Automated Microwave Frequency Control in Dynamic Nuclear Polarization Experiments

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Introduction

- UVa Polarized Targets; Jlab, Fermilab
- Electron beam polarized target experiments
- Aim to create a controller capable of seeking/maintaining ideal frequency for polarization
- Increase the figure of merit (FOM) of DNP experiments

$$FOM = n_t \cdot f^2 \cdot P^2$$

$$n_t = target\ thickness$$

$$f = dilution\ factor$$

$$P = polarization\ measured\ over\ time$$

$$P \uparrow, FOM \uparrow$$

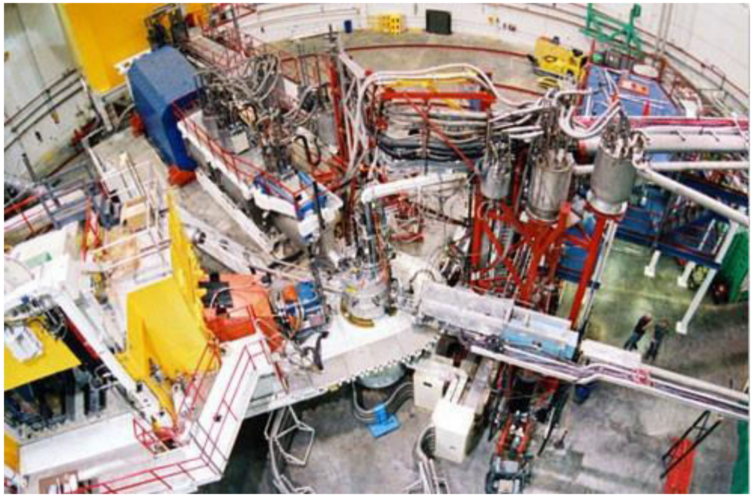
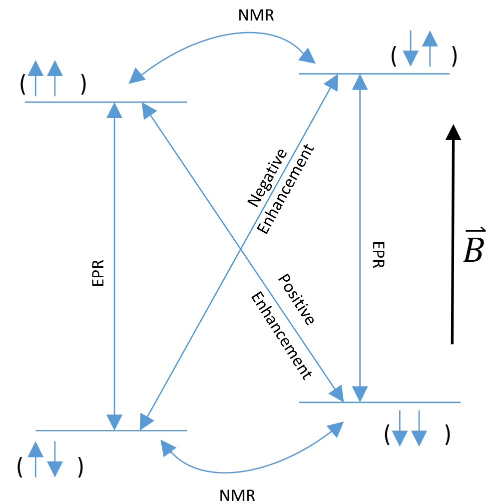


Image: https://www.jlab.org/hall-c

Dynamic Nuclear Polarization (DNP)

- Polarization: Alignment of the spin of particles in a given direction (typically $\overrightarrow{B_o}$)
- DNP: Transfer of electron spin polarization to the nucleus
- Illustrating with Solid Effect (DNP mechanism)
- Additional electrons are added when material doped with beam irradiation
- Signal picked up through NMR coil



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

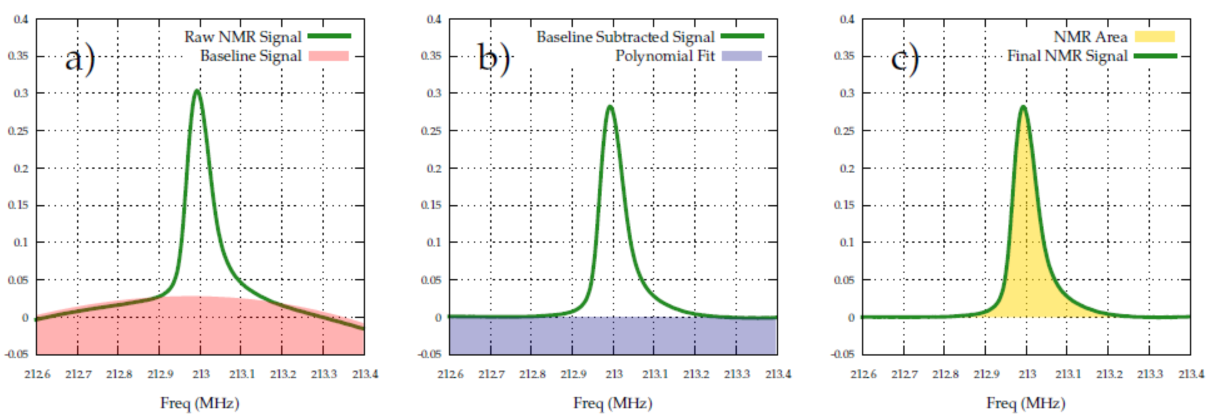
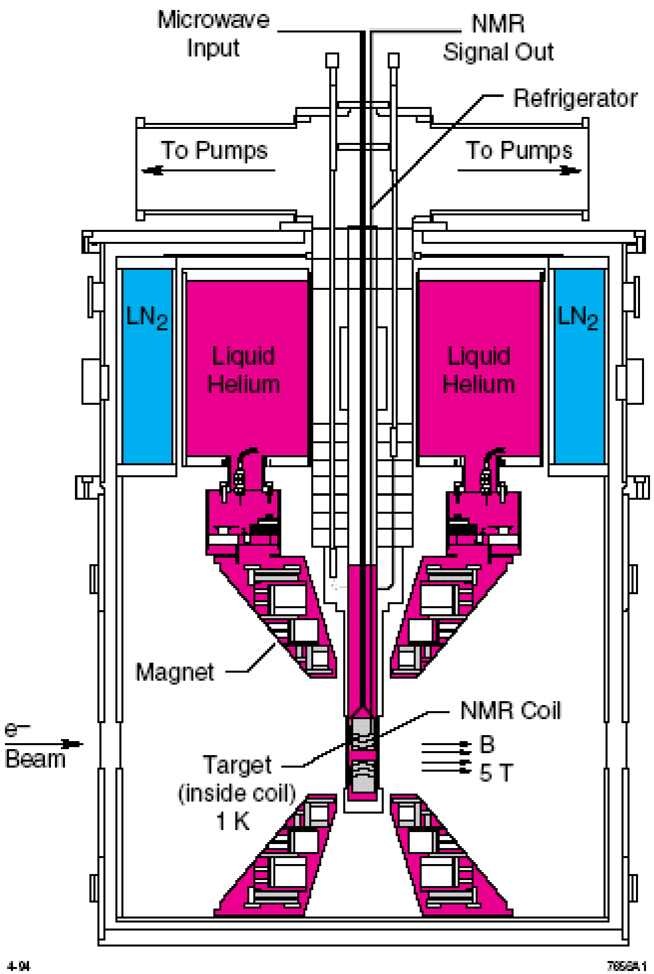


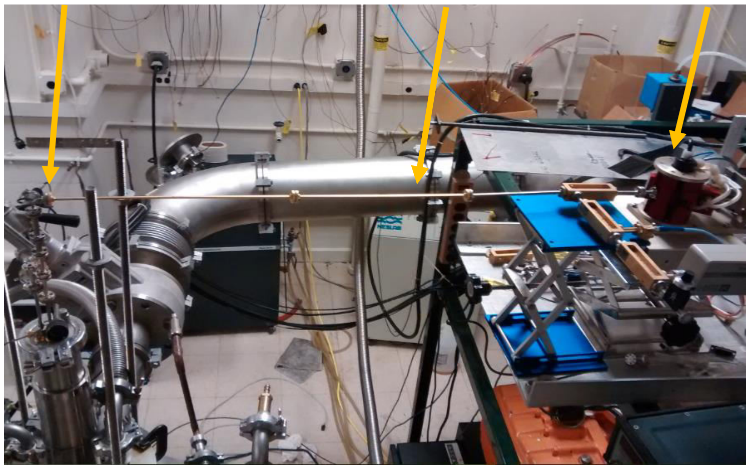
Image: Maxwell, J.(2011). Probing Proton Spin Structure: A Measurement of - at Four- Momenentum Transfer of 2 to 6 GeV2. Retrieved from http://libra.virginia.edu/catalog/libra-oa:5202

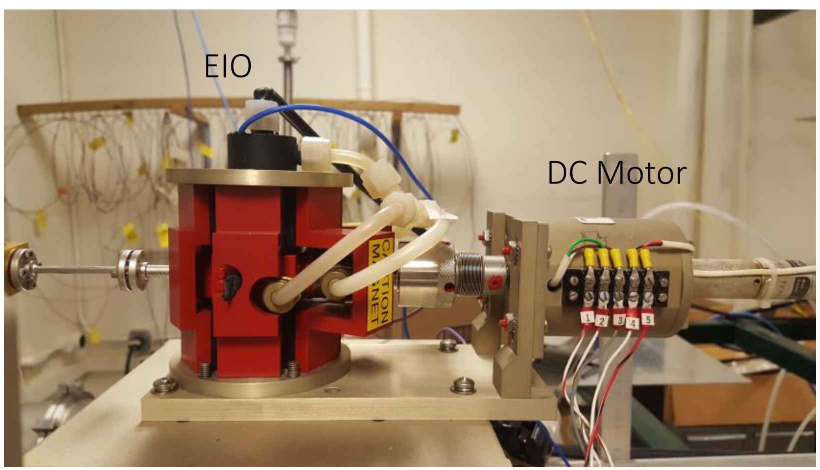
DNP

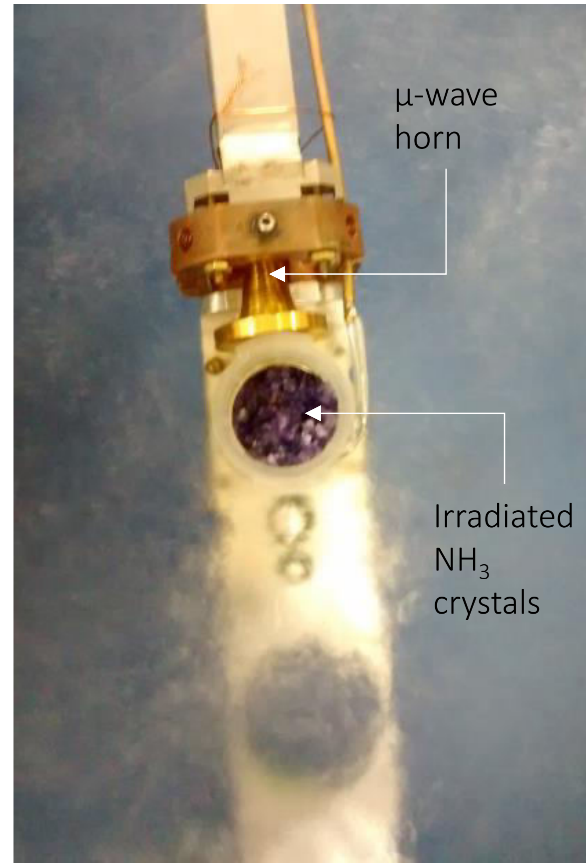

Microwave Input
NMR Signal Out
Refrigerator
To Pumps
To Pumps
LN_2
Liquid Helium
Liquid Helium
LN_2
Magnet
NMR Coil
e−
Beam
B
5 T
Target
(inside coil)
1 K
4-94


OXFORD

DNP


To magnet
Microwave Line
EIO


EIO
DC Motor
CAUTION MAGNET


µ-wave horn
Irradiated NH_3 crystals

Microwave Frequency

- Dictated by difference in nuclear Larmor and electron paramagnetic resonance frequencies (EPR)
- [140.0 GHz – 140.4 GHz for NH_3 @ 5T] / [69.7 GHz – 70.1 GHz @ 2.5 T] for positive polarization
- [140.4 GHz – 140.8 GHz for NH_3 @ 5T] / [70.1 GHz – 70.5 GHz @ 2.5 T] for negative polarization

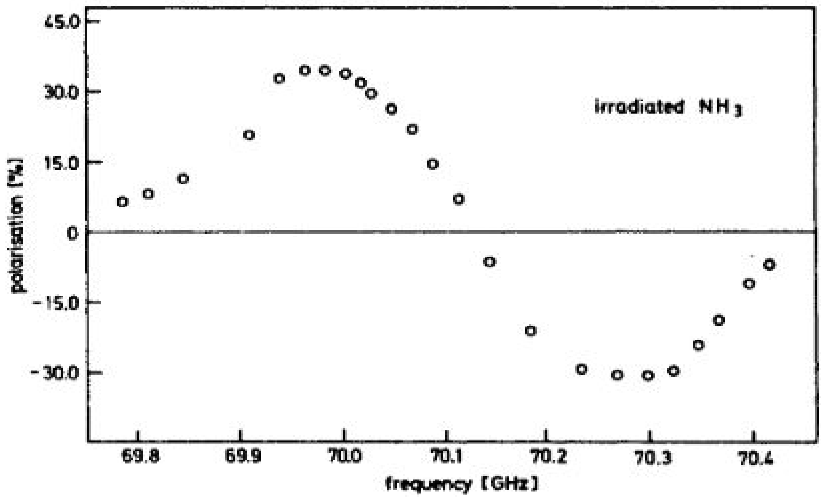


Image: Riechert, H. (1983). Polarization Properties of irradiated ammonia (NH3 and ND3) at 1K and 25 kG. AIP Conference Proceedings 95, 520 .

"Frequency Drift"

- Optimal frequency for positive and negative polarization is *not* constant

- Changes take place as more centers are created in the material as a result of irradiation.

- Steady state of polarization at a particular frequency also vulnerable to other variables such as temperature, microwave power, number of anneals, etc.

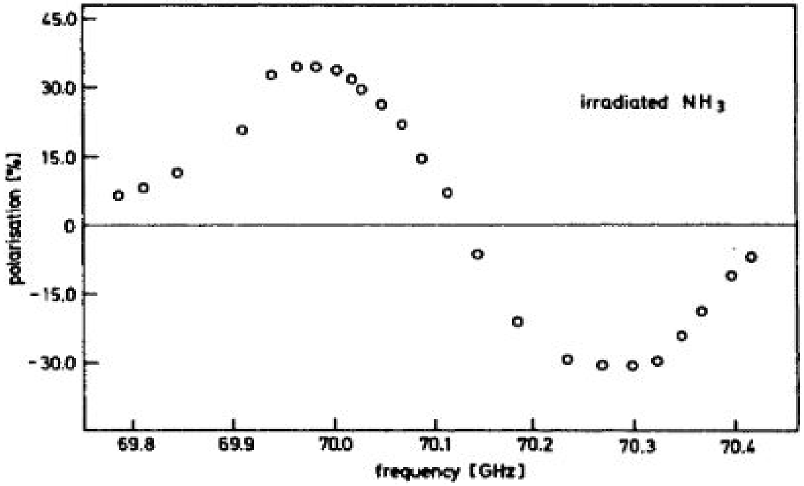
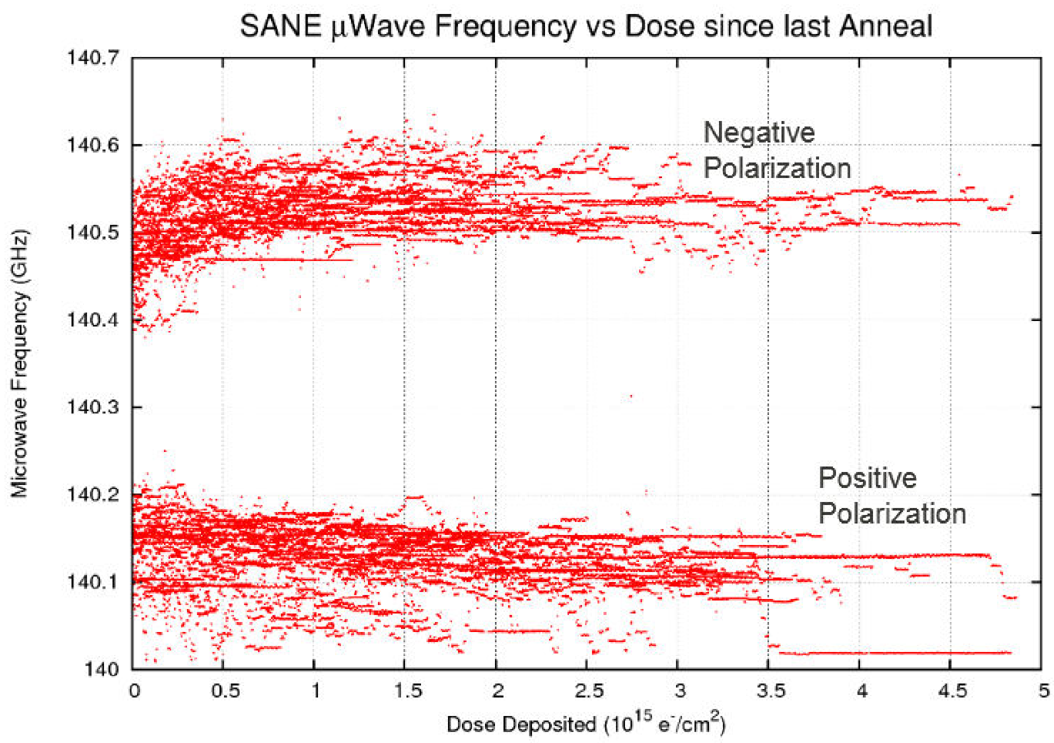
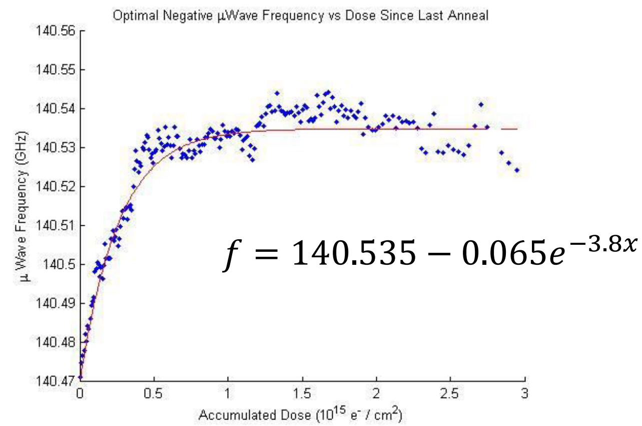


Image: Riechert, H. (1983). Polarization Properties of irradiated ammonia (NH_3 and ND_3) at 1K and 25 kG. AIP Conference Proceedings 95, 520 .

“Frequency Drift”

For the 5T field





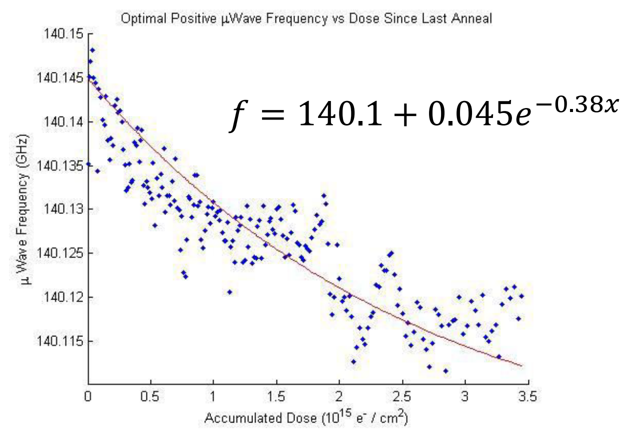
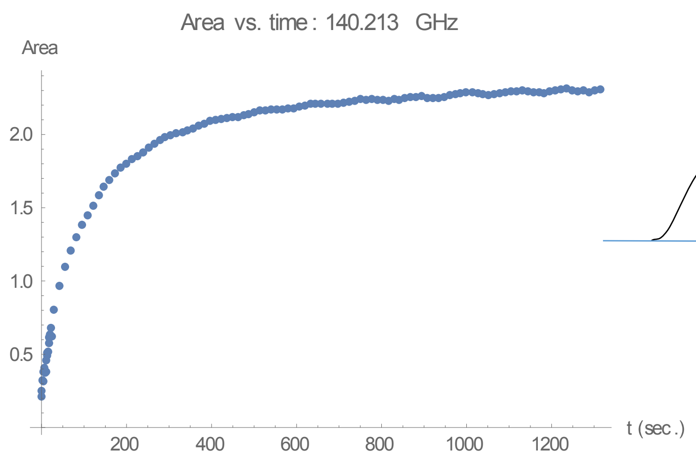
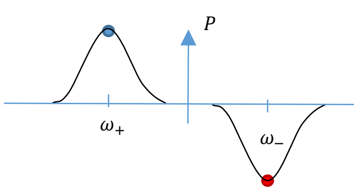


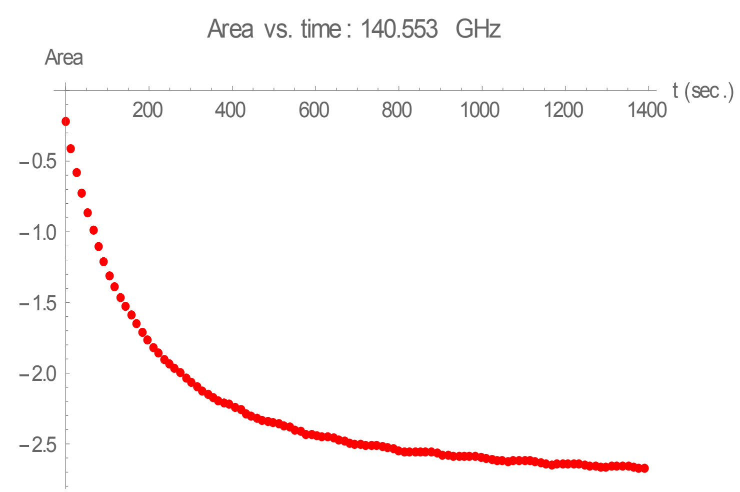
Image: https://www.jlab.org/Hall-C/talks/01_22_10/maxwell.pdf

Maintaining Highest Polarization

- Manually maintaining optimal polarization is tedious, error prone
- If characteristics of polarization growth/decay are understood, process can be automated
  - Input = EIO voltage divider value ∝ μ-wave frequency
  - Output = Polarization value from NMR analysis software



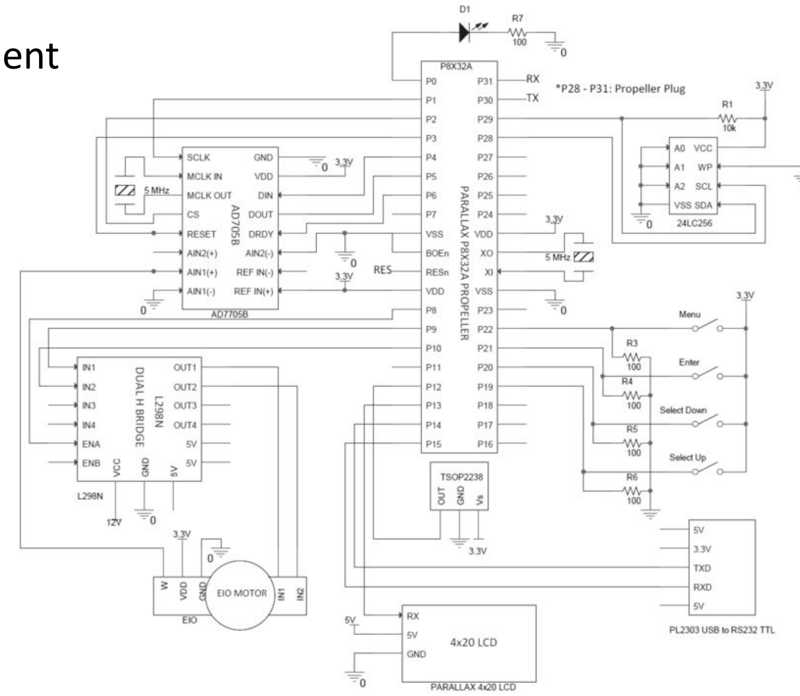




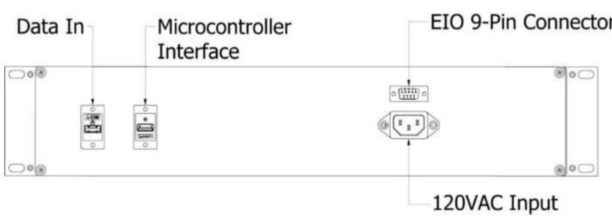
Types of Motors

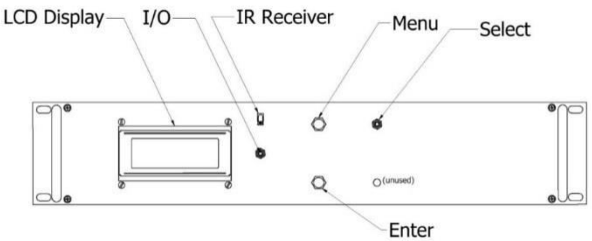
- Two motor types used with EIO
- Continuous DC motor
  - Most common motor currently in use (standard)
  - Shaft rotates continually whenever a voltage is applied
    - Movements are not very precise (can over shoot)
- Stepper motor
  - Applying voltage causes the motor to “step” by a couple degrees, and then stop
    - Allows for much more controlled movements
  - For continuous motion, a series of pulses is used

Standalone Controller (for standard motor)



- Built to replace traditional manual frequency adjustment
- Components
  - Standard 2U Rack-mount hardware
  - Parallax P8X32A microcontroller
  - PL2303 USB to RS232 TTL serial communication
  - Parallax 4x20 LCD display
  - L298N H-Bridge motor controller
- Features
  - Front-panel readout and user interface
  - Remote control support
  - Automatic and manual control of motor
  - Works with different EIOs via calibration
- Required for use with "traditional" motor

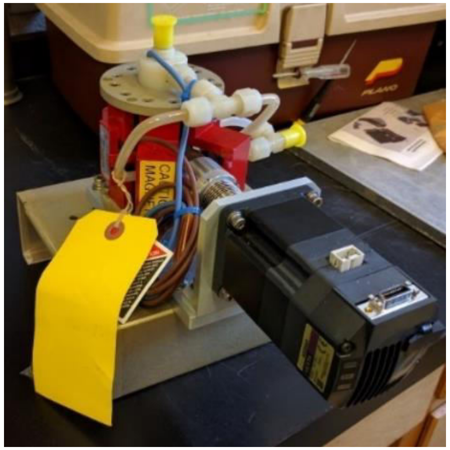




Software controller

For Polarized Drell-Yan experiment with Sea Quest (E1039)

- New hardware available from CPI: stepper motor and power supply
- Stepper motor: benefits over "traditional" motor
  - Much more precise bellows position control
  - Amount to move can be directly specified
  - Controlled directly through RS232 serial
  - EIO power supply is also controlled via serial
  - System control via LabVIEW

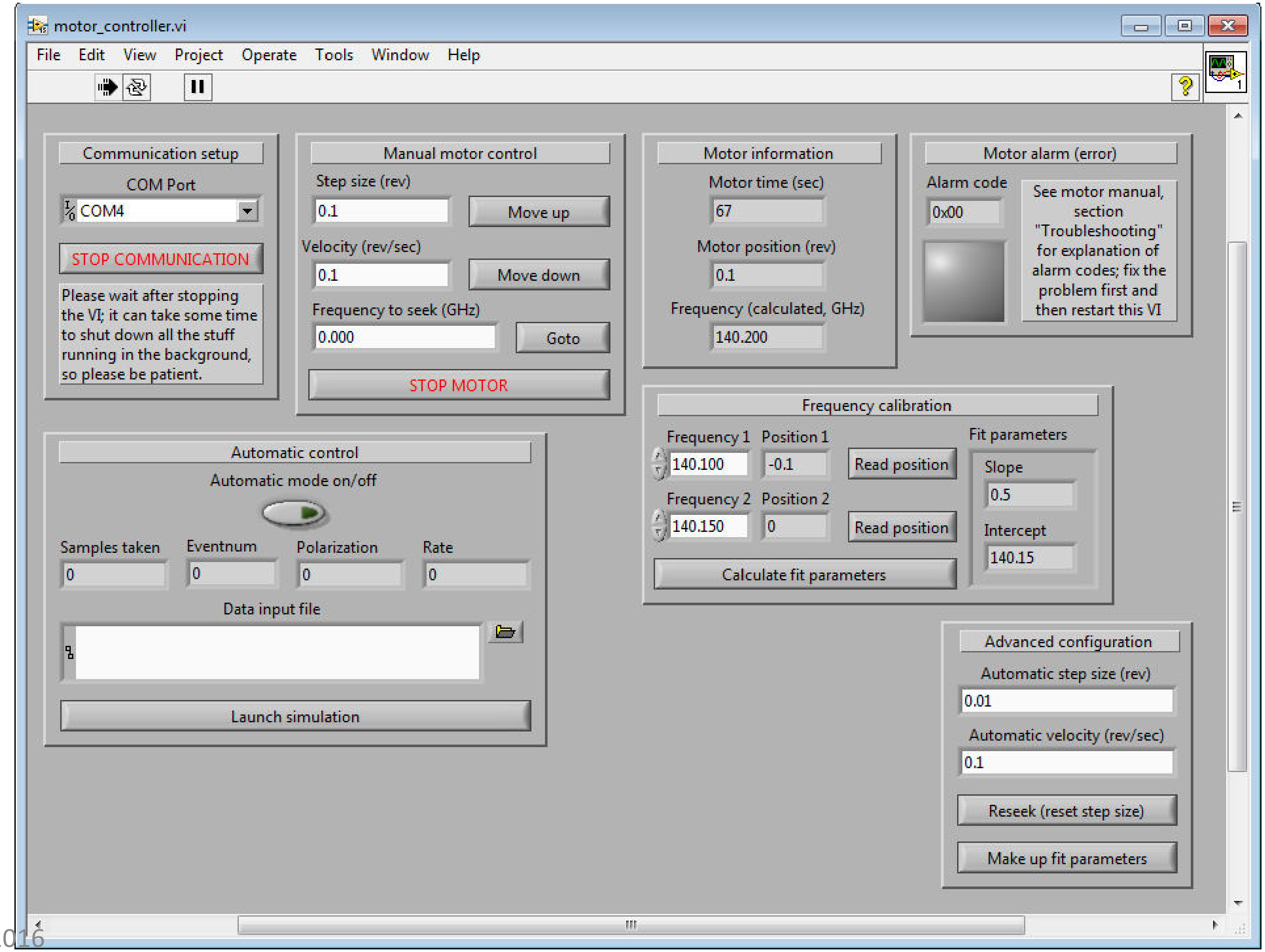


- New software controlled microwave power supply
  - Software controlled transmit/standby, power
  - Software controlled cathode, anode and filament voltages
  - Monitor cathode, anode and helix currents
  - System control via LabVIEW

Automation Control

- Must seek optimal microwave frequency
  - Uses real-time polarization
  - Change position or stay fixed
  - Switch between positive and negative
- Must perform well given external variations
  - Thermal fluctuations
  - Beam trips
  - Decay from beam irradiation
  - Microwave power variations
- Developed (and still in progress) Monte Carlo for testing efficiency and optimization under all these dynamics

LabVIEW Controller



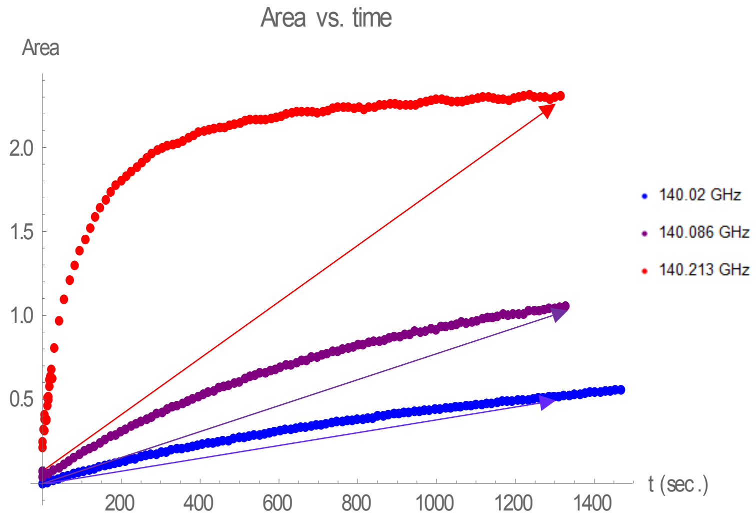
Seek Algorithm

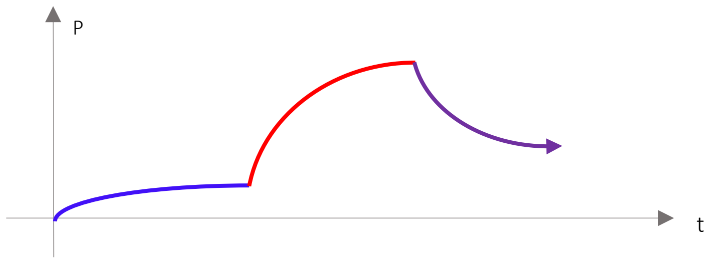
- Motion of the motor should be based on the rate of polarization increase
  - An increase in the rate implies that the motor is moving in the right direction; a decrease implies that the motor should return to a previous position

- Rates calculated using three (or more) data points (pairs of polarization and time values)
  - Calculate slope connecting adjacent data points, and then average rates:

$$rate = \frac{\frac{P_3 - P_2}{t_3 - t_2} + \frac{P_2 - P_1}{t_2 - t_1}}{2}$$

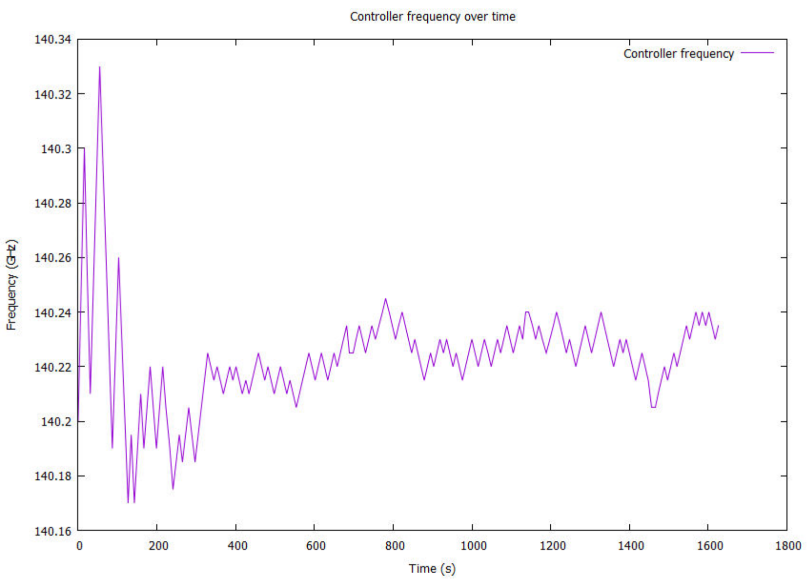
- Averaging the rates gives better results when the polarization experiences fluctuations (due to thermal effects)

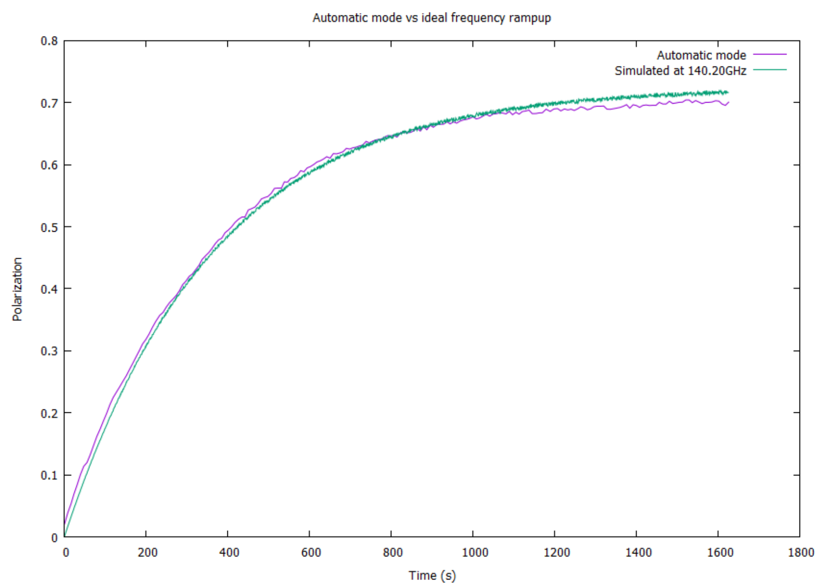




Optimal vs Seeking Algorithm

- Efficiently automates the process of a person seeking the ideal frequency
- Accurately converges to ideal frequency relatively quickly (~5 minutes)
- Quick "ramp-ups" when starting from good frequency
- Plots below taken from a run of the LabVIEW stepper motor controller, interfacing with simulation
    - Results from standalone controller box should be similar (uses same seek algorithm)





System Model

Behavior of ramp-up and decays are based on Differential Solid Effect

- Model for spin ½ from Leifson and Jeffries, 1961
  - Set of coupled differential equations for nuclear (P_n) and electron (P_e) polarizations:

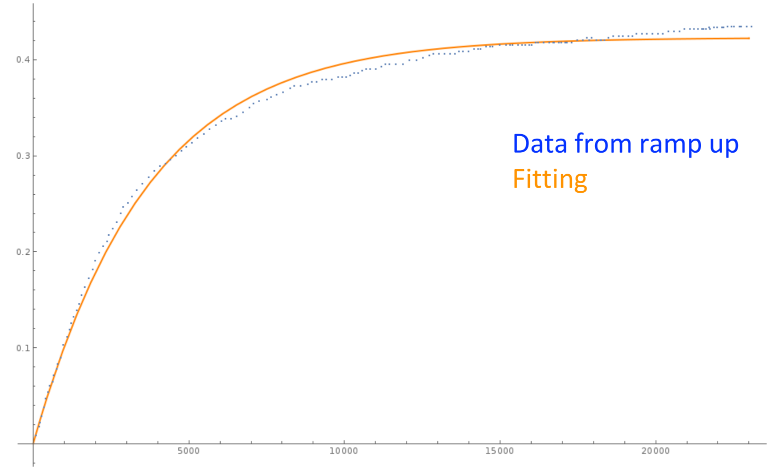
$$T_{1e}\frac{dP_n}{dt} = \left(-\frac{T_{1e}}{T_{1n}} - \frac{C\alpha}{2} - \frac{C\beta}{2}\right)P_n + \left(\frac{C\alpha}{2} + \frac{C\beta}{2}\right)P_e$$

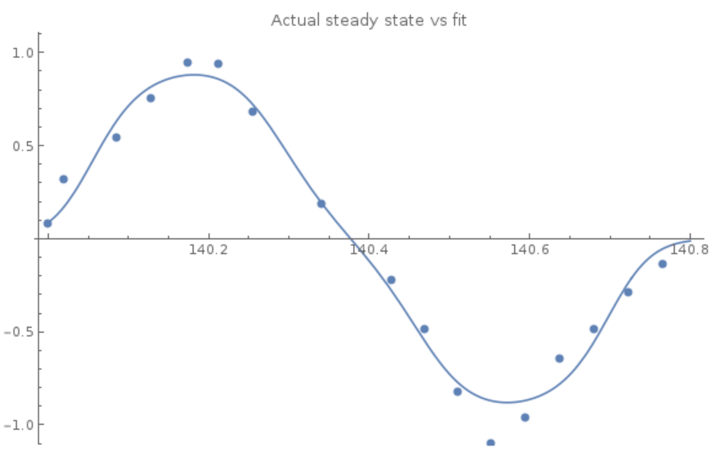
$$T_{1e}\frac{dP_e}{dt} = \left(\frac{\alpha}{2} - \frac{\beta}{2}\right)P_n + \left(-1 - \frac{\alpha}{2} - \frac{\beta}{2}\right)P_e + P_0$$

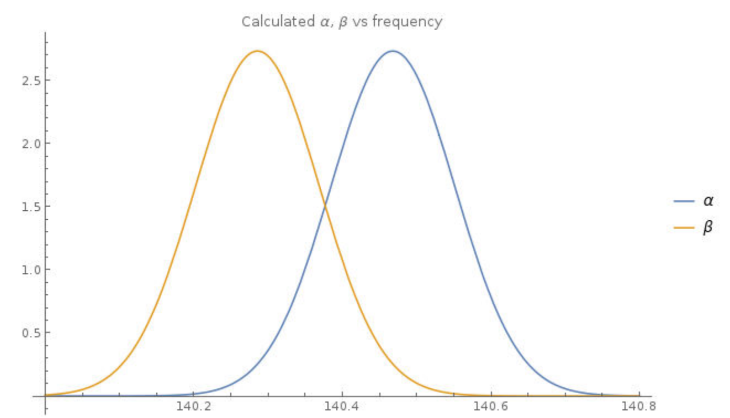
  - α and β are parameters corresponding to transitions (induced by microwave), α drives negative while β drives positive for given frequency
  - Steady state family of solutions overlap in frequency distributions
  - C is the ratio of electrons to nuclei
  - T_{1e}, T_{1n}, and P_0 are constants
  - General 'reduced' solution is of the form $P_n(t) = A + Be^{-k_1 t} + De^{-k_2 t}$

Simulation

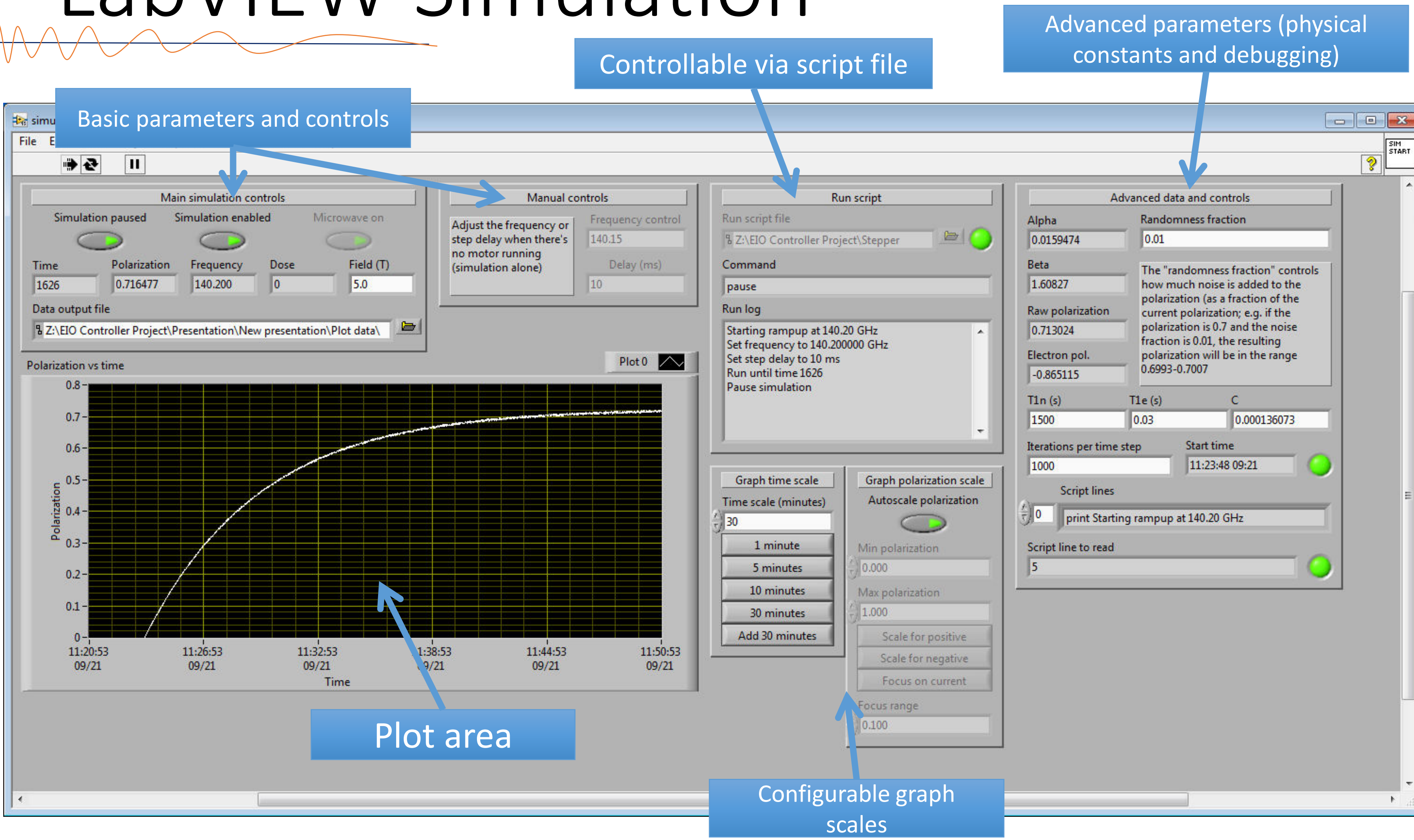
- Written in LabVIEW to work with stepper motor
  - Can also be run by itself to produce data
- Implements model
  - Parameters α and β calculated from frequency
  - Uses experimental fit to steady state P_n





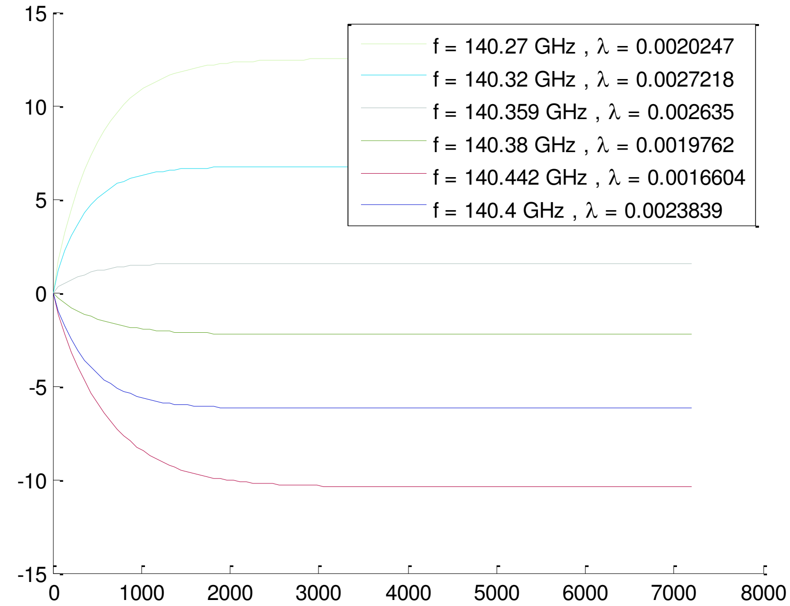


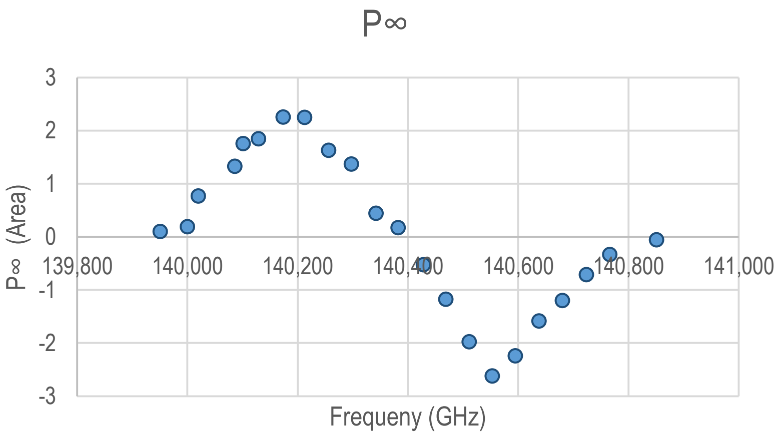
LabVIEW Simulation

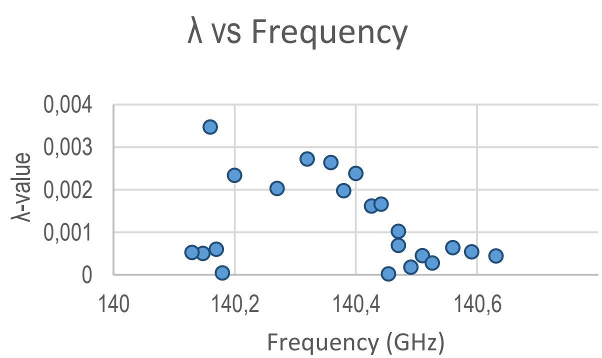


Single Exponential Approximation

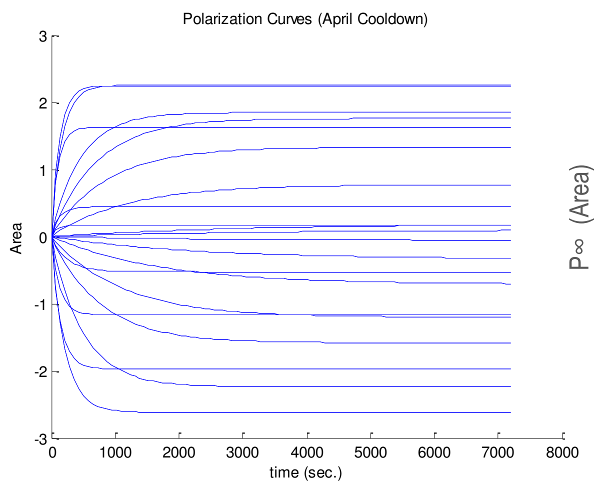
- Fit experimental data to function of the form $P_n(t) = P_\infty + Ae^{-\lambda t}$
  - Full model contains two exponential terms, one of which is very small
  - Easier to analyze in this form

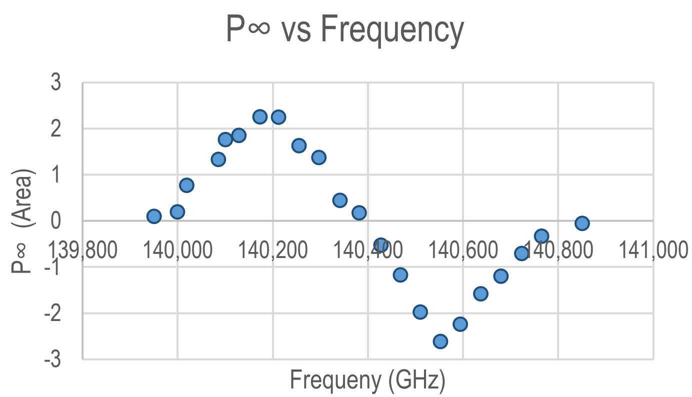


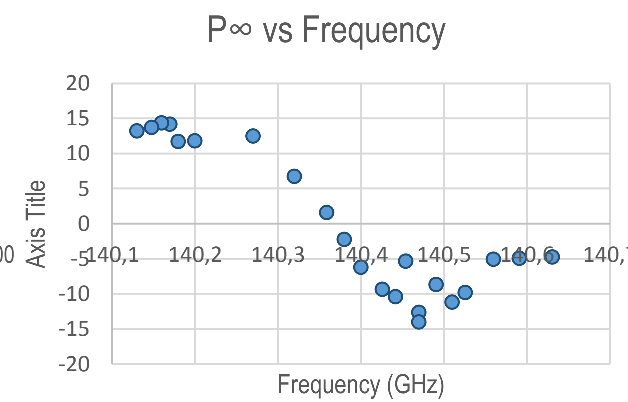


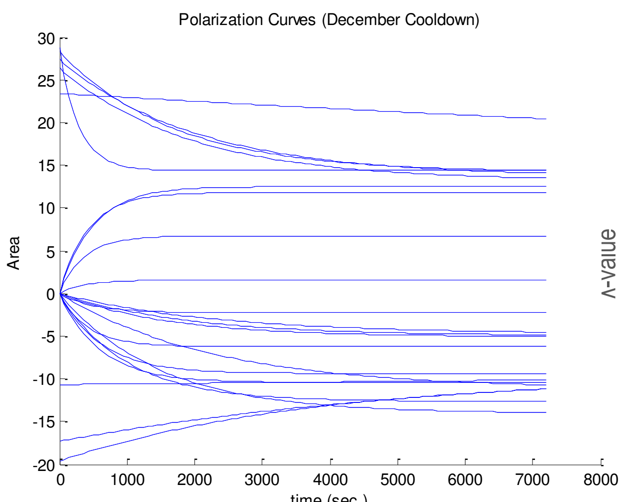


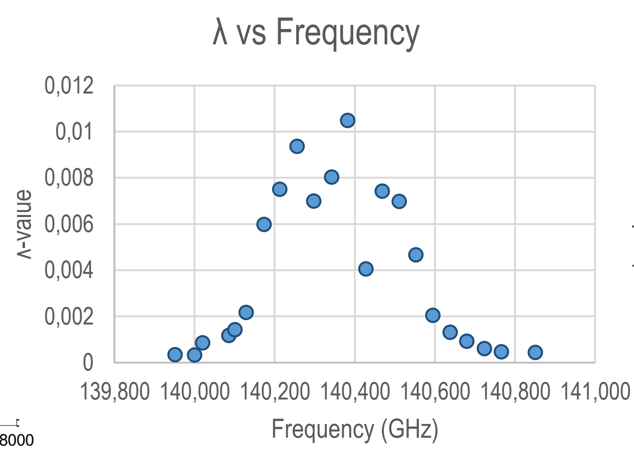
Growth/Decay Data – April and December "Cooldown"

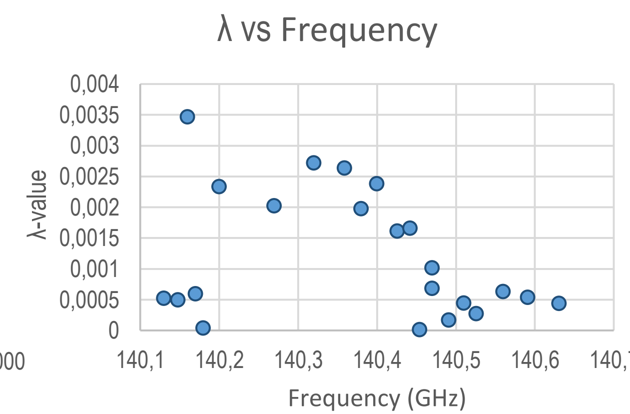






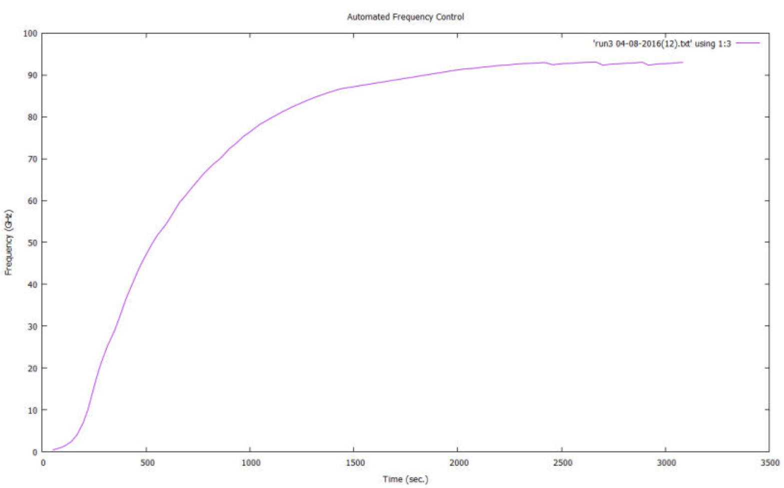






Results

- For DC motor
  - Two calibrations requires
    - One for setting position to frequency
    - One for setting microwave power factors (multiplicative term)
  - Still requires old power supply
  - Incorporates beam trips, thermal fluctuations, radiation damage
- For Stepper motor
    - One calibration
    - Full power supply tube automation still in progress
    - No data tests yet
    - Much to still incorporate



Real automated data from cooldown

Conclusion

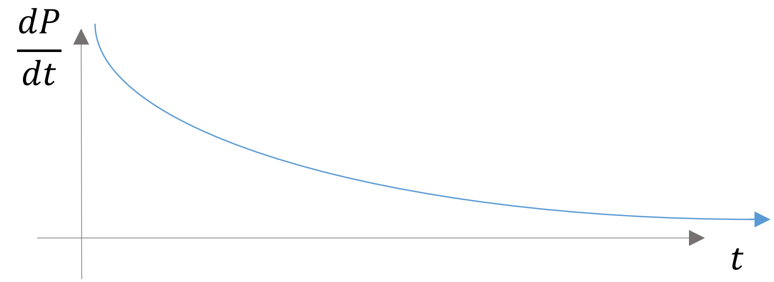
- Two controller systems
  - Standalone controller box supports continuous DC motors (self contained MC)
  - LabVIEW controller supports stepper motors/power supply
  - Both systems offer automatic and manual control of polarization experiments

- Simulation combines theoretical model and experimental data
  - Determine α and β
  - Important to check the seeking algorithm

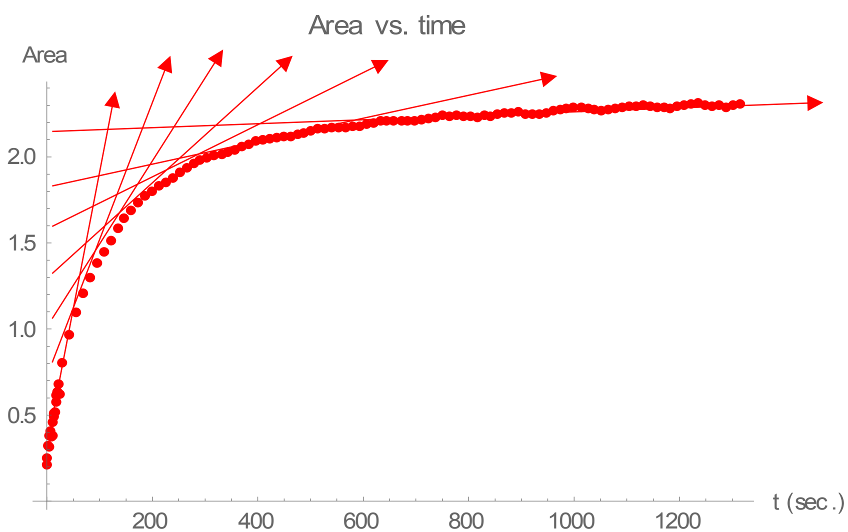
- Future plans
  - Need all radiation and cryogenic effects in full Monte Carlo (expand MC)
  - Need to test both still (stepper version not tested in cooldown)
  - Implement the simulation for spin 1 system
  - Implement tools to control power supply in connection with tube control
  - Lots of cooldown and Monte Carlo testing

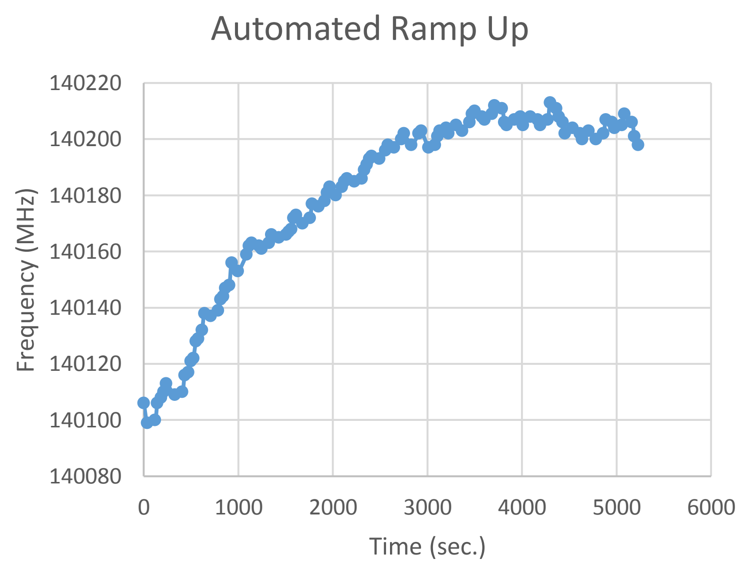
Back up

Limitations

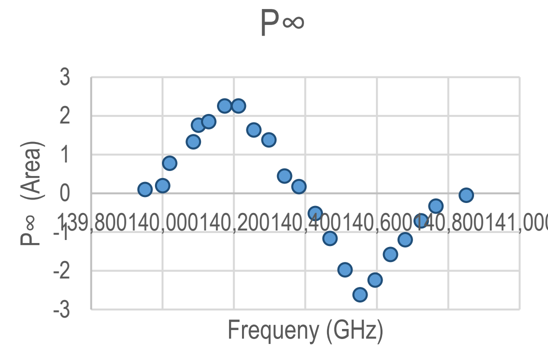


- Fairly slow process, especially when far off of f_{ideal}
- Time *dependent:* $\frac{d}{dt}(-e^{-t}) = e^{-t}$
- Frequently moves in wrong direction
  - Rate is *always* decreasing in exponential growth/decay





Time-independent Seek

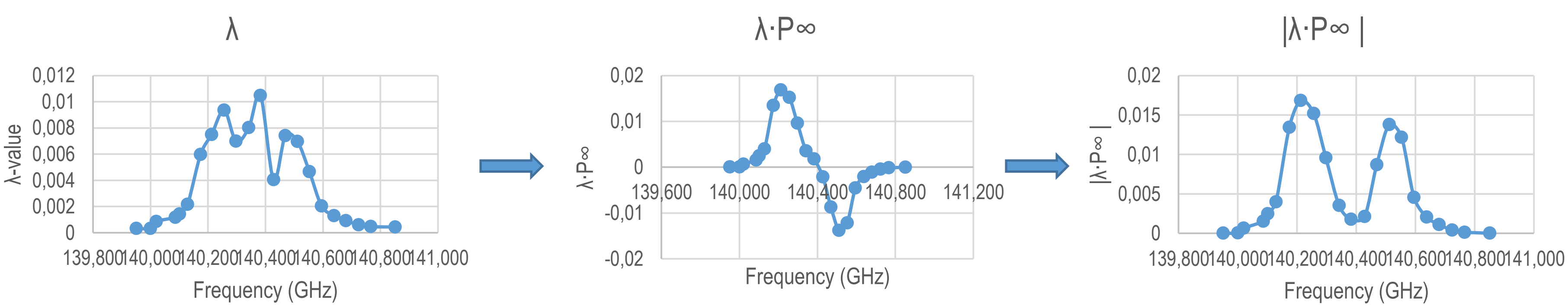


- Seeking frequency by maximizing $|\lambda \cdot P_\infty|$ would eliminate time-dependence
  - Unlike the raw rate of polarization increase, this quantity does not depend on time
- To calculate λ requires the second derivative of $P_n(t)$:

$$P_n'(t) = -A\lambda e^{-\lambda t}$$
$$P_n''(t) = A\lambda^2 e^{-\lambda t}$$

$$\Rightarrow \quad \lambda = \frac{-P_n''(t)}{P_n'(t)}$$

- Works well under perfect conditions, but thermal fluctuations make $P_n''(t)$ very hard to calculate accurately
- Time-dependent seek actually behaves better when fluctuations are present



LabVIEW Controller

- Interfaces directly with motor over RS232
  - No need for standalone controller box
- Features
  - Automatic and manual control
    - Takes advantage of precise motor steps
  - Built-in experimental simulation for testing
  - Data output during automatic mode
  - Easy frequency calibration
- Works only with stepper motor