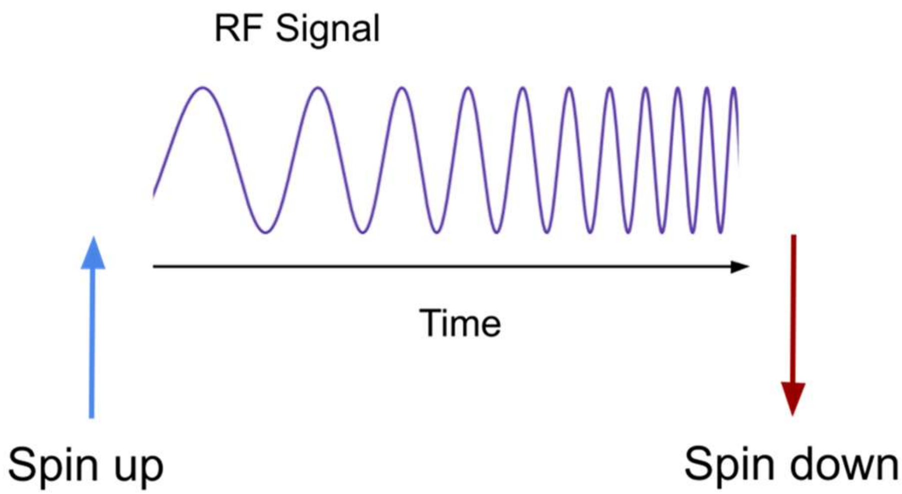


Adiabatic Fast Passage (AFP)

Magnetization of ^{3}He **flipped** by radio frequency (RF) or magnetic field sweep through resonance

Adiabatic Fast Passage (AFP)

Magnetization of ^3He flipped by **radio frequency (RF)** or magnetic field sweep through resonance

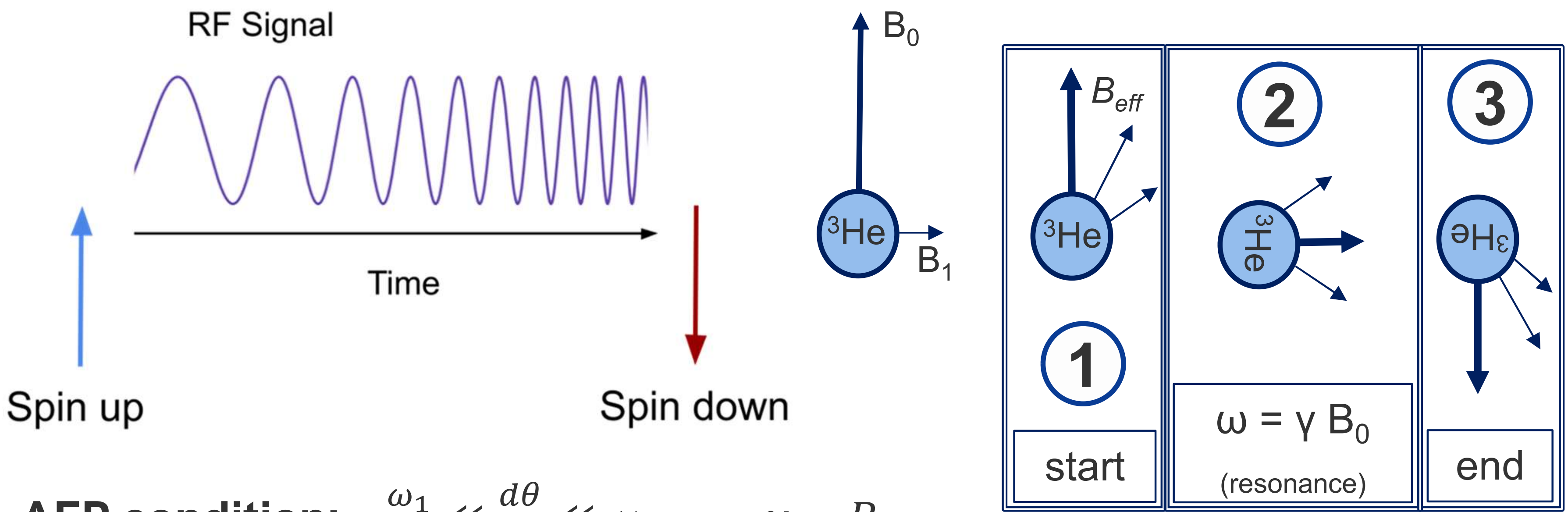


AFP condition: $\frac{\omega_1}{T_2} \ll \frac{d\theta}{dt} \ll \omega_{eff} = \gamma_{He} \, B_{eff}$

Adiabatic Fast Passage (AFP)

Magnetization of ^{3}He flipped by radio frequency (RF) or **magnetic field** sweep through resonance

$$B_{eff} = \sqrt{(B_0 - \omega/\gamma)^2 + B_1^2}$$



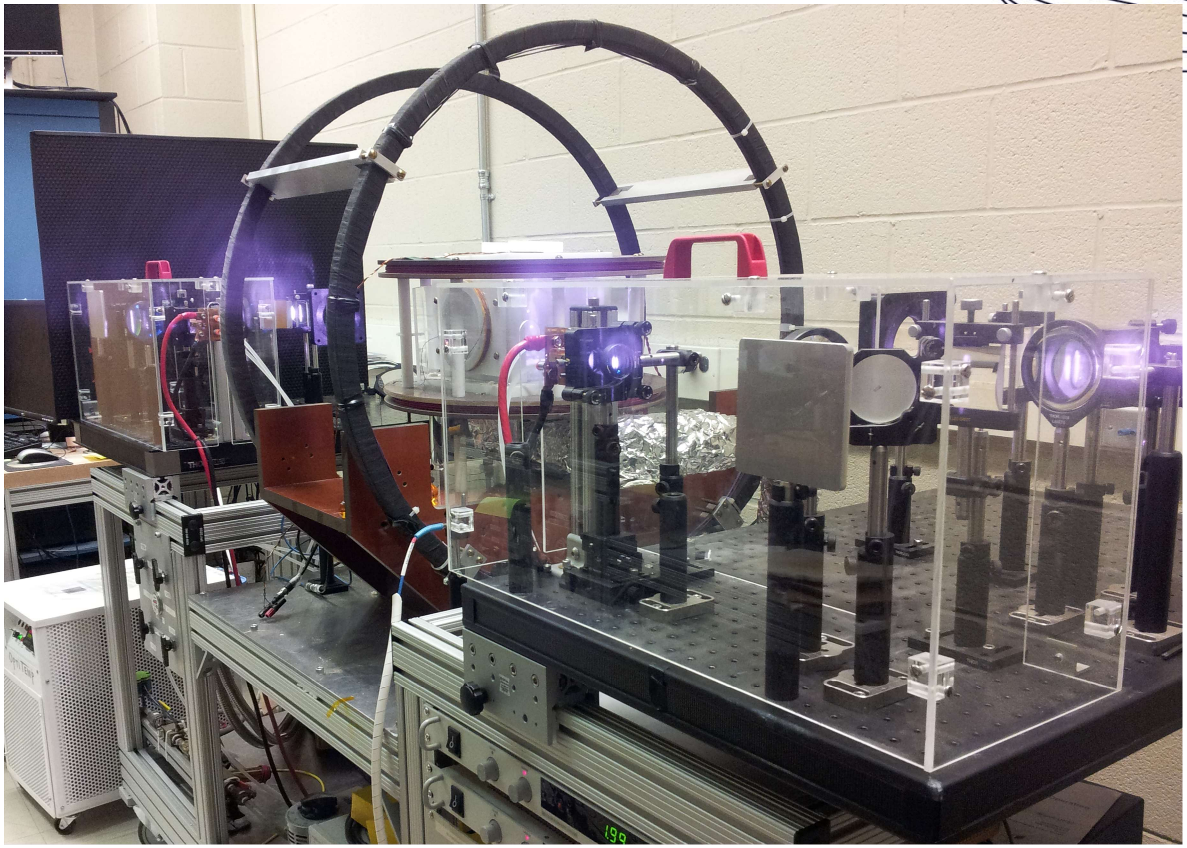
AFP condition: $\frac{\omega_1}{T_2} \ll \frac{d\theta}{dt} \ll \omega_{eff} = \gamma_{He}\, B_{eff}$

03

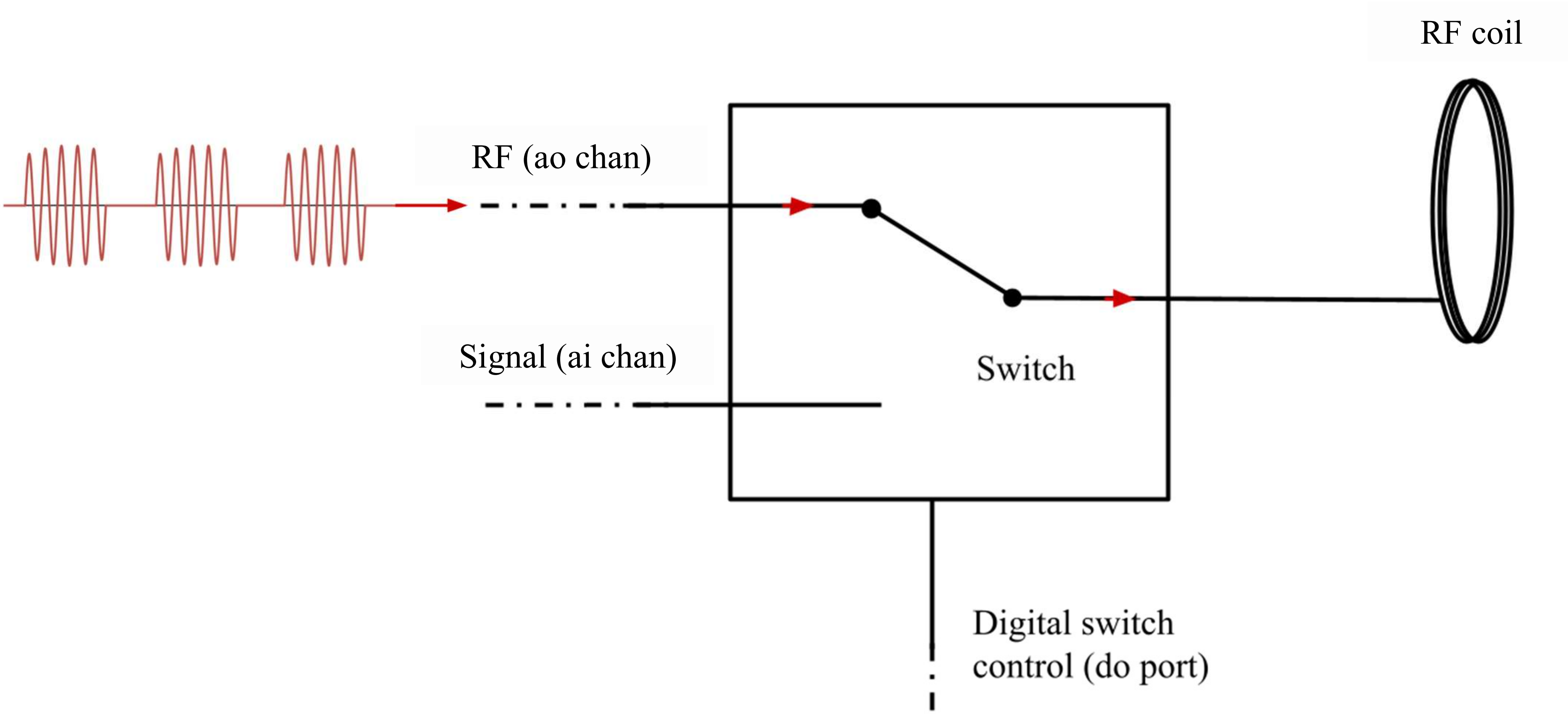
Procedures at NCNR

Lab Setup

- ^{3}He Cell
- Spectrally narrowed diode laser
- Helmholtz coils
  - B_0 holding field
  - Radio frequency (RF) drive
  - Pickup



How Does it Work?



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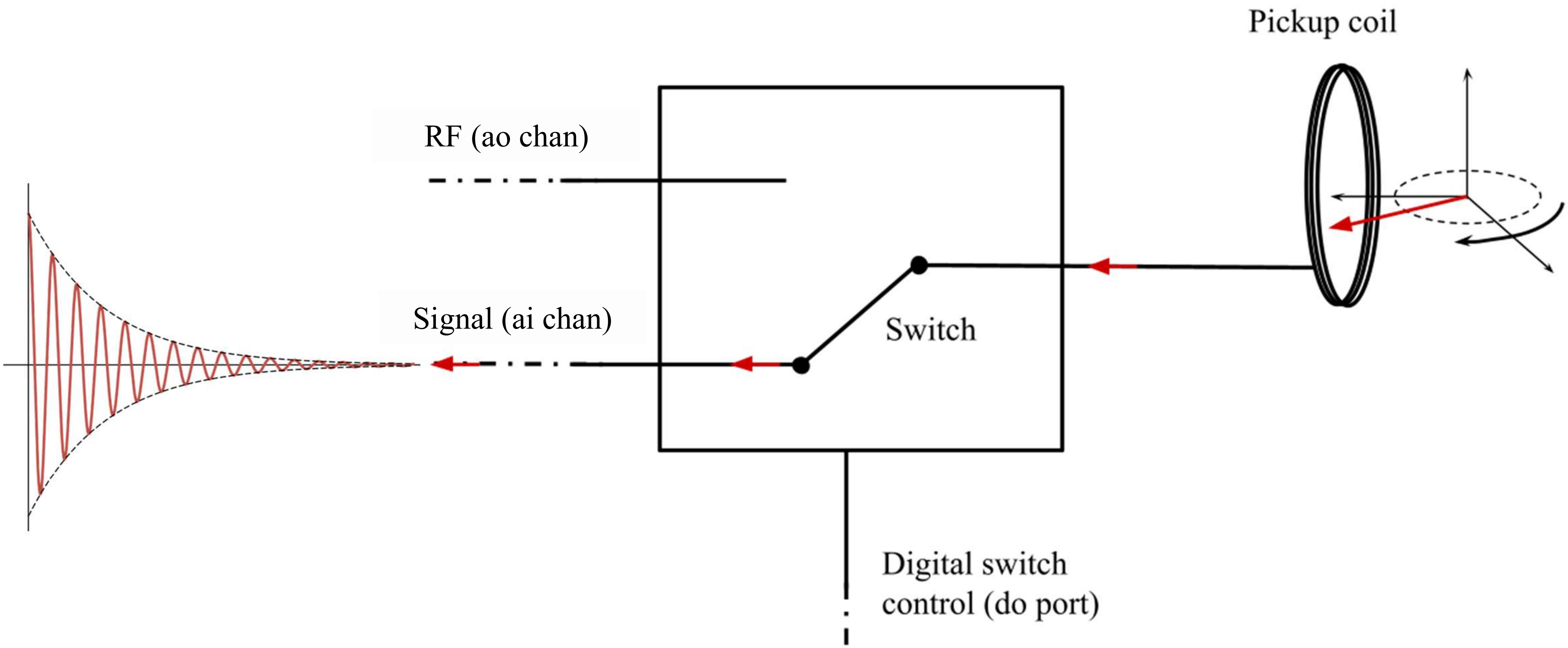


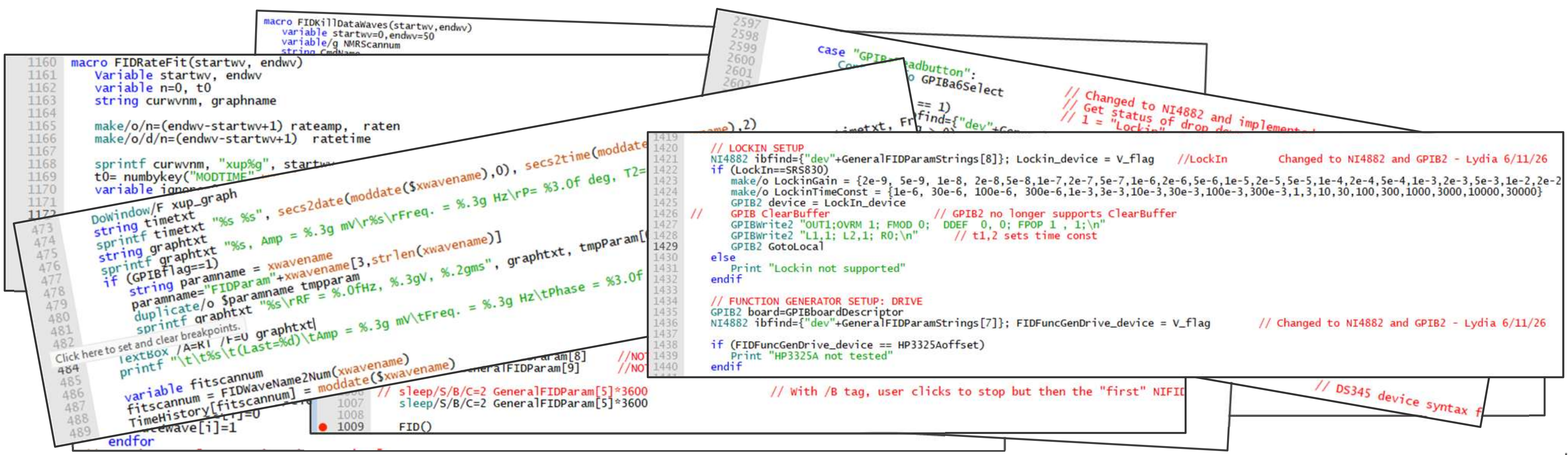
IGOR 6 → IGOR 8

Process:

1. Familiarization with code
2. Updating syntax and structure
3. Run, break, debug, repeat

Challenges:

1. Major hardware communication protocol change from IGOR 6
2. Working in/learning a new language
3. Organization – 4 programs, 3 computers
4. Maintaining high level structure



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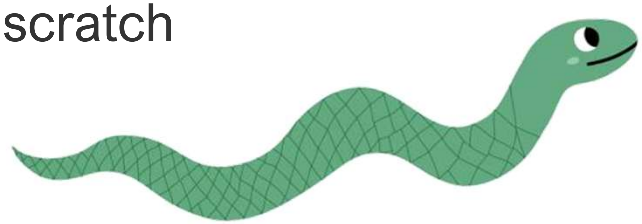
Bonus:
Write it all in python!

- Same challenges
- Plus designing unique program from scratch



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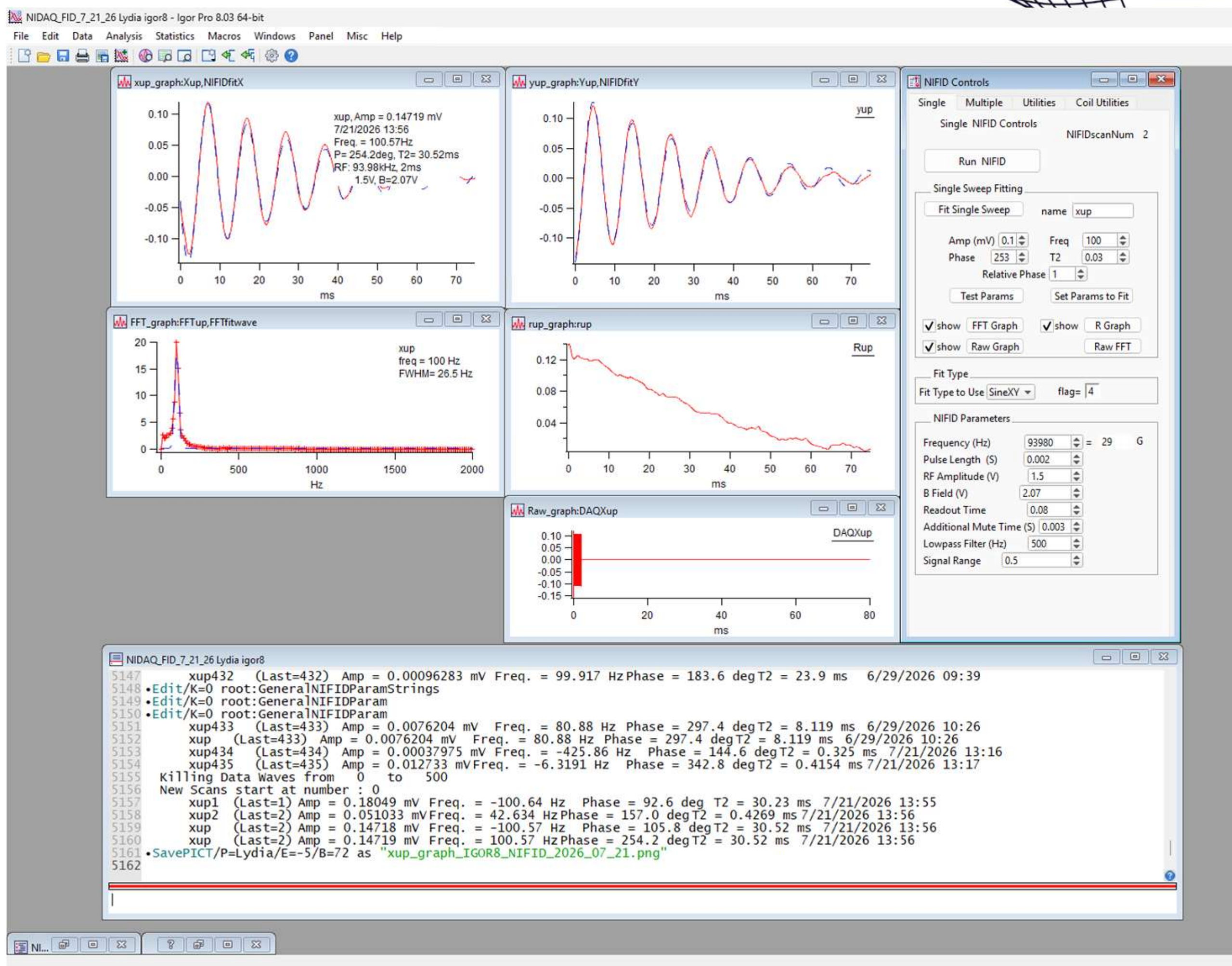
Results

Graphical User Interface



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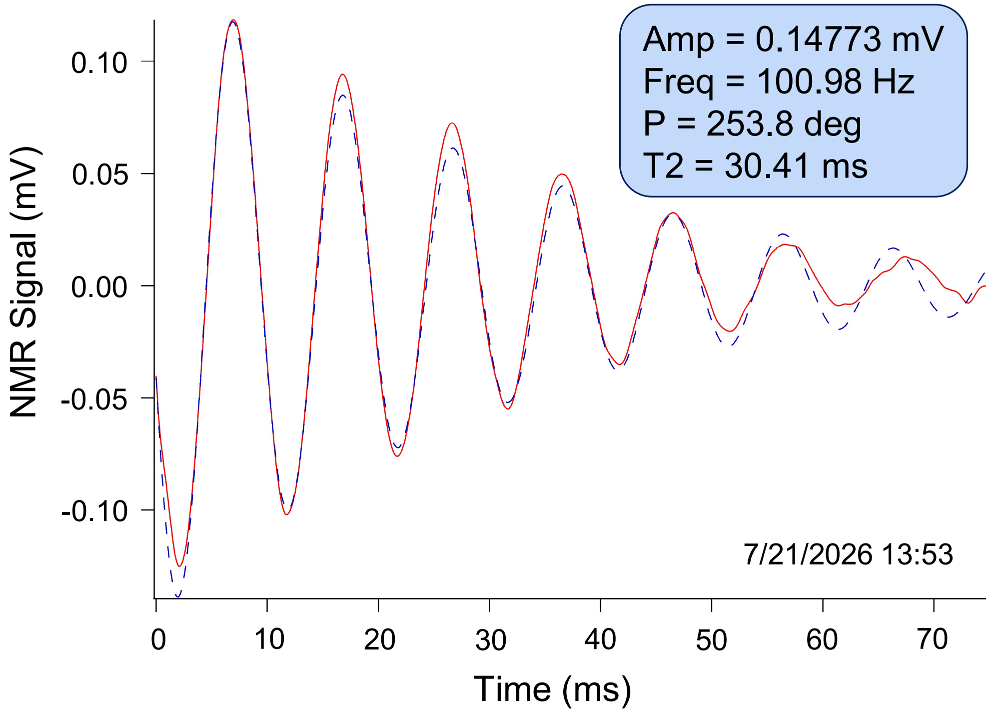
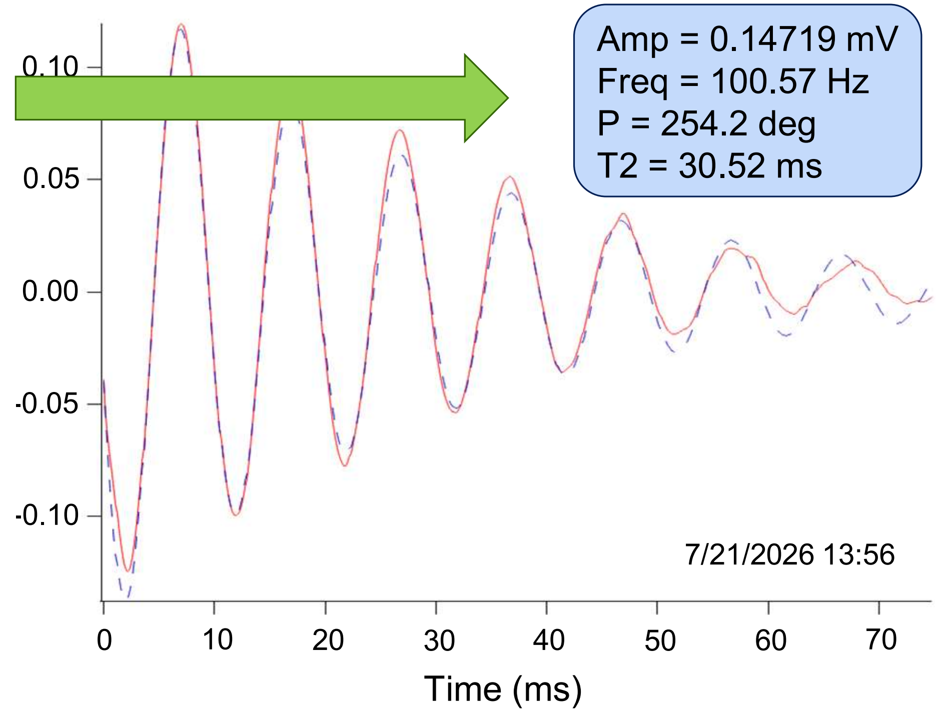
Free Induction Decay

$$f(t) = A\, e^{-\left(\frac{t}{\tau}\right)} \cos(2\pi f t + \phi) + D$$

IGOR 6



IGOR 8

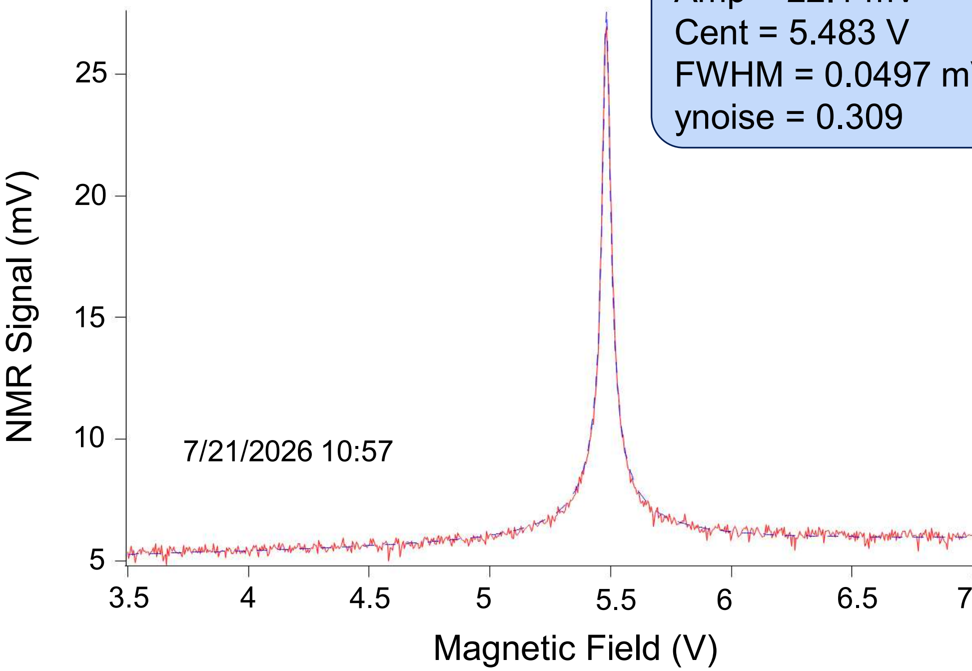


Adiabatic Fast Passage: B-Field

$$g(x) = C_0 + C_1 x + C_2 \Big/ \sqrt{1 + \frac{(x - x_0)^2}{(C_3/2)^2}}$$

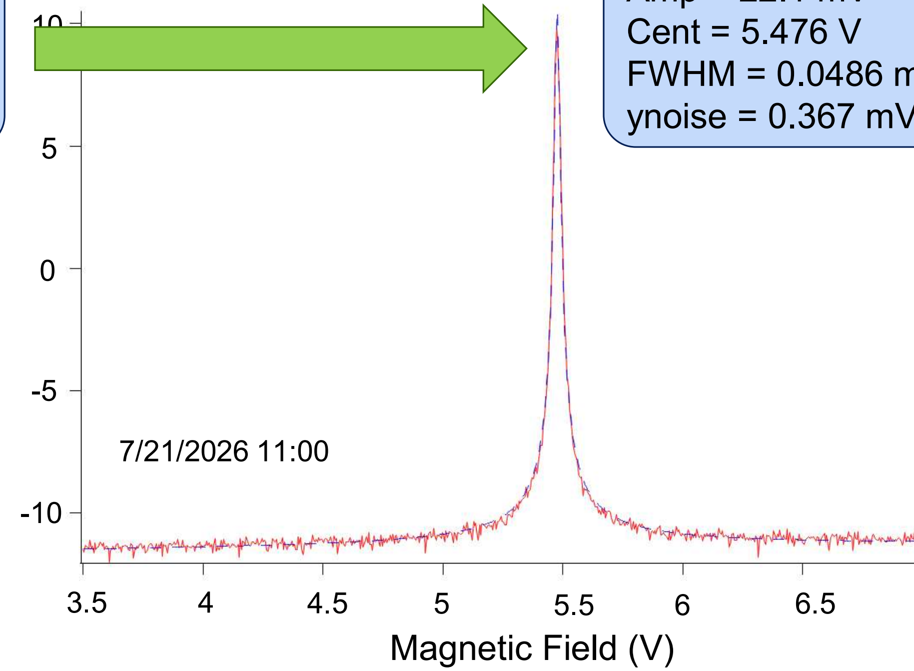
IGOR 6

Amp = 22.1 mV
Cent = 5.483 V
FWHM = 0.0497 mV
ynoise = 0.309



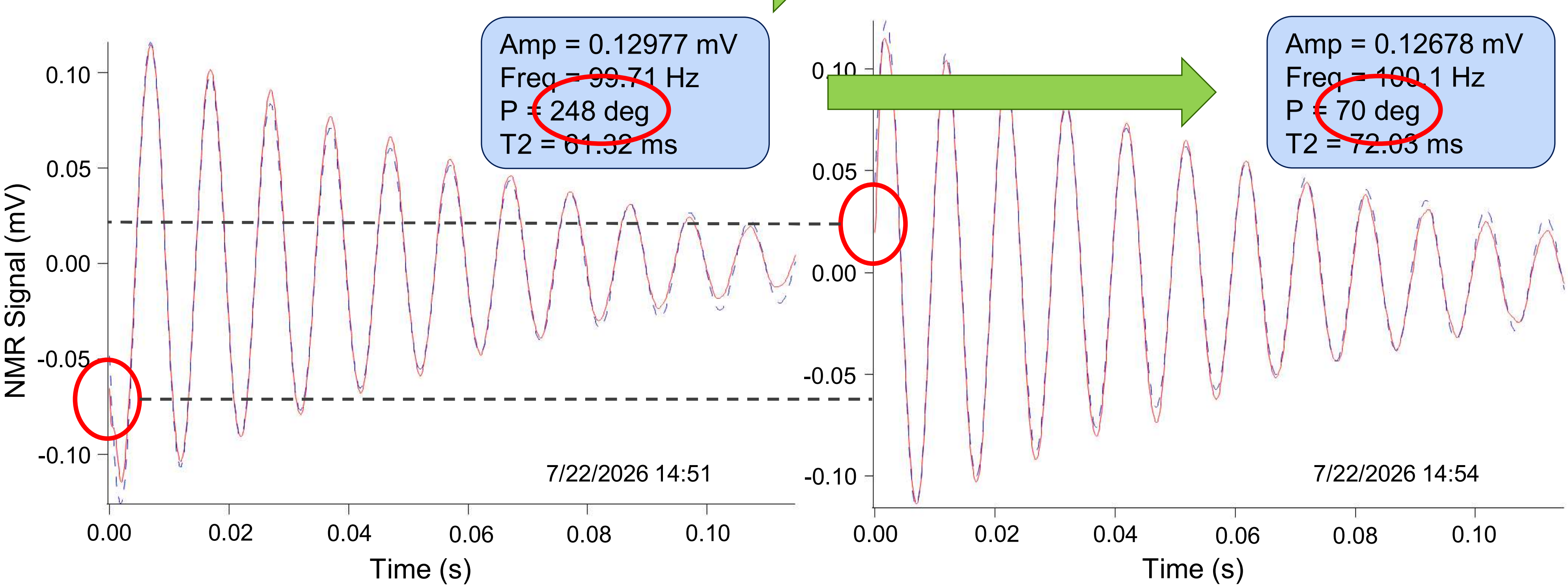
IGOR 8

Amp = 22.1 mV
Cent = 5.476 V
FWHM = 0.0486 mV
ynoise = 0.367 mV

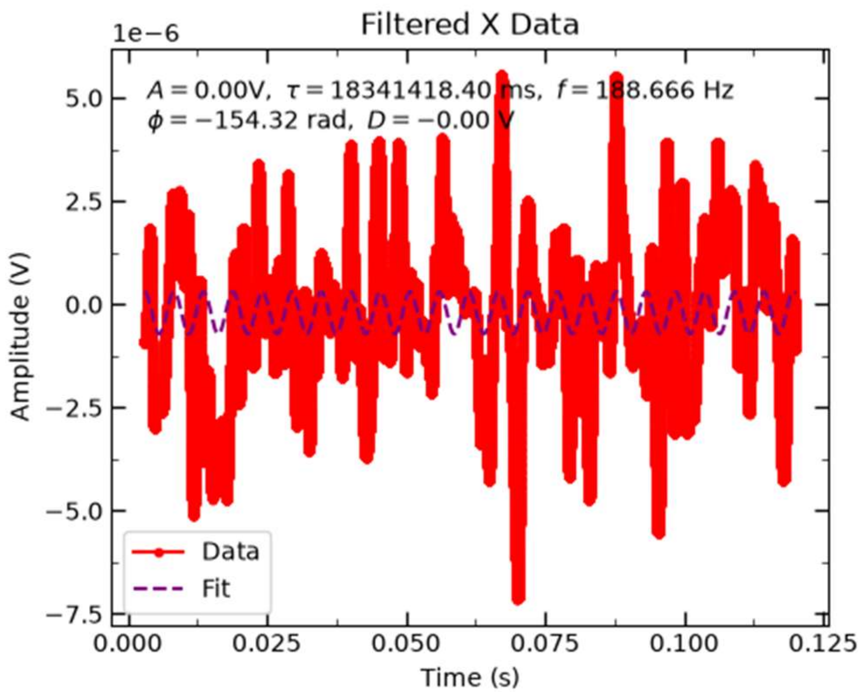


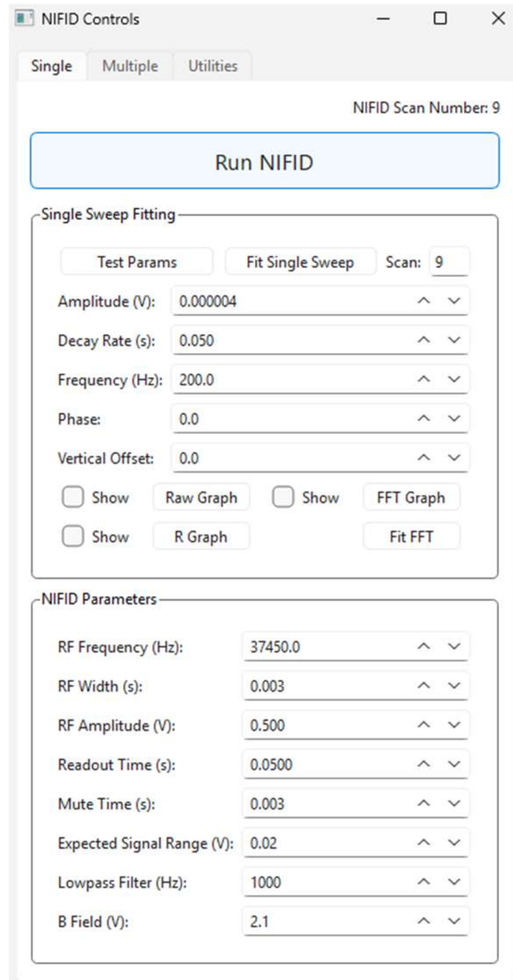
Adiabatic Fast Passage: Radio Frequency

Before **After**



Python

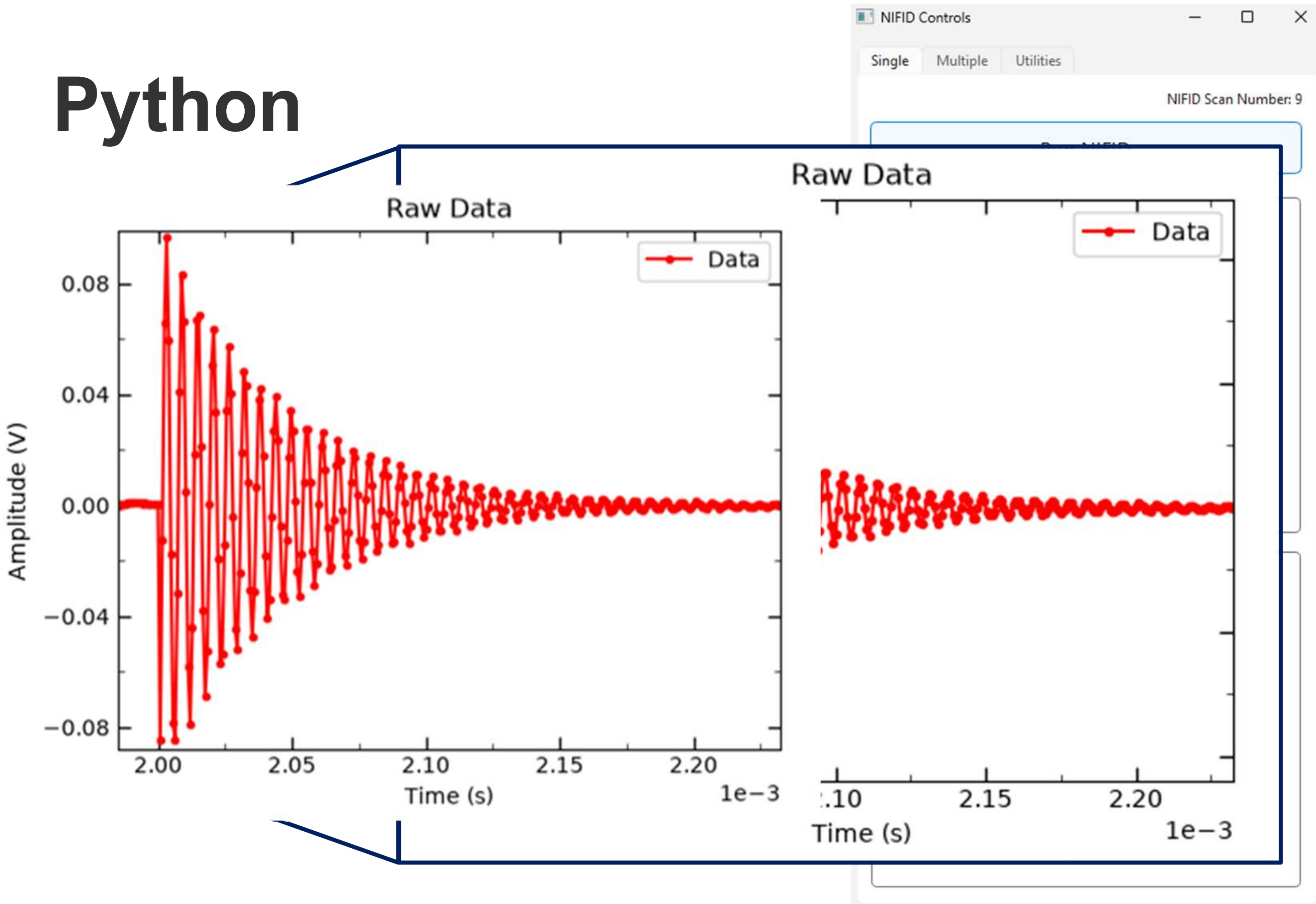




Part 1 of 4: NIDAQ

- Software runs
- Not getting expected FID signal

Python



Part 4 of 4: NIDAQ

- Software runs
- Not getting expected CLE signal
- Evidence of RF pulse

Improvements

- Modular GUI (PyQt6)
- Simplified functions
- OOP design class structure
- Universal coding language

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Conclusion and Future Work

Conclusion

- Polarized neutron scattering experiments at NCNR
- ^{3}He neutron spin filter characterization and control
- IGOR Pro software
  - Learning code and structure
  - Updating software and hardware communication
  - Comparing Results → No differences!
- Python software
  - 1/4 complete
  - FID signal acquisition issues

Future Work

1	Write more involved python capabilities
2	Stay up to date with IGOR

Acknowledgements

Mentors: Wangchun Chen and Shannon Watson

Julie Borchers, Kelsi Rehmann, Cara O’Malley

Gordon Jones at Hamilton College

CHRNS

The Fishbowl and the Shark Tank

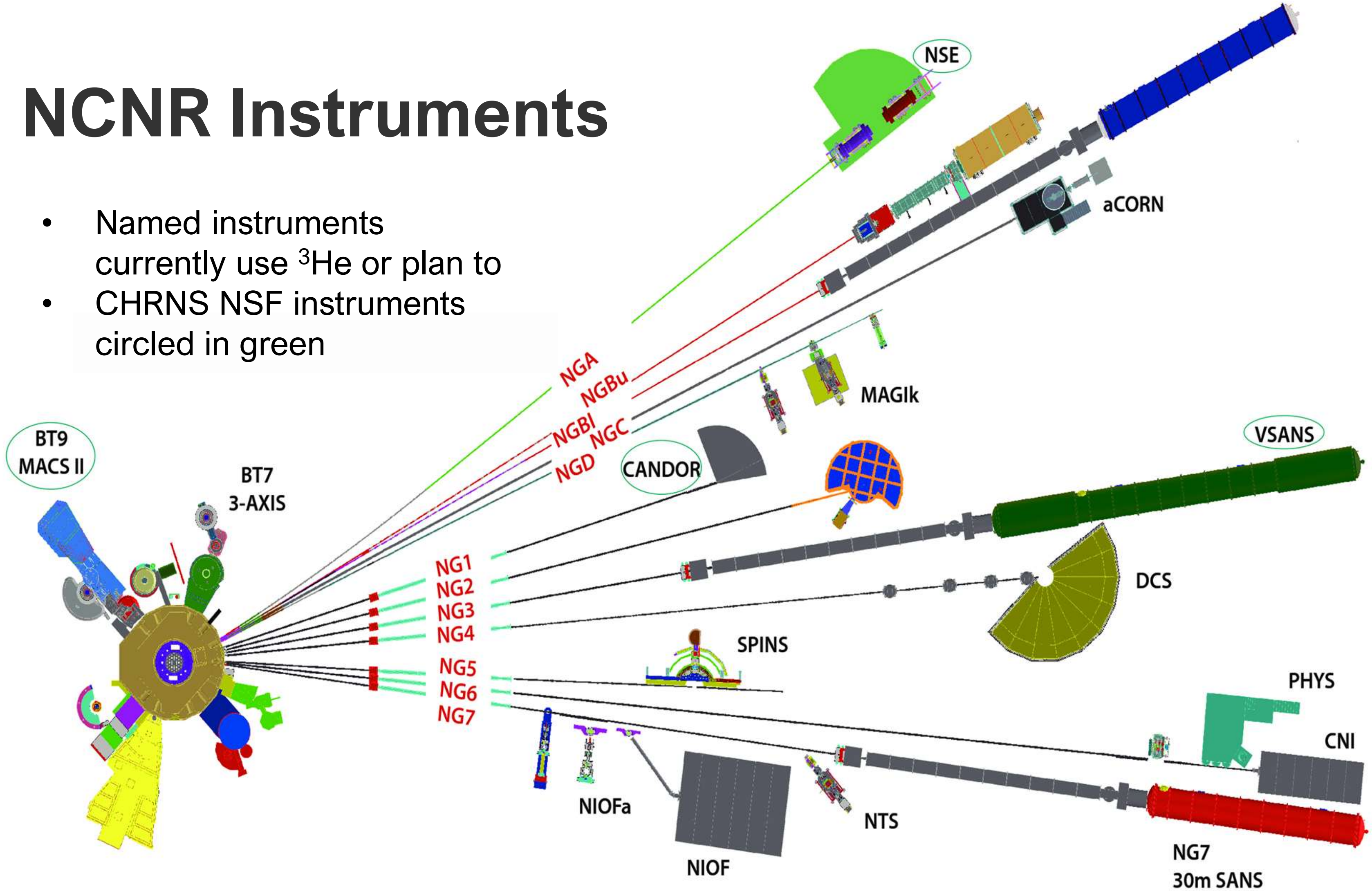
Thank you!

Questions or comments?

lbullock2@wisc.edu

NCNR Instruments

- Named instruments currently use ^{3}He or plan to
- CHRNS NSF instruments circled in green



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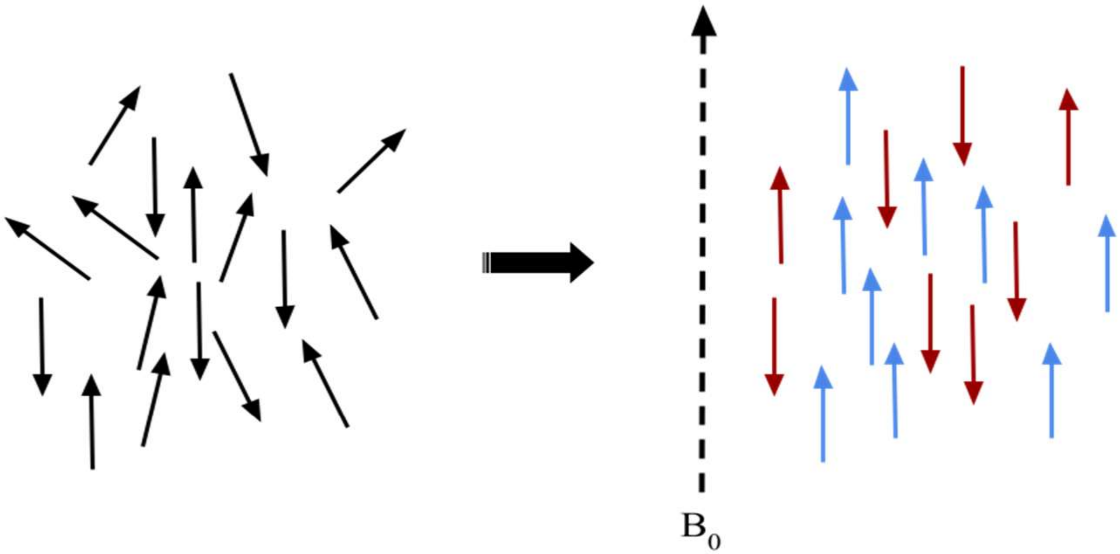
Polarization

- Spin and magnetic moment
- Alignment



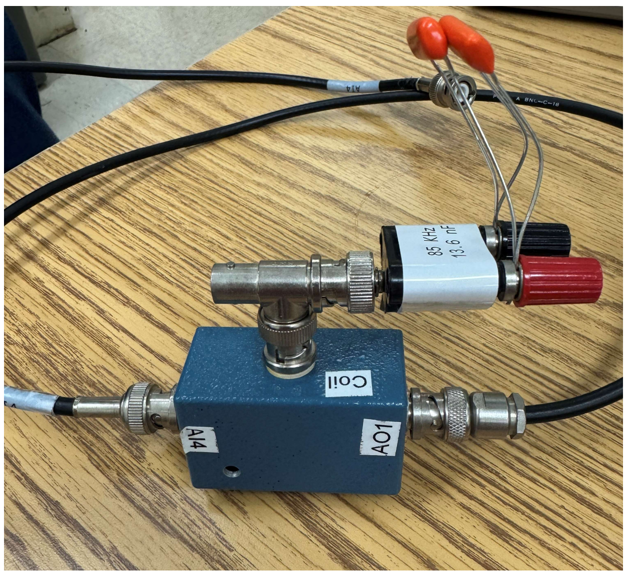
- Net Polarization

$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

Lab Setup

Two methods of FID:

Direct Connection with NIDAQ



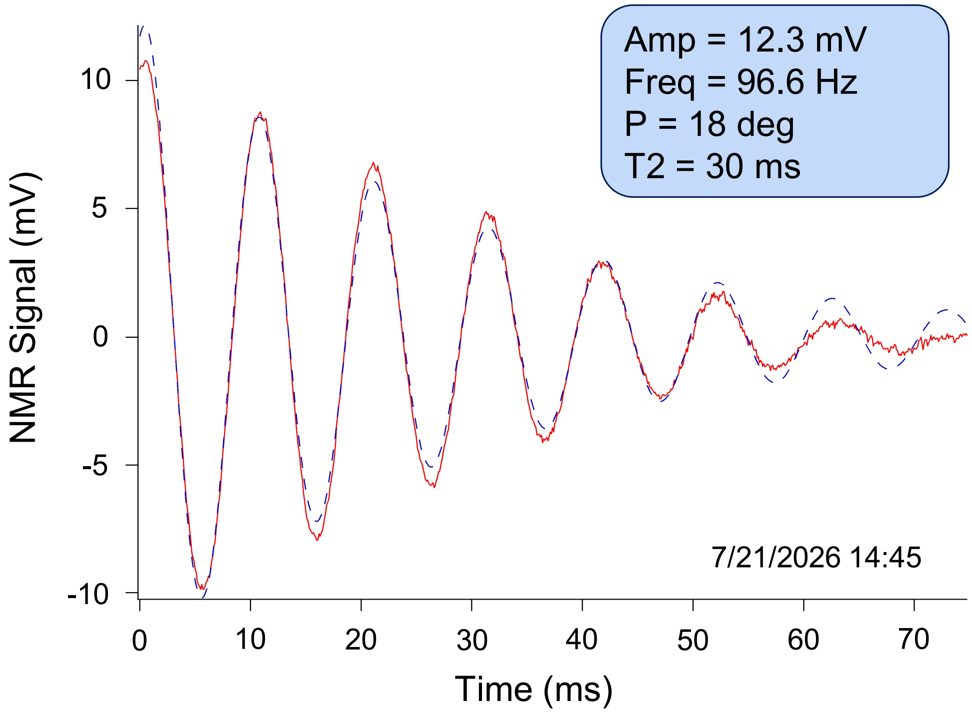
- Small, 3 leads
- Works for stronger signal

Function Generator and Amplifiers

- Requires manual control
- Sensitive to weak signals

Free Induction Decay: Amplifiers $f(t) = A\,e^{-\left(\frac{t}{\tau}\right)}\cos(2\pi f t + \phi) + D$

IGOR 6



IGOR 8