



Research Investigations & Objectives

- ## Background

- FTMW (Fourier transform microwave) spectroscopy measures molecular transitions between quantized rotational energy levels.
- FTMW spectroscopy, when combined with supersonic molecular beams, offers a near collision-free environment to investigate fundamental properties and dynamics of Van der Waal complexes, short-lived intermediates, radicals, combustion/pyrolysis products, etc.
- Diluted analyte is pulsed into a vacuum and excited by short (<1 us) microwave pulses to record rotational spectra
- FTMW spectrometer designed by Dr. Gurusinghe research lab combines Cavity and Chirped pulse FTMW setups in a novel L-shaped design (**Figure 1**) with integrated instruments described in **Table 1/Figure 2**
- Implementation of Python overarching software allows for the development of a multitude of tools through simultaneous instrumentation control on top of ease of spectrometer use



Table 1: Main Instruments (red controlled by software)



```

183   rabeController.start(rabeController.untilIdle());
184
185   valueSteps = (float) (valueRange.getMax() - float(valueRange.getMin())) / (float(valueRange.getMax() - float(valueRange.getMin()))); // Check this with RaviL, do
186   // RabeSteps = (float) (valueRange - startValueRange) / stepInRabe
187   RabeSteps = 1
188
189   //start our run loop
190   oscilloscopeController.startCalibration();
191
192   //start trigger and then calibration
193   SMCController.startTrig();
194
195   while valueController == valueSteps:
196
197       oscilloscopeController.clear();
198
199       threadRabe = threading.Thread(target=rabeController.thread);
200
201       threadAcq = threading.Thread(target=acquireController.thread);
202
203       threadSqr = threading.Thread(target=sqrController.thread);
204
205       #start all
206       threadSqr.start()
207       threadAcq.start()
208       threadRabe.start()

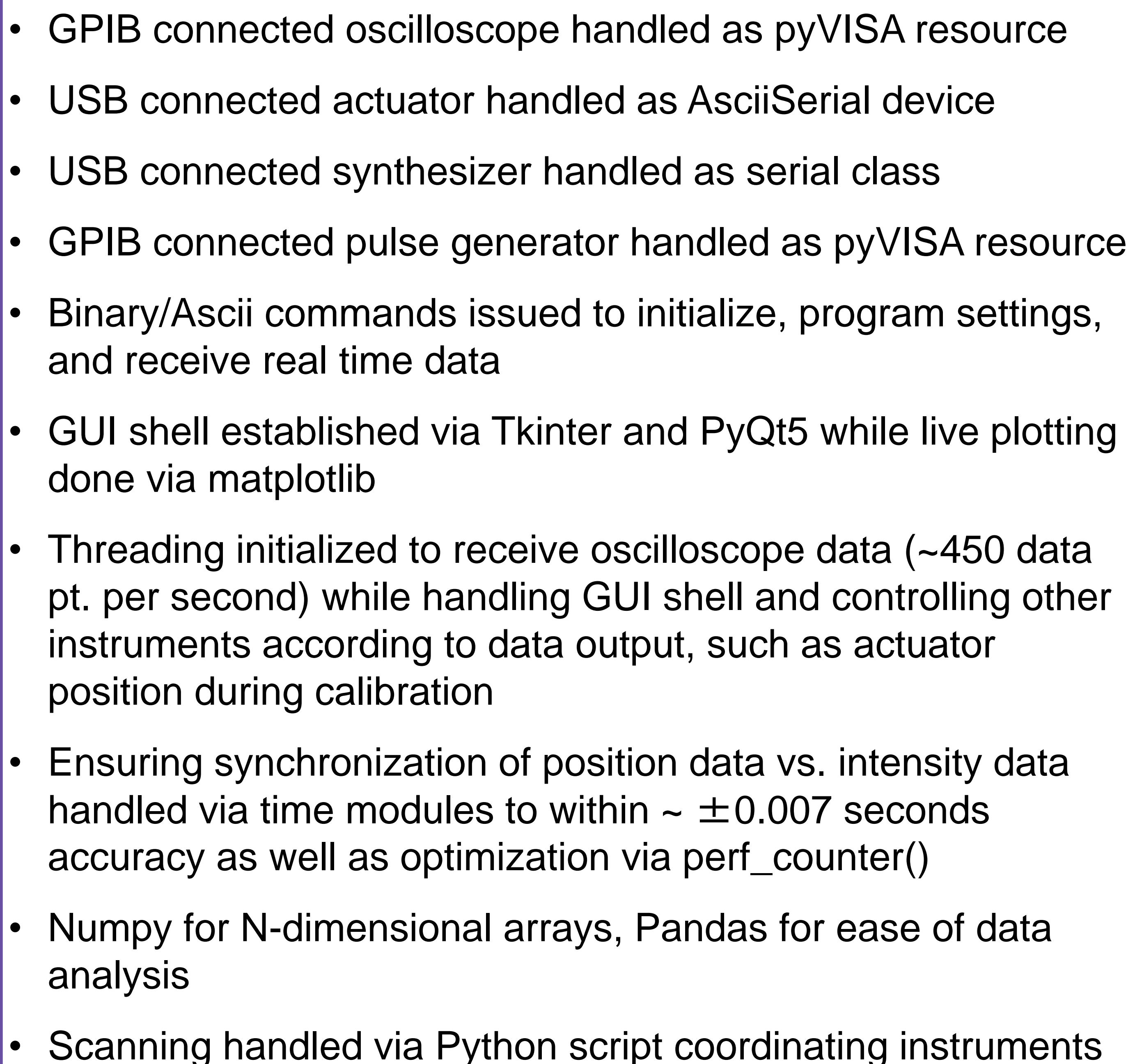
```

Instrument Control & Design

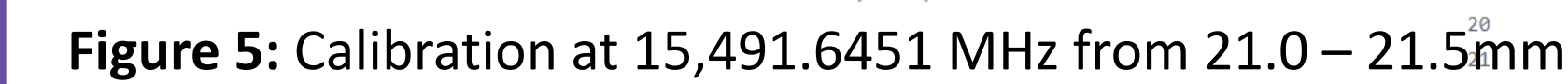
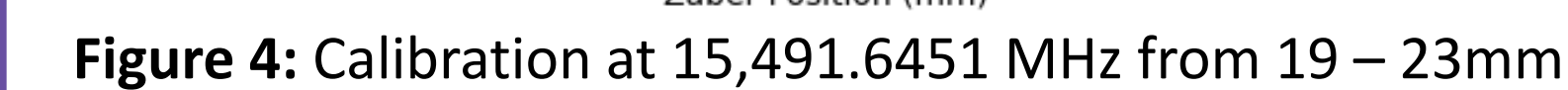
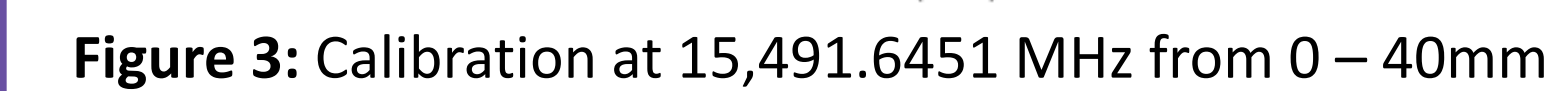
- Microwave pulses are generated using AWG and Valon synthesizers and sent to the MW cavity
- Pulse rate dictated by the delay generator
- Cavity length is dictated by the mirror that Zaber actuator positions
- Collected free induction decay signals are routed to the oscilloscope for signal averaging and Fourier transformation



Software Design



Scanning Results/Conclusions



- Cavity tuning is fully handled by Python software
- For autonomous tuning, waveforms are generated via AWG/synthesizer on initialization of internal trigger by delay generator
- Determines ideal cavity length for a particular frequency for MW experiments
- Maximum is found with ± 0.001 mm accuracy by continuing to refine actuator scan range limits and max actuator velocity
- Mirror actuator position is then fixed in the optimal position for experimentation
- Synthesizer frequency increased for the next run

```

9  def __init__(self, valonConnect):
10     global valonConnect
11
12     #overriding class of valonConnect
13
14     class VSerialPort(serial.Serial):
15
16         def __init__(self, portParam = None):
17             serial.Serial.__init__(self)
18
19             # type
20
21             self.baudrate = 9600
22             self.timeout = 3
23             self.port = port_name
24             self.open()
25             self.setDTR(False)
26             self.flushInput()
27             self.writeDTR(True)
28             self.writeDTR(False)
29
30             response_bytes = self.read(1024) #total bytes expected back from return
31             response_bytes
32             #Hex mode (continuous wave)
33
34             print("-----")
35             print("Serial port for Valon: {port_name} opened successfully.")
36             print("-----")
37             time.sleep(0.5)
38
39             # except self.SerialException as e:
40
41             print("Error opening serial port: {e}")
42
43
44     valonConnect = VSerialPort(port)

```

Future Work & References

- Chirped pulse implementation, improving Big O notation/optimization/settings, and finalizing GUI
- Integrating Tektronix Arbitrary Waveform Generator and generating waveforms via Python

References

- References:**
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 1. R.M. Gursinghe, N. Dias, R. Krueger, A. G. Suits. "Uniform supercyclic flow sampling for detection by chirped-pulse rotational spectroscopy". *J. Chem. Phys.* 156, 014202 (2022).
 2. Park GB, Field RW. Perspective: The first ten years of broadband chirped pulse Fourier transform microwave spectroscopy. *J Chem Phys* 2016;144(20):200901.
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 4. Huckauf, Dr. A. Dr. Jäger's Research Group. <https://www.chem.uolbtra.de/~jaeger/index.htm>
 5. Jo. Thomas, Oleksandr Sulchukov, Wolfgang Jäger, and Yunjie Xu. "Chirped-pulse and cavity-based FTMW spectra of the methyl lactate + ammonia adduct: lock and key selectivity and internal rotational motions." *Angew. Chem.* 125, 4498-4501 (2013). *Angew. Chem. Int. Ed.* 52, 4402-4405 (2013).
 6. Instrumentation Manuals and API documentation.



Acknowledgements: Randi K. Padikoralage, Thusitha Jayasekara, Rusiru P. Rajapaksha, Cadence Miller, Tennessee Technological University



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