OPEN-SOURCE, MODULAR APPROACHES FOR ION MOBILITY SPECTROMETRY

Brian H. Clowers,[1] Gordon A. Anderson,[2] Kelsey Morrison,[1] Peyton Nosbusch,[1] Austen L. Davis[1]

[1] Department of Chemistry, Washington State University, Pullman, WA [2] GAA Custom Engineering, Benton City, WA

INTRODUCTION

- Outside an ionization source and a Faraday plate, a drift tube IMS system is fundamentally comprised of 5 primary components:
  - Reaction/Drift Cell
  - Ion Gate
  - Gate Pulsing Electronics
  - Current to Voltage Converter
  - Data Acquisition System (DAQ)
- Within the IMS research community hardware and DAQ solutions are often custom and rarely replicated exactly.
- In an effort to address this knowledge and resource gap, we outline a range of solutions to the construction and operation of research-grade ion mobility spectrometers.

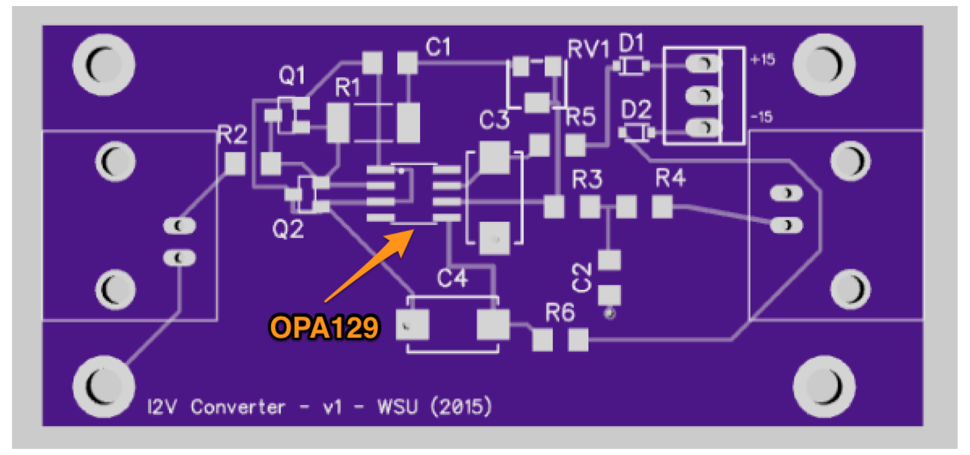


Figure 1. Circuit schematic for a current to voltage amplifier used for gains of 10^8 established through R1. Optimization of the amplifier circuit is required for higher gains. Diptrace and eagle files are located via github (https://goo.gl/82c3Yo)

AIMS

- **Develop and disseminate a series of hardware, software, and DAQ solutions.**
  - **Leverage off the shelf, compact DAQ solutions**
- **Demonstrate the feasibility of a wireless DAQ systems for IMS experiments.**
- **Evaluate performance of floating, wireless ion gate pulsing system.**
- **Encourage collaborative efforts to realize optimum hardware/software solutions for reproducible IMS research.**

SOFTWARE AND HARDWARE TOOLS

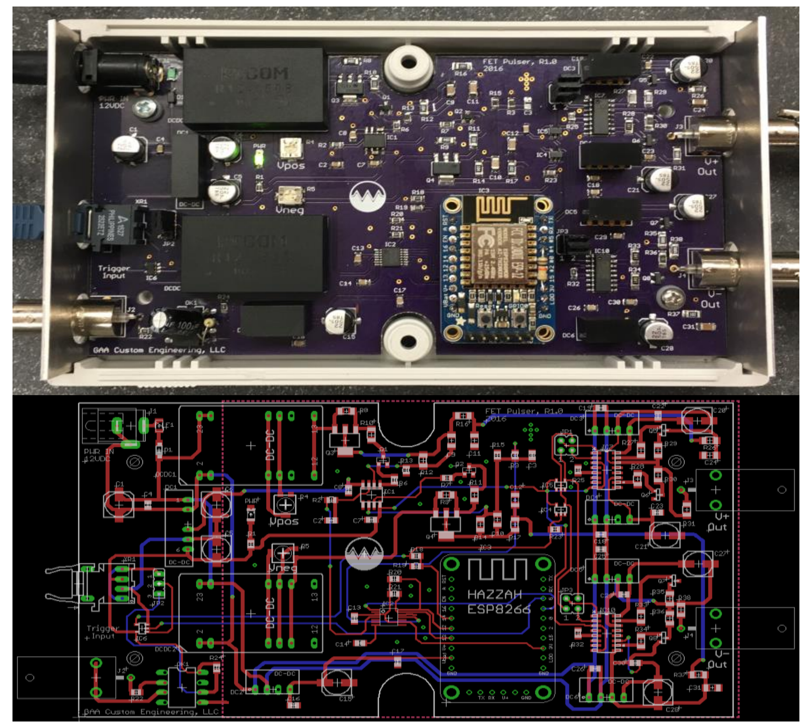
- **DipTrace/Eagle CAD** (electronic design)
- **www.wipy.io**
  - **Open source, wireless, microcontroller**
- **Python**
  - **Cross platform GUI and signal processing**
- **Redis** (results database)

METHODS

- Development of FET pulser was based upon initial designs by WSU employed over the past 25 years.
- Testing of the FET pulser and resulting mobility spectra was acquired using a custom stacked ring IMS system operated at 180 ºC.
  - Initial benchmarking of the pulser was conducted using a 1kHz square wave with a 50% duty cycle (Figure 2).
- Code revisions, design documentation, and updates are currently available through both github and www.clowersresearch.com.

FET Pulser System

- +/- 200 V 0-peak
- 12 Volt Input
- Wireless control of settings
  - ESP8266 (Huzzah Adafruit)
- Fiber Optic Isolation
  - TTL input logic
- Independent channel control
  - http://goo.gl/wqhqrA



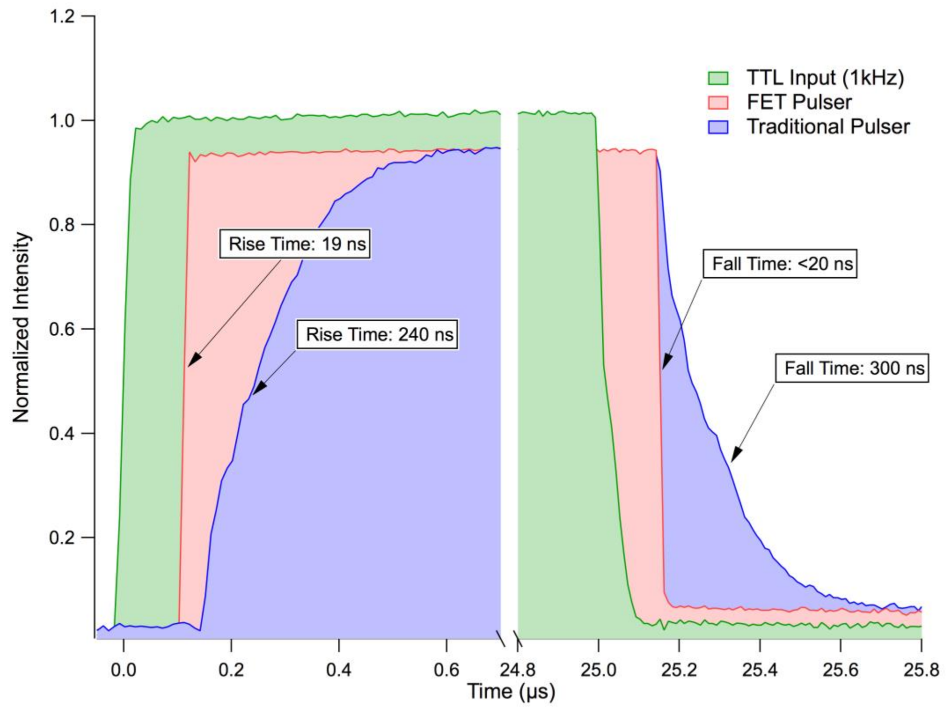


Figure 2. Comparative performance of the newly designed FET pulser illustrates improved rise and fall times when tracking a 1kHz input TTL signal with a 50% duty cycle. The +/- voltage for both the traditional WSU pulser and the newer design was set to 50 V for each output. The performance of the custom, wire-wound transformer, illustrates rise and fall times that approach a few hundred nanoseconds where the newer solid state design yielded pulse transitions in under 20 ns.

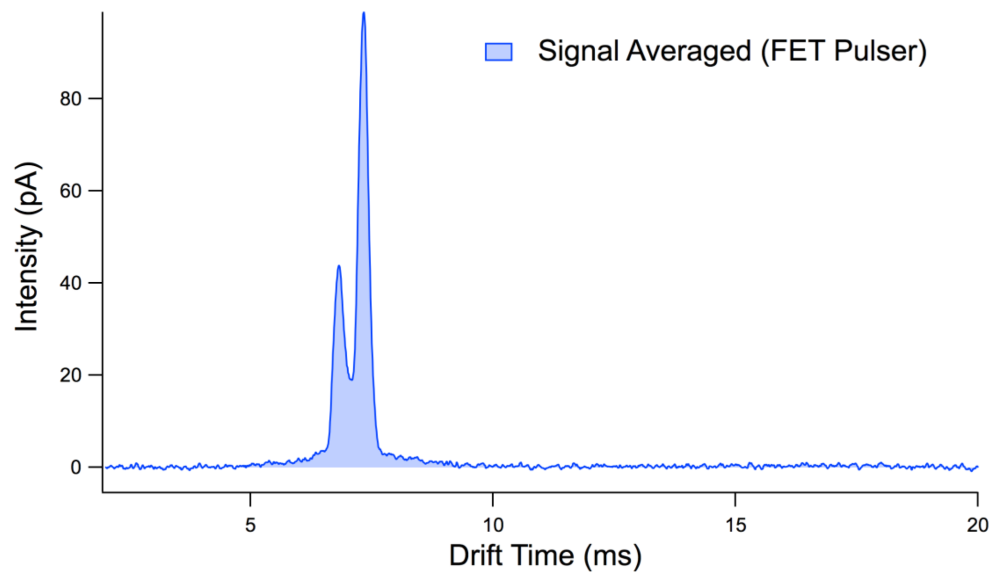


Figure 3. Using a 150 µs gate pulse width as an input, the mobility spectrum to the right highlights the reactant ion peaks obtained using the new FET pulser. The newly design system was floated at 7500 V and operated using a 2200 mAh LiPo battery. Under these conditions the FET pulser was able to operate continuously for ~550 minutes (just shy of initial calculations).

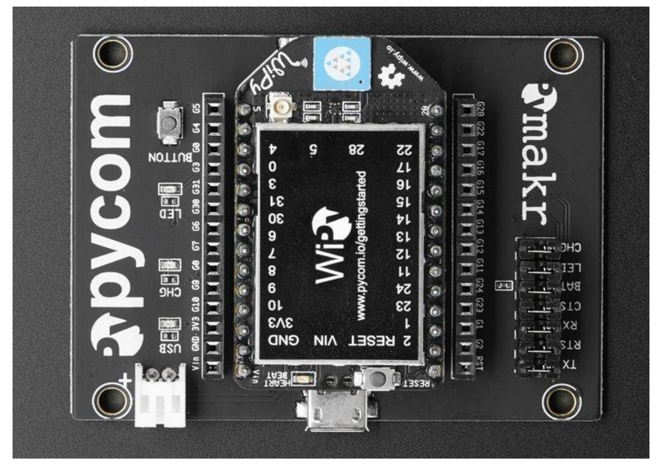


Figure 4. Wipy system mounted to an expansion board providing direct access to I/O pins and an onboard micro SD slot.

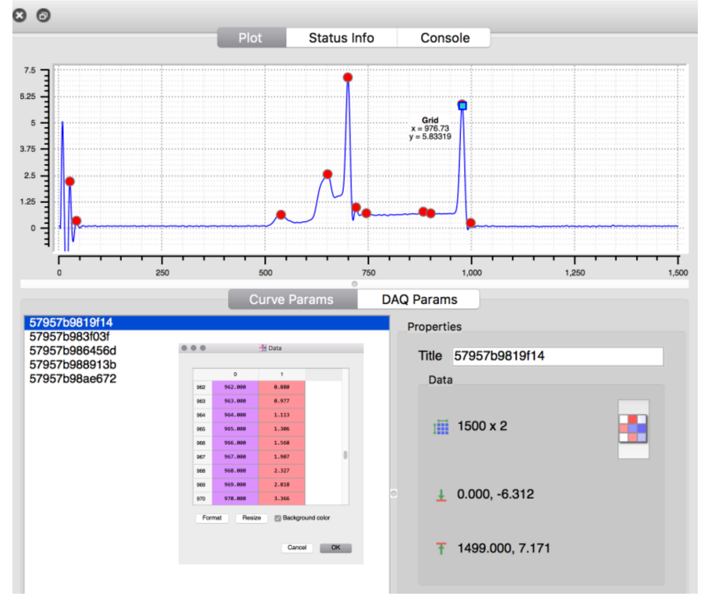


Figure 5. Cross platform GUI providing an interface to the local redis database. Additional features include data export, DAQ parameter uploading, and peak picking.

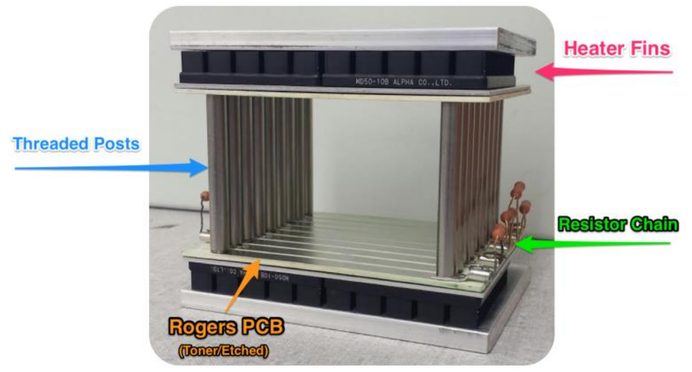


Figure 7. Prototype desolvation region with built-in gas heating. Electrode surfaces are made from Rogers 4350 PCB material and 0.1875 diameter stainless spacers. The dimensions are compatible with grounded insulation to minimize high voltage exposure.

Data Acquisition System

- Wireless microcontroller
  - Cortex-M4 @ 80MHz with RTC
    - RAM: 256 Kbytes
    - Flash: 2 MBytes
  - 4 16-bit timers (16 and 32 -bit)
  - 3 12-bit ADCs (1.8V limit)
  - WiFi: 802.11b/g/n
- Python control environment
  - Standard python modules
  - Excludes floating point numbers
- Hardware based DAQ
  - TTL Trigger
  - FIFO
- Redundant Storage/Transfer
  - Redis server
    - Laboratory computer
  - Direct streaming
  - Onboard SD card

RESULTS

The normalized traces shown in Figure 2 highlighted the ability of the newly designed FET pulser to realized improved rise and fall times. Measured with an oscilloscope probe, the actual peak voltage was routinely lower that expected by approximately 2.1 volts, however, this offset was easily accommodated. The wireless-enabled Wipy platform demonstrated acquisition rates approaching 100 kHz which is more than sufficient for IMS measurements. Challenges to the system remain, specifically, with ADC input voltages limited to 1.8 V. A solution for ion current conversion and amplification highlights gains for 10^8 exists, however, input source matching remains critical. The cross-platform GUI is compatible to any redis server and may prove useful for a wide range of DAQ efforts.

CONCLUSIONS

- Using github as a repository, a series of hardware and software solutions are presented and open for improvement.
- The solid-state, floating ion gate pulser marks an improvement over the performance of historical pulsers.
  - Continuous battery operation at high voltage is possible for ~9 hours.
- The DAQ platform is highly customizable, relatively inexpensive ($50 USD), and demonstrates data acquisition rates sufficiently high for IMS measurements.
- The use of the asynchronous redis server maintains a repository of data but is compatible with real-time streaming from the wipy device and can also be used to push DAQ settings.
  - Redundant data storage is accomplished with the wipy using an onboard SD card.
- A cross-platform data viewing and processing platform was developed that leverages a redis server which features direct data export and peak picking.

FUTURE DIRECTIONS

- Improve data streaming and pulsing control across the wipy and pulser platforms.
- Integrate thermoelectric trickle charger to harvest excess heat from the IMS cell.

ACKNOWLEDGEMENTS

Support for this work was supported in part by the NSF (CMI-1506672) and ARO (W911NF-15-1-0619). The authors would also like to recognize the assistance of both Wenjie Liu and Eric Davis.

WASHINGTON STATE UNIVERSITY

BRIAN H. CLOWERS, PH.D.
brian.clowers @ wsu.edu
www.clowersresearch.com