AXIe Helps Unlock the Secrets of Astrochemistry

By Larry Desjardin, Modular Methods

I had the fortune to speak with Dr. Steven Shipman, a chemistry professor at New College of Florida. He's a rotational spectroscopist, which means he watches how molecules rotate, and uses that to learn about them. A molecule's rotation is a function of its three dimensional shape, so its rotational spectrum acts as a "molecular fingerprint", unique to it. While rotational spectroscopy has many applications, Dr. Shipman's research focuses on astrochemistry. He is trying to find out how and why complex molecules formed in interstellar space, and ultimately how our life-bearing planet came to be the way it is. Along the way, he also has interest in continually pushing the technology to make better and faster measurements. That's where AXIe comes in.

To understand the measurement challenge, it is important to understand how rotational spectroscopy measurements are made. A chirped pulse is created that shifts from 0 to 5GHz in 250ns. To create this chirped pulse, Dr. Shipman uses an AXIe Arbitrary Waveform Generator, the Agilent M8190A. It is a two channel AWG in a double-wide AXIe module that can sample up to 12Gs/s. This pulse is filtered, frequency shifted up to 26.5GHz, and amplified using a variety of external microwave components.

This amplified signal interacts with the rotating molecule, which then generates its own phase-coherent signal. This is digitized by a digitizer or oscilloscope. The main challenge is that the signals are both extremely weak and short-lived (10 microseconds at most). An enormous amount of averaging is required to achieve the signal-to-noise ratio needed to study the molecules in detail. Dr. Shipman noted that they historically averaged two million cycles, which required roughly seven hours. This was tedious for Dr. Shipman's students, who spent hours doing the data collection instead of doing coursework or focusing on the basic research itself.

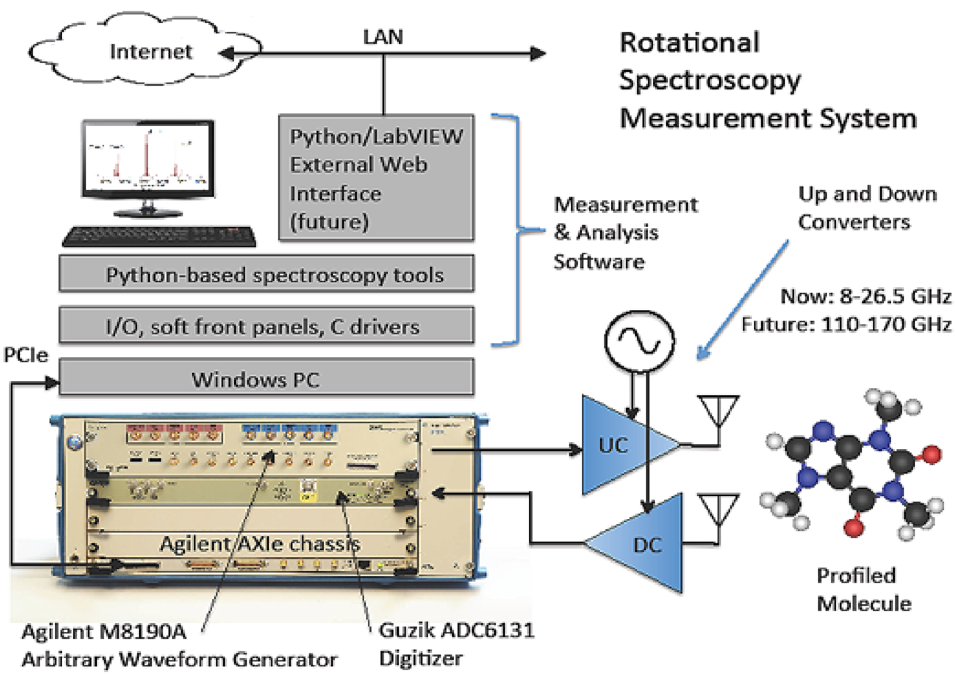
The averaged signals were then analyzed using publicly available spectroscopy programs, or scripts that Dr. Shipman and others have written in Python. Fourier transforms are key elements to the analysis.

The throughput bottleneck was the overhead of off-board averaging techniques. This was a key reason for Dr. Shipman's selection of the Guzik ADC6131 AXIe digitizer. The ADC6131 captures signals at 40Gs/s with 13GHz of bandwidth and 8 bits of resolution. Each single-slot module has 64GBytes of on-board memory, a PCIe (PCI Express) Gen 2 backplane interface, and a high-speed local bus. Most importantly, it also includes an on-board FPGA-based signal processing system based on Altera FPGAs.

The on-board FPGAs proved crucial, as the digitizer performed the averaging itself, and sent the averaged data to the computer. The speed improvements were impressive. "It used to take me approximately 3.5 hours to collect a million averages," Shipman claimed," I can now do this in roughly 12 seconds with the new digitizer."

Besides freeing up time for him and his students, the fast measurement and average times also give Dr. Shipman other options. While an average of two million samples was the previous standard, the system has shown excellent phase stability out to one billion averages. The results match precisely the results from his previous system, but the added averaging improves the signal to noise ratio even further.

The figure below shows a block diagram of the new system.



The AXIe subsystem is the core of the measurement system, and consists of the Agilent M9505A 5-slot AXIe chassis, the Agilent AWG, and the Guzik digitizer. The AWG creates a 0-5GHz chirped signal, which is upconverted to between 8 and 26.5 GHz. This interacts with the molecule under test, which creates its own phase-coherent signal, but for 10 microseconds or less. It is downconverted and then digitized by the Guzik digitizer. This cycle is quickly repeated until the critical number of averages is achieved.

The AXIe system is connected to a Windows PC via PCIe Gen 2. This is an extremely fast low-latency connection. Dr. Shipman uses VISA as the I/O layer, delivered with the Agilent drivers. While C drivers (such as IVI-C) could be used to control the instruments, Dr. Shipman's first system is being used manually. He controls the

Agilent AWG using the soft front panel software delivered with the product, and receives the averaged information from the Guzik digitizer using a simple C driver.

The data is then analyzed with public domain and internally generated Python tools that do the actual spectroscopy measurements. Dr. Shipman plans to make the system available over the web to other researchers through a remote control interface. For this they are developing a web interface based on Python and LabVIEW. By changing the upconverters and downconverters, Dr. Shipman plans to upgrade the system to cover 110 to 170 GHz in the future.

Now, back to astrochemistry. Once the spectra of various molecules have been collected, many different things can be done with the data. Of particular interest to Dr. Shipman is the mapping of molecules in the interstellar medium with radio telescopes. By determining exactly where molecules are located, it is possible to see which compounds are correlated or anti-correlated with each other. This in turn gives clues about how the molecules are formed and destroyed, which may eventually lead back to why the planet Earth is the way it is.

Besides astrochemistry, rotational spectroscopy has applications in trace gas detection in environmental monitoring. This is useful for understanding atmospheric chemistry, and monitoring industrial processes to ensure they are operating correctly.

Dr. Shipman can be contacted via email at shipman@ncf.edu, and his other contact information is available at the New Florida College website here. While Shipman's test system is a particularly unique application, the desire for performance and speed is shared by many engineers. Dr. Shipman has demonstrated the performance capability of a multi-vendor AXIe system in a dramatic fashion. His own words sum it up well, "The speed with which it can acquire data is still breathtaking."