

# An Automated, Open-Source Calibration System for Peroxyacyl Nitrates

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**Abstract.** A fully automated, open-source calibration system was developed to control the separation and quantification of peroxyacyl nitrates (PANs) using gas chromatography (GC). The system communicates with three data acquisition (DAQ) boards: Measurement Computing's USB-1408FS, USB-1608FS, and National Instruments' USB-6009. These DAQ boards controlled mass flow controllers, performed timed valve switching, and acquired  
10 analog signals. The software replaces proprietary LabVIEW code while offering precise control of PAN injections. The system proved to be reliable and robust through multiple tests, including successful isolation of PAN from a mixture containing acryloyl peroxyacrylate (APAN) and other atmospheric contaminants. A stress test showed stability and reliability under long term continuous operation. Additionally, the platform allows flexible configuration of flow and timing sequences, requires no licensing, and is portable across compatible Windows  
15 systems. Minor usability limitations were identified but did not impact analytical performance, allowing this system to be an effective and reproducible tool for laboratory research of PAN-type compounds.

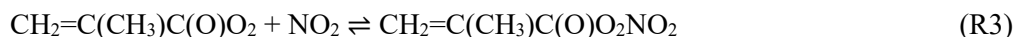
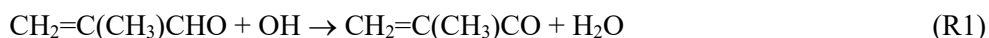
## 1. Introduction

Peroxyacyl nitrates (PANs), with the general chemical formula  $RC(O)O_2NO_2$ , are a class of nitrogen containing organic peroxides synthesized in the troposphere through the photochemical oxidation of volatile organic  
20 compounds (VOCs) in the presence of nitrogen oxides ( $NO_x \equiv NO + NO_2$ ). Elevated levels of PANs are usually observed in environments impacted by photochemical smog or biomass burning emissions, both of which indicate degraded air quality (Grosjean et al., 1993; Gaffney and Marley, 2021). In such environments, human exposure to PANs has been linked to unfavourable health effects, particularly eye discomfort and irritation (Altshuller, 1978). PANs are relevant in tropospheric photochemistry since they act as reservoirs for reactive nitrogen oxides. Unlike  
25  $NO$  and  $NO_2$ , which react and deposit near their emission sources, PANs are thermally more stable under colder conditions and can persist for hours to days, allowing the transportation of  $NO_x$ . Once transported to warmer

regions, they thermally decompose, releasing NO<sub>2</sub> and peroxy radicals which enhance local ozone production (Roberts, 1990).

While acetyl peroxyxynitrate (also known as peroxyacetyl nitrate or PAN) is usually the most abundant, other PAN-type species such as propionyl peroxyxynitrate (PPN), acryloyl peroxyxynitrate (APAN), methacryloyl peroxyxynitrate (MPAN), i-butyryl peroxyxynitrate (PiBN), n-butyryl peroxyxynitrate (PnBN), benzoyl peroxyxynitrate (PBzN), and furoyl peroxyxynitrate (fur-PAN) have also been detected (Roberts et al., 2022).

A representative example of PAN formation is methacryloyl peroxyxynitrate, which is produced from methacrolein (2-methylprop-2-enal) (Mielke & Osthoff, 2012). The mechanism begins with abstraction of the aldehydic hydrogen by the hydroxyl radical, forming an acyl radical. This radical reacts with molecular oxygen to form a peroxyacyl radical, which then combines with NO<sub>2</sub> to produce MPAN. The reaction sequence is as follows:

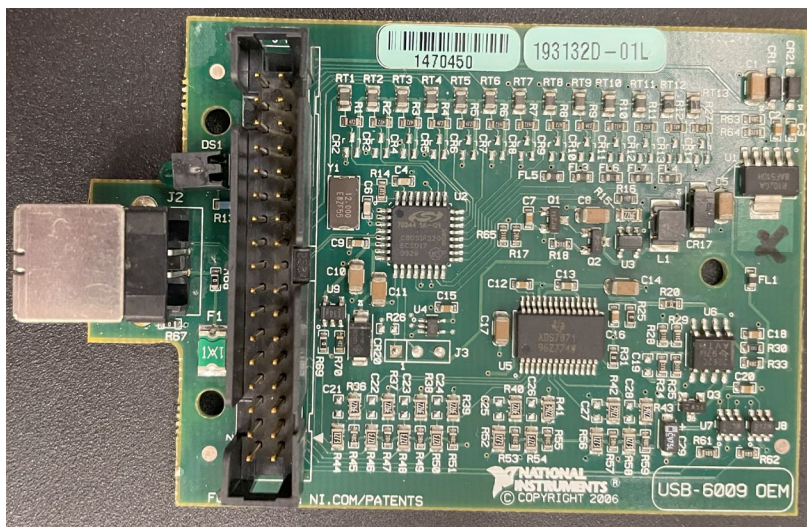


Mixing ratios of PANs in ambient air have been quantified using gas chromatography with electron capture detection (GC-ECD) (Darley et al., 1963; Flocke et al., 2005; Tokarek et al., 2014) and thermal dissociation chemical ionization mass spectrometry (TD-CIMS) (Slusher et al., 2004; Zheng et al., 2011; Mielke & Osthoff, 2012). These methods require calibration as instrumental response varies between compounds.

Synthesis of PANs for use as standards is limited by their instability. For example, diffusion sources often produce mixed or impure outputs, especially for compounds like APAN or MPAN which have a reactive double bond in the side chain. As a solution to this, PANs have been generated by the photolysis of a carbonyl compound in the presence of NO<sub>x</sub>. Carbonyl compound precursors include ketones such as 2-propanone and 3-pentanone (Warneck & Zerbach, 1992; Furgeson et al., 2011; Rider et al., 2015; Pätz et al., 2002), aldehydes such as ethanal or propanal (Volz-Thomas et al., 2002), and acyl chlorides such as acryloyl and methacryloyl chloride (Veres and Roberts, 2015). A recent example of PAN formation using the photochemical source is APAN, which is produced from acrolein (prop-2-enal) (Gomez et al., 2025).

Separation of PAN-type compounds prior to detection is important for two reasons. First, the thermal dissociation cavity ring-down spectroscopy (TD-CRDS) instrument used for quantification is unable to distinguish between overlapping species within the same chemical family. It only measures the thermally dissociated product nitrogen dioxide, so without prior separation, the signals from different species overlap and cannot be resolved. Therefore, a preparatory-scale gas chromatography has been used beforehand to separate analytes prior to their quantification (Roberts et al., 2022).

National Instruments (NI) LabVIEW has served the Osthoff group as a software platform for instrument control and data acquisition (Tokarek et al., 2014). LabVIEW's graphical interface and integration with NI data acquisition (DAQ) devices (also referred to as "boards"), such as the USB-6008/6009 (Figure 1) and Measurement Computing Corporation's USB-1408FS/1608FS (Figure 2) have made it a convenient solution for acquiring data from analytical instruments. However, after NI's acquisition by Emerson in 2023 and changes of its licensing model to a subscription model, LabVIEW has become expensive to maintain for university laboratories.



**Figure 1.** National Instruments USB-6009 OEM board used for data acquisition and control of actuators within LabVIEW environments.



**Figure 2.** The Measurement Computing USB-1408FS DAQ board. Commonly used in LabVIEW based setups for analog and digital control.

To address these limitations, open-source alternatives such as Python may be used. Python is an open-source programming language that is commonly used in science and engineering due to its simplicity, readability, and broad range of applications. This programming language is particularly well-suited to research environments, as it allows chemists to automate experiments, control hardware, process data, and generate graphical user interfaces (GUI) within a single environment.

Python can control laboratory instruments through libraries such as “mcculw”, which supports Measurement Computing devices (e.g., USB-1408FS or USB-1608FS), or “nidaqmx”, which communicates with National Instruments hardware (e.g., USB-6008 or USB-6009). These tools make it possible to replace all of LabVIEW’s functions, such as voltage measurements, signal timing, and valve control. Additionally, Python’s compatibility with data analysis and graph plotting libraries (e.g., “numpy”: for efficient computation, “matplotlib”: a data visualization library) makes it a powerful tool for researchers who value transparency and long-term sustainability in the lab.

In this work, we demonstrate that a custom-built calibration system programmed in Python provides a functional alternative to proprietary software such as National Instruments’ LabVIEW. The Python-based control system was implemented to actuate a 2-position valve for sample collection, allowing the separation of PAN-type compound

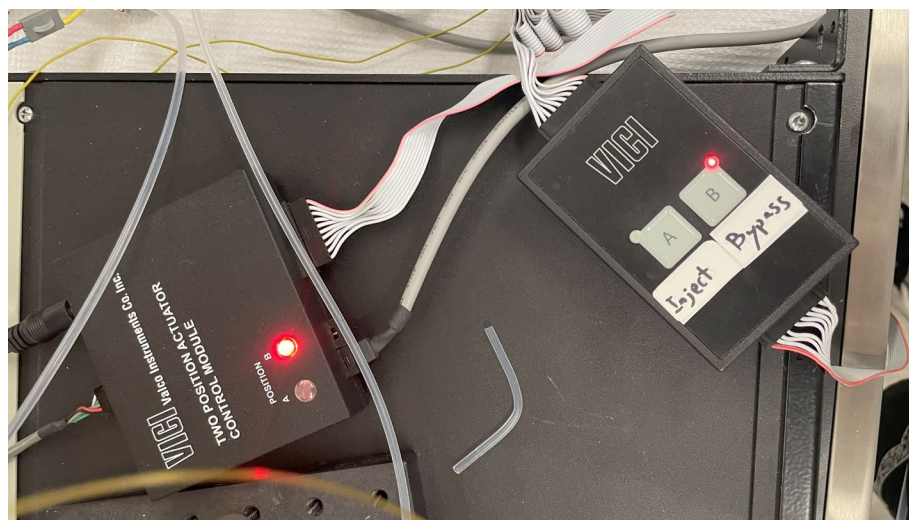
mixtures using a preparatory scale gas chromatography column. This setup that enables automation of valve switching and data acquisition without the licensing constraints associated with commercial software.

## 2. Methods

90 The main instrument used in this project was the GC-ECD, which was used for the separation and detection of PAN-type compounds (Tokarek et al., 2014). Although a TD-CRDS (Taha et al., 2018) is available in the lab and relevant for future work, it was not used in this project. However, the software developed here is compatible with TD-CRDS and can be adapted to automate its operation as well.

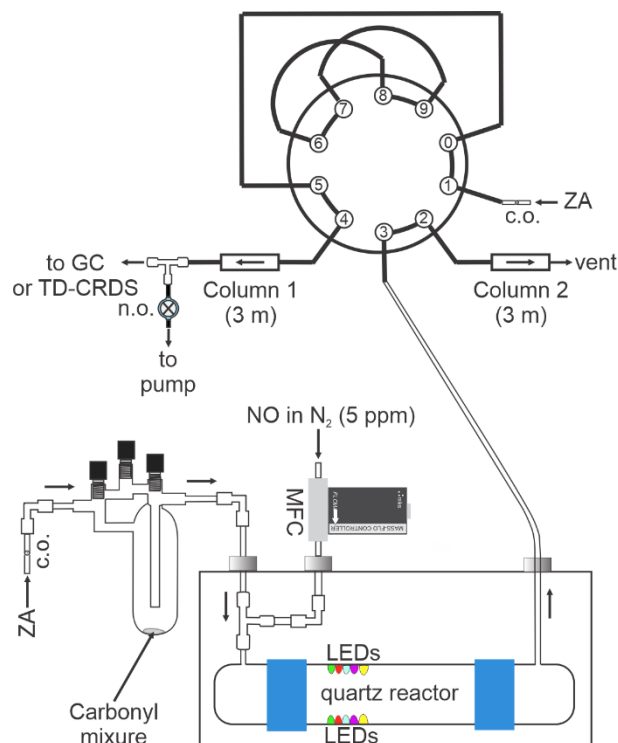
A Valco Instruments Company Inc. (VICI) two-position microelectric actuator was used to control switching in  
95 the GC-ECD (Figures 3A, 3B). This actuator rotates a multi-port valve between two fixed positions and can be triggered either manually or through a digital input/output port that is set to either on (5 V input) or off (0 V input). We controlled the actuator electronically by sending an electrical signal from the DAQ board to the actuator's input pins. Specifically, sending 0 V to pin 5 activated position A, while sending 0 V to pin 6 activated position B (Figure 4). The actuator itself was powered through a 24 V power supply.

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**Figure 3A.** A VICI two-position actuator control module used to switch flow between the bypass and separation lines. The illuminated indicator corresponds to the active flow path.

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**Figure 3B.** Schematic of the GC-ECD experimental setup with a two-position VICI microelectric actuator for valve switching. The actuator alternates the valve between two positions, directing flow either through column 1 (to detector) or column 2 (to vent). Abbreviations: ZA: zero air; c.o.: critical orifice.

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## Digital Control of the Actuator

### Digital Communication Protocol

Pins 1 and 2 provide ground and +5 volt outputs, respectively; pins 3 and 4 are TTL outputs for Position A and Position B, and are considered asserted at 0 volts and deasserted at 5 volts. (This is sometimes referred to as "negative true logic".) Pins 5 and 6 are digital inputs for switching to Position A and Position B. They can be driven either by 5 volt TTL/CMOS logic or by contact closure to ground (Pin 1). Isolated contact closure outputs are available at Pins 7 and 8 for Position A and Pins 9 and 10 for Position B. If there is a positioning error due to valve sticking, clamp ring slippage, etc., the output is set to "0" (all lines high for a negative true output).

Digital I/O Cable	
Pin #	Signal Description
1	Ground
2	+5 VDC
3	Position A output
4	Position B output
5	Position A input
6	Position B input
7	Position A relay contact output
8	Position A relay contact output
9	Position B relay contact output
10	Position B relay contact output



**Figure 4.** Digital input/output pin assignments for the VICI two-position microelectric actuator (VICI, 2009).

The VICI valve was an on/off switch between two flow paths (Figure 4): the bypass line and the separation loop.

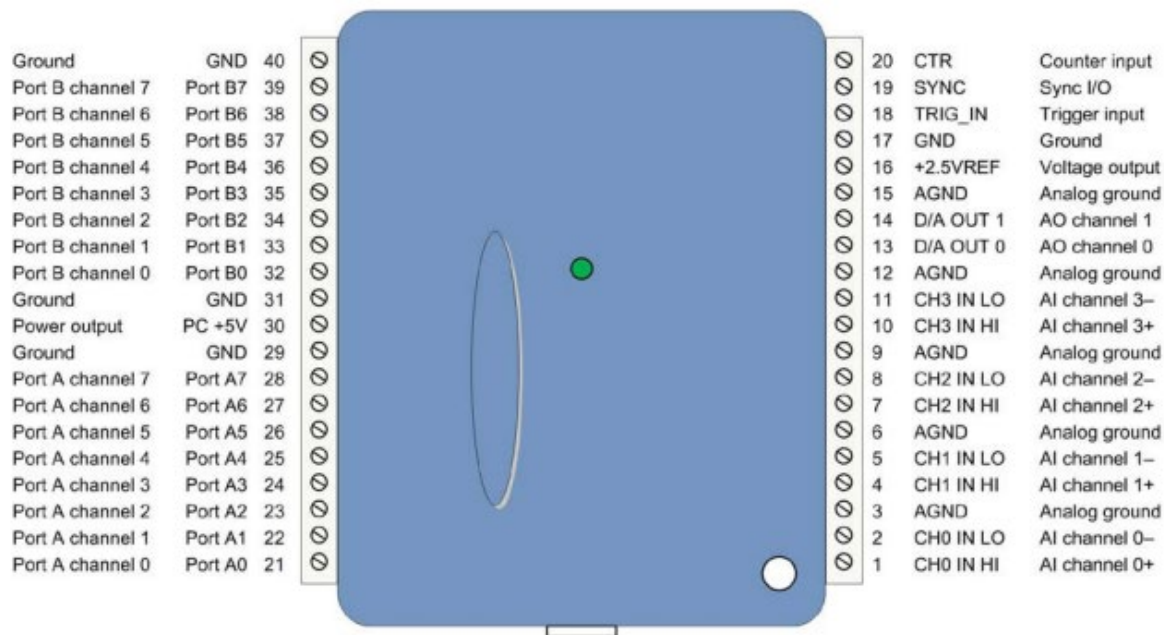
115 The separation loop directs flow to the instrument (either GC or TD-CRDS), while the bypass line vents to the fume hood. The GC also contains a second internal VICI valve which governs sample injection onto the column.

## 2.1. Measurement Computing's USB-1408FS

120 An automated, open-source software platform was written in Python (v3.13) using the PyCharm integrated development environment to control valve switching and perform real-time signal acquisition during chromatographic experiments. The program interfaces with a Measurement Computing USB-1408FS DAQ board via the "mcculw" library, allowing direct communication between both analog and digital inputs and outputs. The system was debugged and refined using generative AI to optimize both code structure and graphical interface behaviour.

125 The USB-1408FS can be used in experiments requiring signal acquisition and timed valve switching. It provides four single-ended analog input channels, two analog outputs, and sixteen digital input/output lines (Figure 5). In this application, analog input channel 0 was connected to the signal output of the GC-ECD, and digital output lines 0 and 1 on port A were connected to the VICI valve controller.

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**Figure 5.** Pinout diagram of the Measurement Computing USB-1408FS DAQ board. (Measurement Computing Corporation, 2023a)

135 The software was modularized into five core components: valve control, data acquisition, GUI display, user configurable settings, and a main launcher script. This was designed to be modular, which allows the user to configure experimental parameters without the GUI in case an unforeseen issue arises. The GUI was developed using the “tkinter” package, a Python toolkit for building windows-based GUIs. Two tabs were provided: configuration and control. The configuration tab allows users to specify hardware channels (analog/digital outputs) and select which DAQ board to control, in case there is more than one DAQ board connected. The control tab displays the experiment progress in real time. Elements displayed consisted of elapsed time, signal voltage readings and graph, the valve switching schedule and manual override buttons to switch valves.

Two valves were controlled by the USB-1408FS DAQ board. Two digital output lines were used to operate valve positions A and B. These valves were toggled by changing the voltage on individual pins. Digital valve control was achieved by setting the appropriate output line “low” (0 V) which the VICI valve controller interprets as a signal to switch (Figure 6). For example, to activate position A, we set its port to “low” state to complete a circuit. To deactivate position A, we return the line to a “high” (5 V) state.



```

# Function to switch to Position A (open Valve A, close Valve B)
def set_valve_position_a(self) -> None:
    if not self._hardware_available:
        print("Simulating valve A open")
        return

    try:
        ul.d_bit_out(self.board_num, DigitalPortType.FIRSTPORTA, 0, 0) # Valve A ON
        ul.d_bit_out(self.board_num, DigitalPortType.FIRSTPORTA, 1, 1) # Valve B OFF
    except Exception as e:
        print(f"Error setting valve A: {str(e)}")

# Function to switch to Position B (open Valve B, close Valve A)
def set_valve_position_b(self) -> None:
    if not self._hardware_available:
        print("Simulating valve B open")
        return

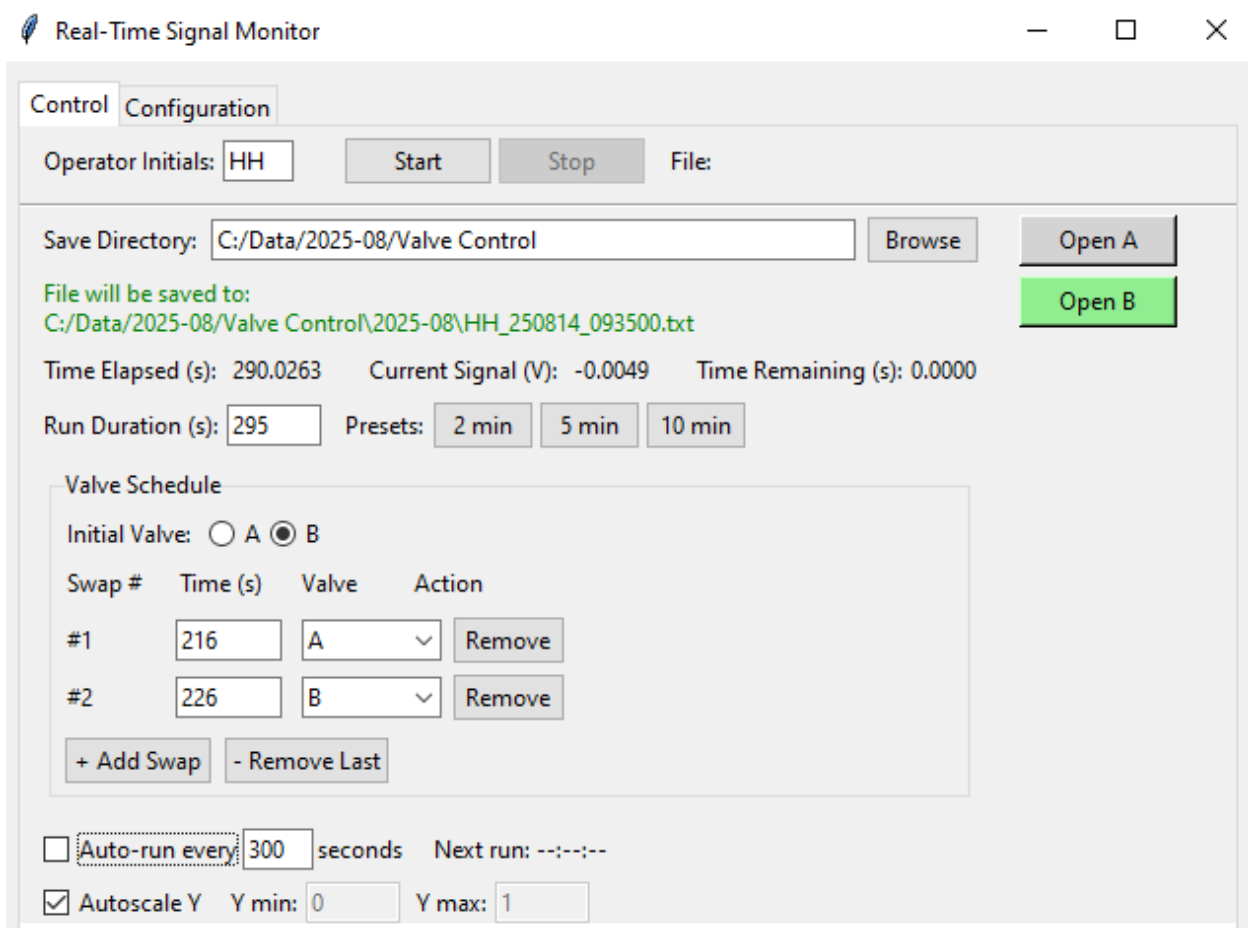
    try:
        ul.d_bit_out(self.board_num, DigitalPortType.FIRSTPORTA, 0, 1) # Valve A OFF
        ul.d_bit_out(self.board_num, DigitalPortType.FIRSTPORTA, 1, 0) # Valve B ON
    except Exception as e:
        print(f"Error setting valve B: {str(e)}")

```

150 **Figure 6.** Python functions used to control valve A and valve B through digital output lines on the USB-1408FS DAQ board. Each function selectively sets the appropriate digital lines to either a low or high state. `set_valve_position_a()` activates valve A while ensuring valve B remains deactivated. Conversely, `set_valve_position_b()` activates valve B while ensuring valve A remains deactivated. These operations prevent both valves from being activated at the same time and avoid interference with other unused digital lines.

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Valve transitions could be scheduled through the GUI using a timing table (Figure 7). These time points were stored as a schedule and executed automatically relative to the experiment start time. Multiple swaps were allowed and configurable in case more than one compound needed to be separated.



**Figure 7.** Custom Python-based GUI for scheduling valve transitions. The software allows timed switching between valve positions A and B, with configurable swap times and run durations. Execution timings were relative to the start of data acquisition.

165 If the DAQ board or the VICI valve controller was not detected, the system entered a simulation mode, and the valve commands were printed to console rather than physically executed. This allowed offline testing and debugging.

Voltage signals were sampled from an analog channel at 10 kHz. Data were collected in blocks of 100 samples, and the average voltage of each block was used for display and storage.

170 Run durations were user-configurable, where the user enters the desired run duration in seconds as seen in Fig. 7. Preset buttons for 2-, 5-, or 10-minute runs also exist as these run durations were commonly used in the group. An auto-run mode feature was introduced which allowed repeated data collection at fixed intervals. This is intended

for unattended operation during long term experiments. To ensure consistent organization of data files and alignment with time-based protocols, each run begins precisely at a time that is an exact multiple of the run duration. For instance, if the run duration is set to 300 s (5 min), data collection would begin at timestamps such as 13:05:00, 13:10:00, 13:15:00, etc. The software continuously calculates the time remaining until the next scheduled run and starts it automatically at the appropriate moment.

After an experimental run, all data is recorded to a tab delimited text file with time values expressed in seconds since January 1<sup>st</sup>, 1904. Although an unusual time format, this epoch format is commonly used in scientific computing. In our case, Igor Pro uses January 1<sup>st</sup>, 1904, as a reference date for time calculations (Figure 8). The data file is named using the group's convention "UI\_YYMMDD\_HHMMSS" where "UI" represents user's initials, YYMMDD represents the current date (year/month/day), and HHMMSS represents the current time (HH:MM:SS, 24-hour format).

```
# Generate filename for this run
initials = settings.operator_initials.upper()
stamp = datetime.now().strftime("%y%m%d_%H%M%S")
self.current_filename = f"{initials}_{stamp}"

# File I/O
def writeData(self, data: list[tuple[float, float]]) -> None:
    if not data or not self.filename:
        return

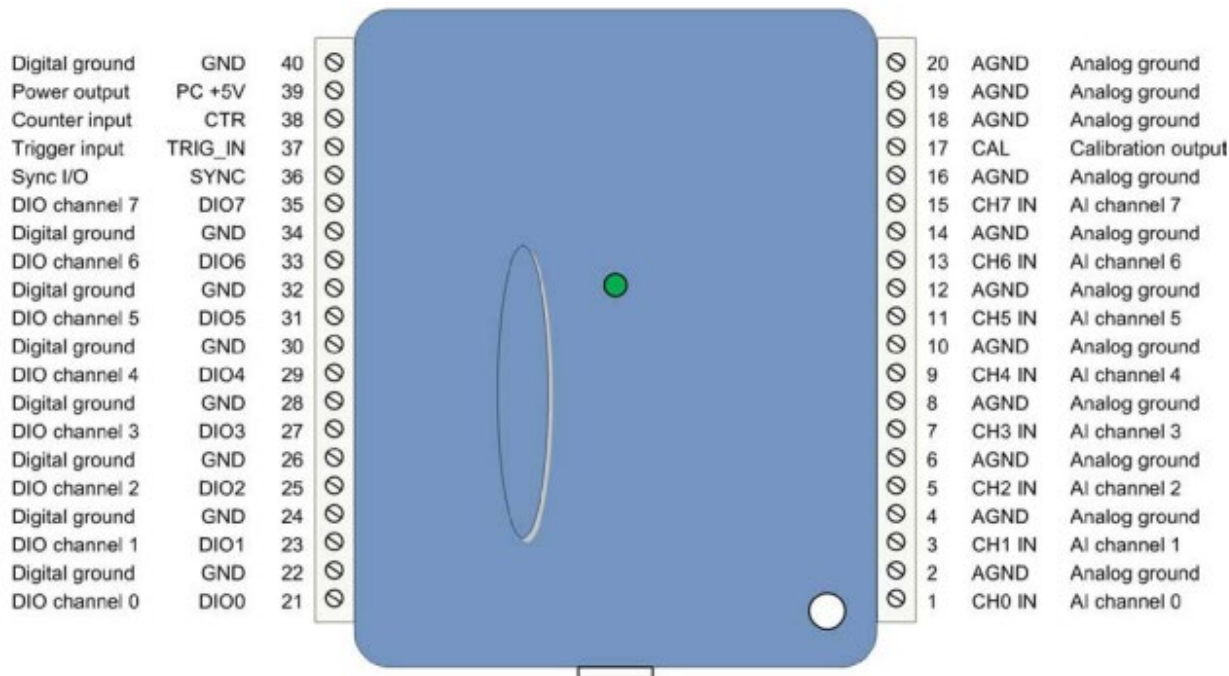
    with open(self.filename, "w", encoding="utf-8") as file:
        for epoch, v in data:
            #format: "[time since Jan 1st 1904] TAB [Signal up to 4 decimal places]"
            file.write(f"{epoch:.4f}\t{v:.4f}\n")
    print(f"Saved {len(data)} rows to {self.filename}")
```

**Figure 8.** Python script that automatically generates filenames using operator's initials and timestamp in the format YYMMDD\_HHMMSS (top). Python function writeData() used to save experimental results to a tab delimited text file (bottom).

This software enables chemists to run time-resolved chromatography experiments on Measurement Computing's USB-1408FS DAQ board with precise valve control, real-time signal monitoring, and automated data logging, without relying on proprietary software such as LabVIEW. The open-source design, GUI accessibility, and the fallback simulation mode make it suitable for both research and teaching laboratories.

2.2. Measurement Computing’s USB-1608FS

195 A second version of the software was developed for compatibility with Measurement Computing USB-1608FS  
DAQ board. Although similar in function to the USB-1408FS, the USB-1608FS features a different pinout and  
analog input configuration compared to the USB-1408FS (Figure 9). This required slight modifications to the  
software due to how analog input signals were handled and which ports were used to control the valves. The user  
interface and experimental procedure remained the same, but switching to the USB-1608FS required internal  
200 reassignment of digital lines.



**Figure 9.** Pinout diagram of the Measurement Computing USB-1608FS DAQ board. (Measurement Computing Corporation, 2023b)

205 The board was connected to the GC-ECD using the same principle as the USB-1408FS, but with modifications to  
account for the USB-1608FS pin layout (Figure 10). Analog channel 0 was connected to the analog signal output  
from the electron capture detector, just like the USB-1408FS. Valve control was achieved through digital output  
lines DIO3 and DIO1 on the DAQ board. These lines were wired to the GC’s internal VICI valve controller where  
it switches the columns.

```

def _set_valve(self, a_state: int, b_state: int):
    """Set both valve control lines to specified states"""
    if not self._hardware_available:
        return

    try:
        # Set Position A control (DI03)
        ul.d_bit_out(self.board_num, DigitalPortType.AUXPORT, 3, a_state)
        # Set Position B control (DI01)
        ul.d_bit_out(self.board_num, DigitalPortType.AUXPORT, 1, b_state)
    except Exception as e:
        print(f"Error setting valve states: {str(e)}")

```

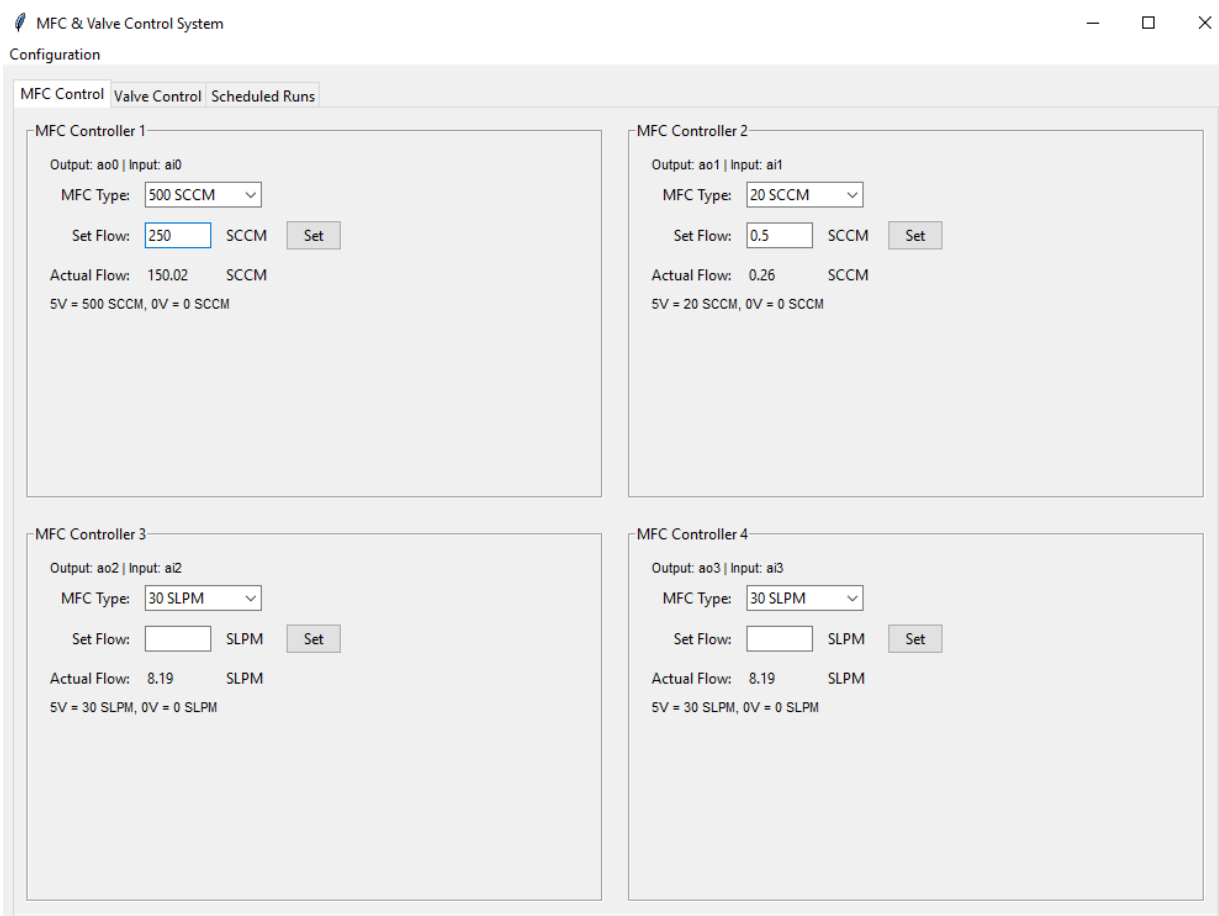
**Figure 10.** Python function `_set_valve()` used to control valve states via digital outputs on the USB-1608FS DAQ board. Same logic as for the USB-1408FS, but different lines.

Despite having different ports and channels, the GUI, experimental procedure, and software logic remained the same. All other features, including run scheduling, auto-run mode, and data storage conventions, were kept identical between versions. The modular software design allowed both boards to be supported simultaneously with no adjustments. This ensured that users could operate either DAQ board interchangeably within the same experimental set up, without requiring reconfiguration or changes to their established GC-ECD procedures.

## 2.3. National Instruments' USB-6008 and USB-6009

The Osthoff group uses an in-house-designed mass flow and valve control boxes powered by a National Instruments USB-6008 or USB-6009. Analog output from the DAQ is used to set and read supplied voltages to mass flow controllers (MFCs), while digital outputs are used to toggle up to four extra valves in the lab.

For this project, MFCs were used to control the flow of NO gases into the PAN generator and the instrument system. Each MFC has a specific range of flow rates, either 30, 15, 5 or 1 standard liters per minute (SLPM), or 500, 100, 20, 10 standard cubic centimeters per minute (SCCM). Normalization allows experiments to be compared throughout different temperatures and pressures. Each MFC has a linear response between the input voltage and its corresponding flow rate. For example, a 30 SLPM MFC delivers its maximum flow (30 SLPM) when supplied with 5 V. Supplying 2.5 V to that same device produced half the flow (15 SLPM). Similarly, a 500 SCCM MFC would output 250 SCCM when provided 2.5 V (Figure 11).



**Figure 11.** The MFC control user interface. Each panel corresponds to one MFC channel, where the user can select the MFC type, input a target flow rate, and monitor the actual flow. The system accepts SLPM or SCCM depending on the selected MFC and linearly maps the analog voltage to the maximum flow rate of the device.

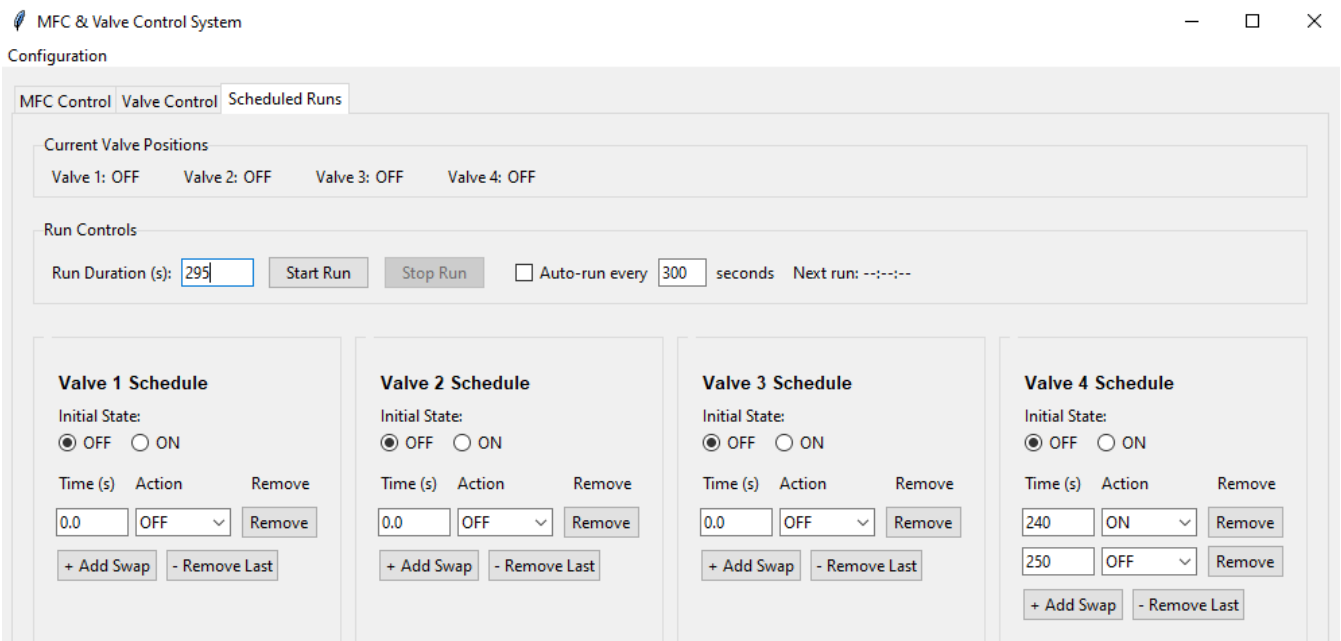
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The bottom of each panel displays flow rate to voltage conversions for reference.

240

Valve toggling was handled by digital output lines, where each line was assigned to a valve. Similarly to both Measurement Computing’s DAQ boards described previously, the valves connected to the NI USB-6009 could be scheduled to switch states at user-defined times. A GUI allowed users to input swap times relative to the experiment start time, enabling precise control over gas routing sequences (Figures 12, 13). The implementation of time based digital valve control provided a consistent and automated method to coordinate gas delivery and separation across multiple instruments.





**Figure 12.** The “Scheduled Runs” tab within the MFC and Valve Control System GUI. Each valve can be individually scheduled to swap states (ON/OFF) at specified times. The run duration and swap times are relative to the experiment start time. An auto-run mode allows repetition of runs for unattended operation.

```
def cancel_schedules(self):
    """Cancel all scheduled jobs for this valve"""
    for job_id in self.swap_job_ids:
        self.master.after_cancel(job_id)
    self.swap_job_ids = []

def set_valve_state(self, state):
    """Set valve state and track current state"""
    self.current_state = state
    self.daq.write_digital(self.port_line, state)

def turn_off(self):
    """Turn off this valve"""
    self.current_state = False
    self.daq.write_digital(self.port_line, False)
```

**Figure 13.** Example implementation of valve control in Python. Functions allow cancellation of scheduled events

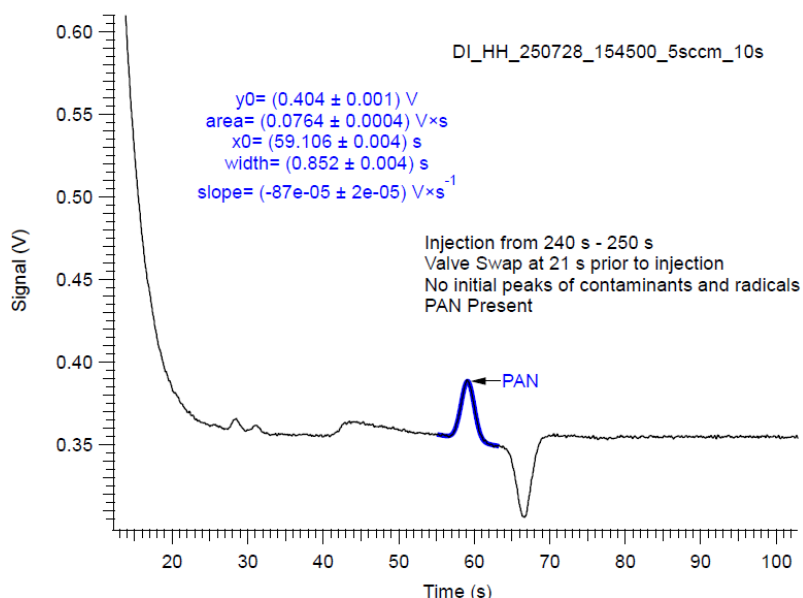
250 (cancel\_schedules), setting a valve state (set\_valve\_state), and shut down (turn\_off). These functions are implemented with the DAQ digital output lines to enable automated toggling of valves during experiments.

### 3. Results and Discussion

#### 3.1. System Testing and Performance

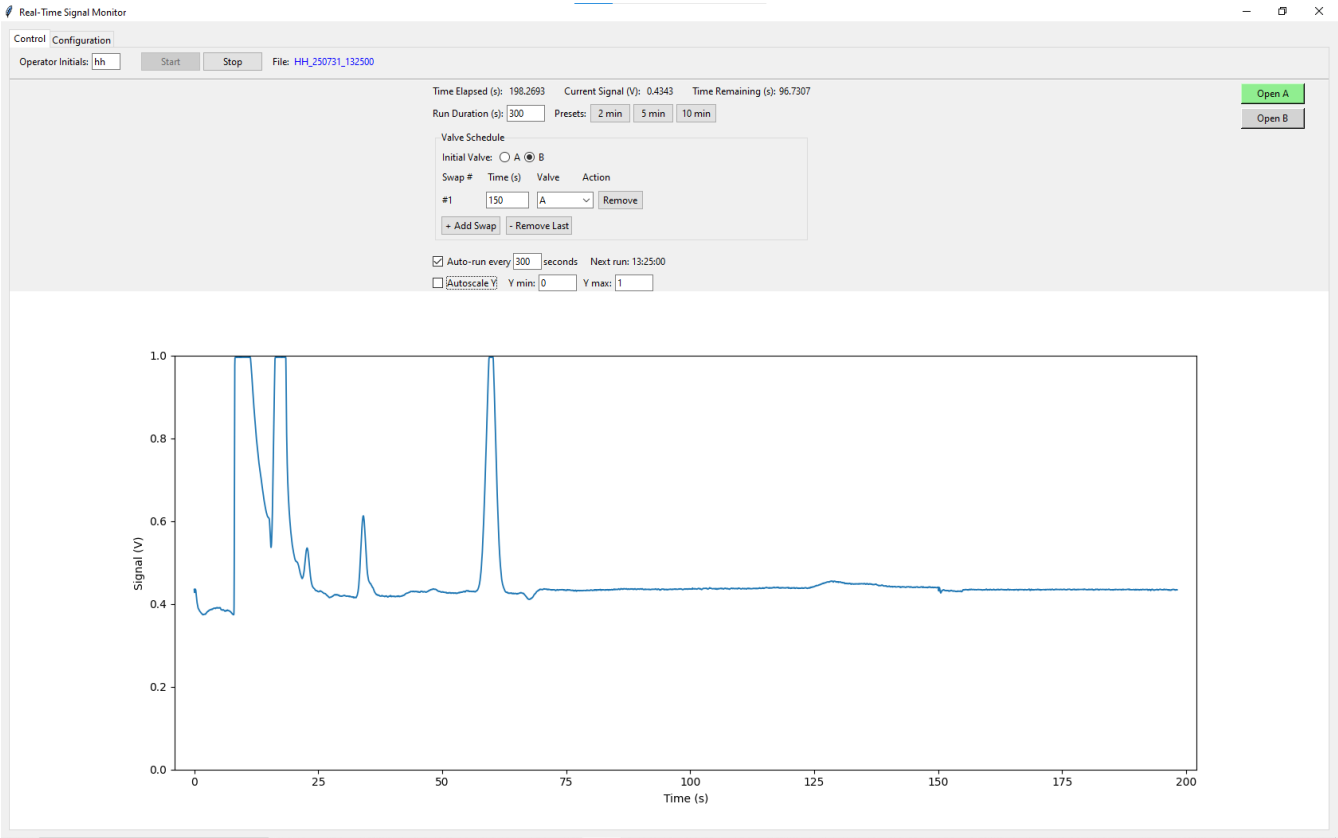
The Python program was tested across multiple days and configurations to assess its performance in instrumental control and separating PAN-type compounds from mixtures using the setup shown in Fig. 3B.

On July 28<sup>th</sup>, a successful injection of a PAN mixture into the GC using the external valve was demonstrated (Fig. 14). The external valve regulated how much of the mixture entered the GC column. This setup was sufficient to direct gas pulses into the column and provided sharp chromatographic peaks. During this testing phase, one computer tested the external valve swaps while another computer was controlling the interior GC valves and the MFCs. Valve synchronization testing revealed a consistent offset of 21 s between system clocks of the two computers used during this phase. This was compensated by delaying one system's swap, achieving synchronized injection.



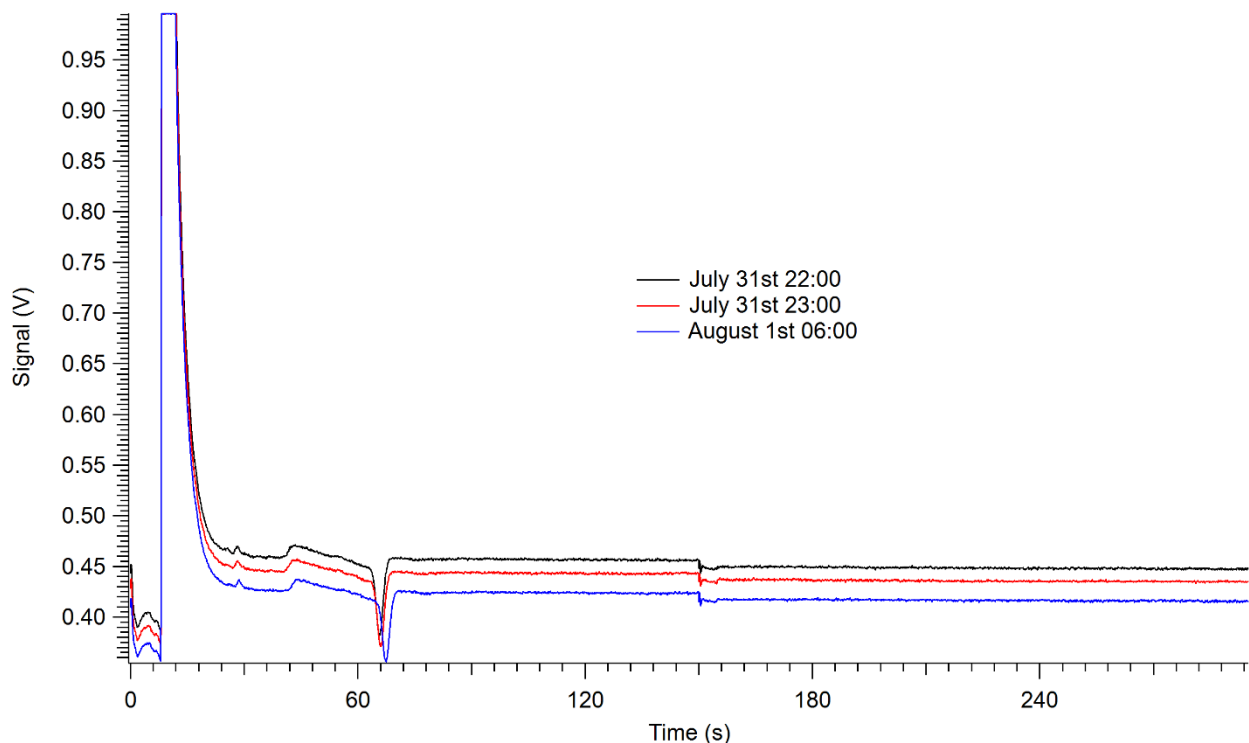
**Figure 14.** Chromatogram shows successful PAN injection using the external valve. The injection occurred  
265 between 240-250 seconds, with a 21 second valve swap delay used to compensate for clock offsets between two computers controlling the system.

By July 31<sup>st</sup>, complete software control of the GC system (both external and internal valves) was achieved through Python code using both USB-1408FS and USB-1608FS (Figure 15). This milestone marked a full transition away from LabVIEW for the GC side of the setup. The Python-based system enabled automated and precise injection controls and bypass switching.



**Figure 15.** Screenshot taken on July 31<sup>st</sup>, 2025 (file: HH\_250731\_132500) showing the first successful chromatographic peaks from fully Python controlled GC injections and valve switching.

Between July 31<sup>st</sup> and August 1<sup>st</sup>, a 24 hour stress test was conducted to determine the system's robustness under extended operation (Figure 16). Blank injections were repeatedly scheduled via the Python control system using the auto-run feature. These tests confirmed that the software could maintain accurate timing, perform valve toggling, and log data continuously without error.

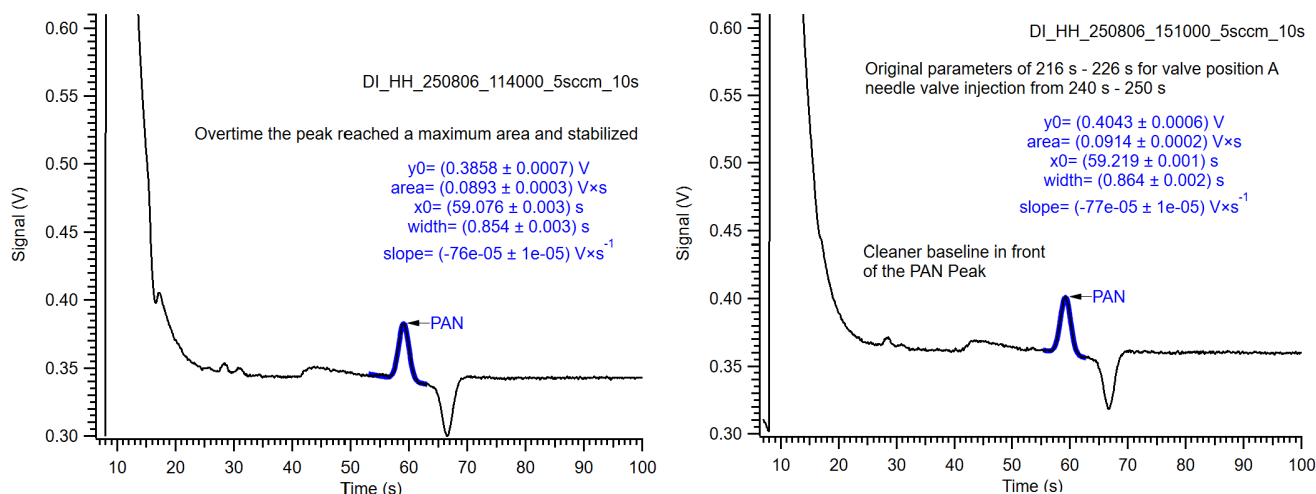


**Figure 16.** Overlay of three arbitrary blank runs taken during a 24 hour continuous stress test between July 31<sup>st</sup> and August 1<sup>st</sup>, 2025. Blank runs were triggered at regular intervals using the auto-run feature of the program. The internal GC valve swap was triggered at 150 s of each run. The consistent shape and timing of the valve triggering across all chromatograms confirm software stability.

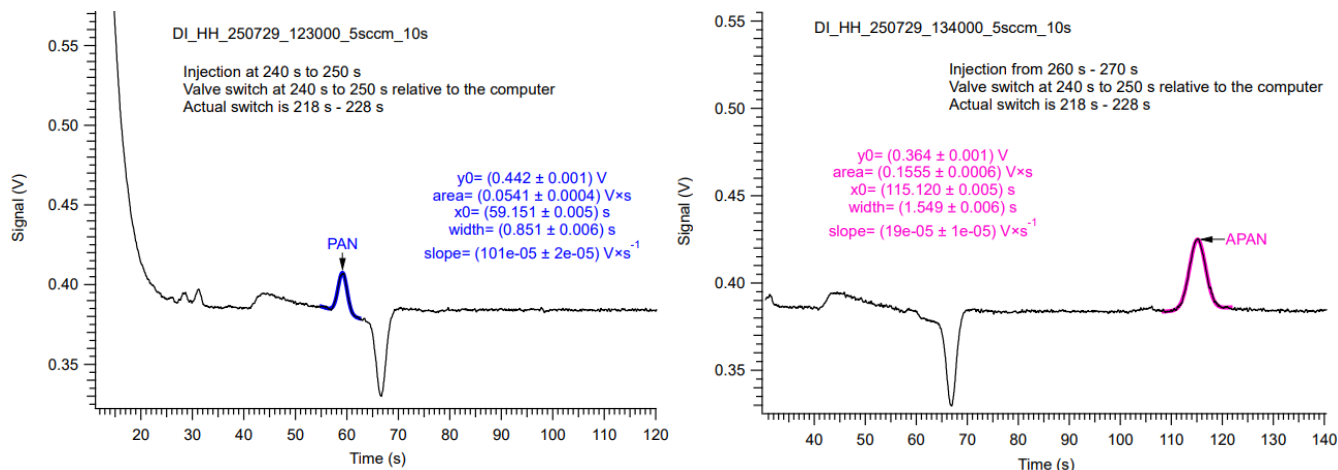
As the physical setup of the instrument was completed prior to my involvement in the project, the specific functions and controls of each valve had to be discovered through a combination of system testing and signal response patterns. During further experimentation, it was determined that the GC system incorporates three valves arranged in series, each responsible for a unique phase of the injection and separation process. In chronological order, the first valve is a VICI actuator responsible for the amount of PANs that enters the pre-column. This valve is controlled by the USB-1408FS. The second valve, a needle valve between the pre-column and the GC, is toggled by a digital output line on the NI USB-6009 DAQ board. The third valve, the internal GC injection valve, is controlled by the USB-1608FS with another VICI actuator.

The needle valve, controlled by the NI DAQ, plays a role in separating individual PAN-type compounds. By precisely controlling the timing of when gases pass from the pre-column into the GC, it determines which species

are injected. For example, PAN can be isolated from contaminants by changing the needle valve injection timing as seen in Fig. 17. Additionally, if PAN and APAN are in the same mixture, they can be isolated in the chromatogram (Figure 18). This discovery refined the injection scheduling logic and contributed to the reliable and reproducible separation of PAN-type compounds.



**Figure 17.** Comparison of two chromatograms showing the effect of needle valve timing on PAN peak isolation. Left: Chromatogram showing a PAN peak in a system with no needle valve interference. Right: Chromatogram showing the same PAN peak affected by the needle valve swapping.



**Figure 18.** Comparison of two chromatograms showing the effect of needle valve timing on PAN peak isolation. Left: Chromatogram showing the isolation of PAN from a mixture of PAN and APAN. Right: Chromatogram showing the isolation of APAN from a mixture of PAN and APAN.

### 3.2. Limitations

A limitation of the current implementation is its dependency on specific operating systems and hardware environments. The software could only be successfully run on 64-bit Windows 10 or Windows 11 machines. Compilation on a 32-bit Windows 10 system was unsuccessful since several versions of the “matplotlib” library  
315 failed to compile due to unresolved Microsoft Visual Studio C/C++ build errors.

Attempts to run the program on a Raspberry Pi running Raspbian were also unsuccessful. Within the Raspbian operating environment, the Python libraries "mcculw" and "nidaqmx" do not exist. Measurement Computing provides an alternative library, “uldaq” for the USB-1408/1608FS DAQ boards which is compatible with Linux operating systems. With sufficient time and development effort, refactoring to interface with “uldaq” is a feasible  
320 path in the future.

Currently, the code does not support simultaneous communication with multiple DAQ boards. Each board must have its own instance therefore, synchronized control across multiple DAQ boards may be more difficult.

### 3.3. Conclusion

This work demonstrates that an open-source Python based software can fully replace LabVIEW in operating a GC  
325 setup for PAN-type compound analysis. It successfully controlled all components, including flow controllers, valve toggles, and injections. Three DAQ boards were used: Measurement Computing’s USB-1408FS, USB-1608FS, and National Instruments’ USB-6009. Testing confirmed reliable performance, with features such as synchronized injections, long run time stability, and precise control of compound separation through valve timing.

Compared to the legacy LabVIEW system, the Python code offered better versatility with user defined swap  
330 sequences, and full functionality without licensing constraints. Results include effective separation of PAN from APAN and contaminants, and supported full automation of the GC system. Minor issues, such as overlapping valve indicator lights and a text field bug in the USB-1408FS interface, were identified but did not affect core performance. This system provides a reliable, cost-effective platform for PAN calibration and GC separation workflows.



## 335 **Code Availability**

All code and documentation are uploaded to a GitHub repository (<https://github.com/illiteratewaffle/Analytical-Data-Acquisition>).

### **Measurement Computing's USB-1408FS**

#### **DataAcquisition.py**

```
340 # DataAcquisition.py
import os

import numpy as np
from mcculw import ul
345 from mcculw.enums import ULRange
from mcculw.ul import ULError
import ctypes as ct
import threading, queue, time
from datetime import datetime

350
from Settings import settings

class DataAcquisition:
355     blockSize = 100
        samplingFrequency = 10_000 # Hz

    def __init__(self):
        # Board-specific settings (updated to use settings)
360     self.board_num = settings.ai_board_number
        self.channel = settings.ai_channel
        self.ai_range = ULRange.BIP20VOLTS
        self._hardware_available = False
```

```

365     try:
        # Try to access the board to verify it exists
        ul.get_board_name(self.board_num)
        self._hardware_available = True
    except ULError:
370         print(f'Warning: Analog input board {self.board_num} not found. Running in simulation mode.')
        self._hardware_available = False

        # Pre-allocate one-block buffer
        self._buf = (ct.c_uint16 * self.blockSize)()

375
        # Run bookkeeping
        self.data: list[tuple[float, float]] = []

        # initial file name
380         self.filename = None

        # Threading helpers
        self._queue: queue.Queue | None = None
        self._thread: threading.Thread | None = None
385         self._running = threading.Event()

    def set_filename(self, filename):
        self.filename = filename

390 # Public control surface
def attach_queue(self, q: queue.Queue) -> None:
    """GUI supplies a queue to receive (t_rel, volts)."""
    self._queue = q

```

```

395 def start(self) -> None:
    if self._thread and self._thread.is_alive():
        return
    self._running.set()
    self._thread = threading.Thread(target=self._worker, daemon=True)
400 self._thread.start()

def stop(self, join_timeout: float = 1.0) -> None:
    self._running.clear()
    if self._thread:
405 self._thread.join(timeout=join_timeout)
        self._thread = None
    self.writeData(self.data) # auto-save
    self.data = [] # clear for next run

410 # Background worker — runs in its own thread
def _worker(self) -> None:
    t0 = time.perf_counter()
    while self._running.is_set():
        volts = self.getSignalData()
415 if volts is None:
            continue # skip bad scan, keep running

        t_rel = time.perf_counter() - t0
        epoch1904 = self.getTimeData()
420 self.recordData(epoch1904, volts)

    if self._queue:
        try:
            self._queue.put_nowait((t_rel, volts))
425 except queue.Full: # drop oldest if GUI lags

```

```

        _ = self._queue.get_nowait()
        self._queue.put_nowait((t_rel, volts))
        # a_in_scan blocks  $\approx$  blockSize/samplingFrequency
        # so no extra sleep is needed
430
# Low-level helpers
def getSignalData(self) -> float | None:
    if not self._hardware_available:
        # Simulate a sine wave when hardware isn't available
435        return 2.5 + 2.5 * np.sin(time.perf_counter() * 2 * np.pi * 0.1)

    try:
        ul.a_in_scan(self.board_num,
                     self.channel, self.channel,
440                     self.blockSize, self.samplingFrequency,
                     self.ai_range, self._buf, 0)

        counts = np.ctypeslib.as_array(self._buf).mean()
        return float(ul.to_eng_units(self.board_num, self.ai_range, int(counts)))
445    except ULError as e:
        print("UL error:", e.errorcode, e.message)
        return None

def getTimeData(self) -> float:
450    return (datetime.now() - datetime(1904, 1, 1)).total_seconds()

def recordData(self, epoch1904: float, volts: float) -> None:
    self.data.append((epoch1904, volts))

455 # File I/O. Writes data to file, saves file to computer
def writeData(self, data: list[tuple[float, float]]) -> None:

```

```
if not data or not self.filename:
```

```
    return
```

```
460 try:
```

```
    # Get directory path and ensure it exists
```

```
    dir_path = os.path.dirname(self.filename)
```

```
    if dir_path: # Only try to create if there is a directory component
```

```
        os.makedirs(dir_path, exist_ok=True)
```

```
465
```

```
    # Write the data file
```

```
    with open(self.filename, "w", encoding="utf-8") as f:
```

```
        for epoch, v in data:
```

```
            # Format: "[time since Jan 1st 1904] TAB [Signal up to 4 decimal places]"
```

```
470         f.write(f'{epoch:.4f}\t{v:.4f}\n')
```

```
    print(f'Successfully saved {len(data)} rows to {self.filename}')
```

```
except PermissionError as e:
```

```
475     print(f'Error: Permission denied when writing to {self.filename}: {str(e)}')
```

```
except OSError as e:
```

```
    print(f'Error writing to {self.filename}: {str(e)}')
```

```
except Exception as e:
```

```
    print(f'Unexpected error saving data: {str(e)}')
```

```
480
```

## Display.py

```
▪ import time
```

```
import queue
```

```
import tkinter as tk
```

```
485 from tkinter import ttk, messagebox, filedialog
```

```
import os
```

```

from datetime import datetime, timedelta
import math

490     import matplotlib

matplotlib.use("TkAgg")
from matplotlib.backends.backend_tkagg import FigureCanvasTkAgg
import matplotlib.pyplot as plt

495

from DataAcquisition import DataAcquisition
from Valves import Valves
from Settings import settings

500

class Display:
    """Real-time GUI with variable valve-swap schedules, X/Y autoscaling, and auto-run."""

    OPEN_CLR = "#90EE90"
    CLOSED_CLR = "#D3D3D3"

505

    #


---


    # Construction
    #


---



510

    def __init__(self, root: tk.Tk):
        self.root = root
        self.root.title("Real-Time Signal Monitor")

515

        # Create notebook for tabs
        self.notebook = ttk.Notebook(self.root)

```



```

self.notebook.pack(fill=tk.BOTH, expand=True, padx=10, pady=10)

520     # Create control tab
        self.control_tab = ttk.Frame(self.notebook)
        self.notebook.add(self.control_tab, text="Control")

        # Create config tab
525     self.config_tab = ttk.Frame(self.notebook)
        self.notebook.add(self.config_tab, text="Configuration")

        self.daq = DataAcquisition()
        self.dataQueue = queue.Queue()
530     self.daq.attach_queue(self.dataQueue)

        self.blockMS = max(
            1,
            round(1000 * self.daq.blockSize / self.daq.samplingFrequency),
535     )

        # Run-state
        self.recording = False
        self.maxDuration = settings.effective_run_duration
540     self.currentValve = "A"
        self.swap_job_ids = [] # List to store all swap job IDs

        # Auto-run state
        self.auto_run_job = None
545     self.next_run_time = None

        # Initialize valves after settings
        self.valves = Valves()

```

```

    if not hasattr(self.daq, '_hardware_available') or not self.daq._hardware_available:
550         messagebox.showwarning("Hardware Not Found",
                                f"Analog input board {settings.ai_board_number} not found. Running in
simulation mode.")

    if not hasattr(self.valves, '_hardware_available') or not self.valves._hardware_available:
555         messagebox.showwarning("Hardware Not Found",
                                f"Digital I/O board {settings.dio_board_number} not found. Valve controls will be
simulated.")

    # Build GUI
560     self._build_widgets()

    self.jobId = self.root.after(self.blockMS, self.updateLoop)
    self.root.protocol("WM_DELETE_WINDOW", self.closeWindow)

565     # Start auto-run scheduler if enabled
    if settings.auto_run:
        self._start_auto_run_scheduler()

    #
570


---


    # GUI layout
    #


---



    def _build_widgets(self):
575         # Build configuration tab first
        self._build_config_tab()

        # Build control tab
        self._build_control_tab()

```

580

```
def _build_config_tab(self):  
    """Build the configuration tab"""  
    config_frm = ttk.LabelFrame(self.config_tab, text="Board Configuration", padding=10)  
    config_frm.pack(fill=tk.BOTH, expand=True, padx=10, pady=10)
```

585

```
    # AI Board  
    ai_frm = ttk.Frame(config_frm)  
    ai_frm.pack(fill=tk.X, pady=5)  
    ttk.Label(ai_frm, text="AI Board Number:").pack(side=tk.LEFT, padx=(0, 10))  
    self.ai_board_var = tk.IntVar(value=settings.ai_board_number)  
    ai_board_spin = ttk.Spinbox(ai_frm, from_=0, to=15, width=5,  
                                textvariable=self.ai_board_var)  
    ai_board_spin.pack(side=tk.LEFT)
```

590

595

```
    # DIO Board  
    dio_frm = ttk.Frame(config_frm)  
    dio_frm.pack(fill=tk.X, pady=5)  
    ttk.Label(dio_frm, text="DIO Board Number:").pack(side=tk.LEFT, padx=(0, 10))  
    self.dio_board_var = tk.IntVar(value=settings.dio_board_number)  
    dio_board_spin = ttk.Spinbox(dio_frm, from_=0, to=15, width=5,  
                                textvariable=self.dio_board_var)  
    dio_board_spin.pack(side=tk.LEFT)
```

600

```
    # AI Channel  
    chan_frm = ttk.Frame(config_frm)  
    chan_frm.pack(fill=tk.X, pady=5)  
    ttk.Label(chan_frm, text="AI Channel:").pack(side=tk.LEFT, padx=(0, 10))  
    self.ai_channel_var = tk.IntVar(value=settings.ai_channel)  
    ai_channel_spin = ttk.Spinbox(chan_frm, from_=0, to=15, width=5,  
                                textvariable=self.ai_channel_var)
```

610

```

ai_channel_spin.pack(side=tk.LEFT)

# Apply Button
btn_frm = ttk.Frame(config_frm)
615 btn_frm.pack(fill=tk.X, pady=(20, 5))
apply_btn = ttk.Button(btn_frm, text="Apply Configuration",
                        command=self._apply_config)
apply_btn.pack(pady=10)

620 # Status message
self.config_status = tk.StringVar(value="")
ttk.Label(config_frm, textvariable=self.config_status, foreground="blue").pack()

def _build_control_tab(self):
625 """Build the main control tab"""
# Top bar
top = ttk.Frame(self.control_tab, padding=(10, 5))
top.pack(fill=tk.X)

630 ttk.Label(top, text="Operator Initials:").grid(row=0, column=0, sticky="w")
self.initialsVar = tk.StringVar()
ttk.Entry(top, width=5, textvariable=self.initialsVar).grid(
    row=0,
    column=1,
635 padx=(2, 15),
)

self.startBtn = ttk.Button(top, text="Start", command=self.startRecording)
self.startBtn.grid(row=0, column=2, padx=(10, 2))

640 self.stopBtn = ttk.Button(top, text="Stop", command=self.stopRecording, state="disabled")

```

```

self.stopBtn.grid(row=0, column=3)

tkk.Label(top, text="File:").grid(row=0, column=4, padx=(10, 2))
645 self.filenameVar = tk.StringVar(value="")
self.filenameLabel = tk.Label(top, textvariable=self.filenameVar, foreground="blue")
self.filenameLabel.grid(row=0, column=5, sticky="w")

tkk.Separator(self.control_tab, orient="horizontal").pack(fill=tk.X, pady=4)

650

# Main frame
main = tk.Frame(self.control_tab)
main.pack(fill=tk.X, padx=10)

655 info = tk.Frame(main)
info.pack(side=tk.LEFT, expand=True)

# New: Save Directory selection
dir_frm = tk.Frame(info)
660 dir_frm.grid(row=0, column=0, columnspan=6, sticky="we", pady=(0, 5))

tkk.Label(dir_frm, text="Save Directory:").pack(side=tk.LEFT, padx=(0, 5))
self.save_dir_var = tk.StringVar(value=settings.save_directory)
dir_entry = tk.Entry(dir_frm, textvariable=self.save_dir_var, width=40)
665 dir_entry.pack(side=tk.LEFT, fill=tk.X, expand=True)
tkk.Button(
    dir_frm,
    text="Browse",
    width=8,
    670 command=self._select_directory
).pack(side=tk.LEFT, padx=(5, 0))

```

```

# New: File path display
self.file_path_var = tk.StringVar(value="")
675 ttk.Label(
    info,
    textvariable=self.file_path_var,
    foreground="green",
    wraplength=500
680 ).grid(row=1, column=0, columnspan=6, sticky="w", pady=(0, 5))

# Live readouts
ttk.Label(info, text="Time Elapsed (s):").grid(row=2, column=0, sticky="w")
self.timeVar = tk.StringVar(value="0.0000")
685 ttk.Label(info, textvariable=self.timeVar).grid(row=2, column=1, padx=(4, 20))

ttk.Label(info, text="Current Signal (V):").grid(row=2, column=2, sticky="w")
self.signalVar = tk.StringVar(value="0.0000")
ttk.Label(info, textvariable=self.signalVar).grid(row=2, column=3, padx=(4, 20))
690

ttk.Label(info, text="Time Remaining (s):").grid(row=2, column=4, sticky="w")
self.remainingVar = tk.StringVar(value="0.0000")
ttk.Label(info, textvariable=self.remainingVar).grid(row=2, column=5)

695 # Run-duration row
dur = ttk.Frame(info)
dur.grid(row=3, column=0, columnspan=6, sticky="w", pady=(6, 0))

ttk.Label(dur, text="Run Duration (s):").pack(side=tk.LEFT, padx=(0, 2))
700 self.durationVar = tk.StringVar(value=str(settings.run_duration))
self.durationEntry = ttk.Entry(dur, width=7, textvariable=self.durationVar)
self.durationEntry.pack(side=tk.LEFT)
self.durationEntry.bind("<FocusOut>", self._update_duration)

```

```

self.durationEntry.bind("<Return>", self._update_duration)

705
    ttk.Label(dur, text="Presets:").pack(side=tk.LEFT, padx=(10, 2))
    preset_btns = [
        ("2 min", 120),
        ("5 min", 300),
710        ("10 min", 600)
    ]
    for text, sec in preset_btns:
        ttk.Button(
            dur,
            text=text,
715            width=7,
            command=lambda s=sec: self._set_duration(s)
        ).pack(side=tk.LEFT, padx=(0, 2))

720    # Valve schedule controls
    valve_schedule_frm = ttk.LabelFrame(info, text="Valve Schedule")
    valve_schedule_frm.grid(row=4, column=0, columnspan=6, sticky="we", pady=(10, 5), padx=5)

    # Initial valve
725    initial_frm = ttk.Frame(valve_schedule_frm)
    initial_frm.pack(fill=tk.X, padx=5, pady=(5, 0))
    ttk.Label(initial_frm, text="Initial Valve:").pack(side=tk.LEFT, padx=(0, 5))
    self.initialValveVar = tk.StringVar(value="A")
    ttk.Radiobutton(initial_frm, text="A", variable=self.initialValveVar,
730 value="A").pack(side=tk.LEFT)
    ttk.Radiobutton(initial_frm, text="B", variable=self.initialValveVar,
    value="B").pack(side=tk.LEFT)

    # Valve swap table

```

```

735 swap_frm = ttk.Frame(valve_schedule_frm)
swap_frm.pack(fill=tk.X, padx=5, pady=5)

# Table header
header = ttk.Frame(swap_frm)
740 header.pack(fill=tk.X, pady=(0, 5))
ttk.Label(header, text="Swap #", width=8).pack(side=tk.LEFT)
ttk.Label(header, text="Time (s)", width=8).pack(side=tk.LEFT, padx=5)
ttk.Label(header, text="Valve", width=8).pack(side=tk.LEFT, padx=5)
ttk.Label(header, text="Action", width=8).pack(side=tk.LEFT)

745 # Container for swap rows
self.swap_rows_frame = ttk.Frame(swap_frm)
self.swap_rows_frame.pack(fill=tk.X)

750 # Add/remove controls
ctrl_frm = ttk.Frame(valve_schedule_frm)
ctrl_frm.pack(fill=tk.X, padx=5, pady=(0, 5))
ttk.Button(ctrl_frm, text="+ Add Swap", command=self._add_swap_row).pack(side=tk.LEFT)
ttk.Button(ctrl_frm, text="- Remove Last", command=self._remove_last_swap).pack(side=tk.LEFT,
755 padx=5)

# Populate with existing schedule
self.swap_vars = []
for time, valve in settings.valve_schedule:
760     self._add_swap_row(time, valve)

# Auto-run row
auto_run_f = ttk.Frame(info)
auto_run_f.grid(row=5, column=0, columnspan=6, sticky="w", pady=(10, 0))
765

```



```

self.autoRunVar = tk.BooleanVar(value=settings.auto_run)
ttk.Checkbutton(
    auto_run_f,
    text="Auto-run every",
770     variable=self.autoRunVar,
        command=self._toggle_auto_run
    ).pack(side=tk.LEFT)

# Interval entry
775 self.autoIntVar = tk.StringVar(value=str(settings.auto_run_interval))
    self.autoIntEntry = ttk.Entry(auto_run_f, width=5, textvariable=self.autoIntVar)
    self.autoIntEntry.pack(side=tk.LEFT)
    self.autoIntEntry.bind("<FocusOut>", self._update_auto_interval)
    self.autoIntEntry.bind("<Return>", self._update_auto_interval)

780
    ttk.Label(auto_run_f, text="seconds").pack(side=tk.LEFT, padx=(0, 2))

# Next run display
    self.nextRunVar = tk.StringVar(value="Next run: --:--:--")
785    ttk.Label(auto_run_f, textvariable=self.nextRunVar).pack(side=tk.LEFT, padx=(10, 0))

# Y-axis controls
    yctrl = ttk.Frame(info)
    yctrl.grid(row=6, column=0, columnspan=6, sticky="w", pady=(6, 0))
790

    self.autoscaleVar = tk.BooleanVar(value=True)
    ttk.Checkbutton(
        yctrl,
        text="Autoscale Y",
795     variable=self.autoscaleVar,
        command=self._toggleAutoscale,

```

```
).pack(side=tk.LEFT)
```

```
ttk.Label(yctrl, text="Y min:").pack(side=tk.LEFT, padx=(10, 2))
```

```
800 self.yMinVar = tk.StringVar(value="0")
```

```
self.yMinEntry = ttk.Entry(yctrl, width=7, textvariable=self.yMinVar, state="disabled")
```

```
self.yMinEntry.pack(side=tk.LEFT)
```

```
ttk.Label(yctrl, text="Y max:").pack(side=tk.LEFT, padx=(6, 2))
```

```
805 self.yMaxVar = tk.StringVar(value="1")
```

```
self.yMaxEntry = ttk.Entry(yctrl, width=7, textvariable=self.yMaxVar, state="disabled")
```

```
self.yMaxEntry.pack(side=tk.LEFT)
```

```
# Manual valve buttons
```

```
810 valve_f = ttk.Frame(main, padding=(20, 0))
```

```
valve_f.pack(side=tk.RIGHT, anchor="ne")
```

```
self.buttonA = tk.Button(valve_f, text="Open A", width=10, bg=self.CLOSED_CLR,  
command=self.toggleValveA)
```

```
815 self.buttonA.pack(pady=(0, 5))
```

```
self.buttonB = tk.Button(valve_f, text="Open B", width=10, bg=self.CLOSED_CLR,  
command=self.toggleValveB)
```

```
self.buttonB.pack()
```

```
820
```

```
# Matplotlib figure
```

```
self.fig, self.ax = plt.subplots(figsize=(6, 4))
```

```
self.ax.set_xlabel("Time (s)")
```

```
self.ax.set_ylabel("Signal (V)")
```

```
825
```

```
self.line, = self.ax.plot([], [], lw=1.3)
```

```
FigureCanvasTkAgg(self.fig, master=self.control_tab).get_tk_widget().pack(fill=tk.BOTH,  
expand=True)
```

830

```
self.xData = []
```

```
self.yData = []
```

```
#
```

835

```
# Configuration methods
```

```
#
```

---

```
def _apply_config(self):
```

840

```
    """Apply new configuration settings"""
```

```
    try:
```

```
        if self.recording:
```

```
            messagebox.showerror("Error", "Cannot change configuration while recording")
```

```
            return
```

845

```
        # Validate inputs
```

```
        ai_board = int(self.ai_board_var.get())
```

```
        dio_board = int(self.dio_board_var.get())
```

```
        ai_channel = int(self.ai_channel_var.get())
```

850

```
        if not (0 <= ai_board <= 15):
```

```
            raise ValueError("AI board number must be 0-15")
```

```
        if not (0 <= dio_board <= 15):
```

```
            raise ValueError("DIO board number must be 0-15")
```

855

```
        if not (0 <= ai_channel <= 15):
```

```
            raise ValueError("AI channel must be 0-15")
```

```
        # Update settings
```

```

settings.ai_board_number = ai_board
860 settings.dio_board_number = dio_board
settings.ai_channel = ai_channel

# Reinitialize hardware
self.valves = Valves()
865 self.daq = DataAcquisition()
self.daq.attach_queue(self.dataQueue)

self.config_status.set("Configuration updated successfully")
except ValueError as e:
870     messagebox.showerror("Error", f"Invalid configuration: {str(e)}")

#

```

---

```

# Valve schedule management
875 #

```

---

```

def _add_swap_row(self, time_val: float = 0.0, valve_val: str = "B"):
    """Add a new row to the valve schedule table"""
    row = tk.Frame(self.swap_rows_frame)
880 row.pack(fill=tk.X, pady=2)

# Swap number
swap_num = len(self.swap_vars) + 1
tk.Label(row, text=f"#{swap_num}", width=8).pack(side=tk.LEFT)
885

# Time entry
time_var = tk.StringVar(value=str(time_val))
time_ent = tk.Entry(row, width=8, textvariable=time_var)
time_ent.pack(side=tk.LEFT, padx=5)

```

890

```
# Valve selection
valve_var = tk.StringVar(value=valve_val)
valve_cmb = ttk.Combobox(row, width=8, textvariable=valve_var, state="readonly")
valve_cmb['values'] = ("A", "B")
895 valve_cmb.pack(side=tk.LEFT, padx=5)
```

```
# Remove button
remove_btn = ttk.Button(row, text="Remove", width=8,
                        command=lambda r=row: self._remove_swap_row(r))
900 remove_btn.pack(side=tk.LEFT)
```

```
# Store variables
self.swap_vars.append((time_var, valve_var, row))
```

905

```
def _remove_swap_row(self, row):
    """Remove a specific row from the valve schedule"""
    # Find and remove the row from our list
    for i, (time_var, valve_var, row_widget) in enumerate(self.swap_vars):
        if row_widget == row:
            self.swap_vars.pop(i)
            row.destroy()
            break
```

910

```
# Renumber remaining swaps
915 for i, (_, _, row_widget) in enumerate(self.swap_vars):
    swap_num_label = row_widget.winfo_children()[0]
    swap_num_label.config(text=f"#{i + 1}")
```

920

```
def _remove_last_swap(self):
    """Remove the last swap from the schedule"""
```

```

        if self.swap_vars:
            _, _, row = self.swap_vars.pop()
            row.destroy()

925     def _get_valve_schedule(self) -> list[tuple[float, str]]:
        """Get the current valve schedule from the UI"""
        schedule = []
        for time_var, valve_var, _ in self.swap_vars:
            try:
930                 time_val = float(time_var.get())
                valve_val = valve_var.get()
                if time_val >= 0 and valve_val in ("A", "B"):
                    schedule.append((time_val, valve_val))
                else:
935                 messagebox.showerror("Invalid Input",
                                        f"Invalid valve schedule: time={time_val}, valve={valve_val}")
            except ValueError:
                messagebox.showerror("Invalid Input", "Time must be a number")
        return sorted(schedule, key=lambda x: x[0])

940     #

```

---

```

    # Directory selection
    #
945

```

---

```

    def _select_directory(self):
        """Open directory dialog and update save path"""
        dir_path = filedialog.askdirectory(
            initialdir=self.save_dir_var.get(),
950             title="Select Save Directory"
        )

```

```

    if dir_path:
        self.save_dir_var.set(dir_path)
        settings.save_directory = dir_path
955
#
# Duration and interval synchronization
#
960
def _set_duration(self, seconds: float):
    """Set duration without affecting auto-run interval"""
    settings.run_duration = seconds
    self.durationVar.set(str(seconds))
965
def _update_duration(self, event=None):
    """Update from GUI entry"""
    try:
        seconds = float(self.durationVar.get())
970
        settings.run_duration = seconds
    except ValueError:
        pass

def _update_auto_interval(self, event=None):
975
    """Update auto-run interval from GUI"""
    try:
        interval = int(self.autoIntVar.get())
        settings.auto_run_interval = interval
    except ValueError:
980
        pass

#

```

---

```

985     # Auto-run methods
    #

```

---

```

def _toggle_auto_run(self):
    settings.auto_run = self.autoRunVar.get()
    if settings.auto_run:
990         # Update settings from GUI
        try:
            settings.auto_run_interval = int(self.autoIntVar.get())
        except ValueError:
            pass # Keep previous value
995         self._start_auto_run_scheduler()
    elif self.auto_run_job:
        self.root.after_cancel(self.auto_run_job)
        self.auto_run_job = None
        self.next_run_time = None
1000        self.nextRunVar.set("Next run: --:--:--")

def _calculate_next_run(self):
    """Calculate next run time at exact second interval."""
    now = datetime.now()
1005    interval_seconds = settings.auto_run_interval

    # Calculate next time that is multiple of interval seconds
    current_seconds = now.hour * 3600 + now.minute * 60 + now.second
    remainder = current_seconds % interval_seconds

1010    if remainder == 0:
        # Already at interval, run immediately
        next_seconds = current_seconds

```



```

else:
1015     next_seconds = current_seconds + interval_seconds - remainder

    # Convert seconds back to time
    next_hour = next_seconds // 3600
    next_minute = (next_seconds % 3600) // 60
1020     next_second = next_seconds % 60

    # Create next run time
    next_run = now.replace(hour=next_hour, minute=next_minute, second=next_second,
microsecond=0)

1025

    # Handle day rollover
    if next_hour >= 24:
        next_run = next_run + timedelta(days=1)

1030     return next_run

def _start_auto_run_scheduler(self):
    if not settings.auto_run:
        return

1035

    # Calculate next run time
    self.next_run_time = self._calculate_next_run()
    self.nextRunVar.set(f"Next run: {self.next_run_time.strftime('%H:%M:%S')}")

1040

    # Calculate delay in milliseconds
    now = datetime.now()
    delay_ms = int((self.next_run_time - now).total_seconds() * 1000)

    # Schedule next run

```

```
1045         if self.auto_run_job:
            self.root.after_cancel(self.auto_run_job)
            self.auto_run_job = self.root.after(delay_ms, self._execute_auto_run)
```

```
def _execute_auto_run(self):
1050     if not settings.auto_run:
        return
```

```
        # Start recording
        self.startRecording()
```

```
1055     # Schedule next run after current run completes
        self.auto_run_job = self.root.after(
            int(settings.auto_run_interval * 1000), # Use full interval
            self._start_auto_run_scheduler
1060     )
```

```
        #
```

---

```
        # Valve helpers
1065     #
```

---

```
def _setValveState(self, valve: str):
    if valve == "A":
        self.valves.set_valve_position_a()
1070     self.buttonA.config(bg=self.OPEN_CLR)
        self.buttonB.config(bg=self.CLOSED_CLR)
    else:
        self.valves.set_valve_position_b()
        self.buttonB.config(bg=self.OPEN_CLR)
1075     self.buttonA.config(bg=self.CLOSED_CLR)
```

```

        self.currentValve = valve

#
1080
# Autoscale toggle
#

def _toggleAutoscale(self):
1085     state = "disabled" if self.autoscaleVar.get() else "normal"
        self.yMinEntry.config(state=state)
        self.yMaxEntry.config(state=state)

#
1090
# Start / Stop
#

def startRecording(self):
1095     if self.recording:
        return

    # Set operator initials from GUI
    settings.operator_initials = self.initialsVar.get().strip() or "NULL"
1100

    # Generate filename for this run
    initials = settings.operator_initials.upper()
    stamp = datetime.now().strftime("%y%m%d_%H%M%S")
    self.current_filename = f"{initials}_{stamp}"
1105

    # Generate directory path

```

```

base_dir = self.save_dir_var.get()
yyyy_mm = datetime.now().strftime("%Y-%m")
full_dir = os.path.join(base_dir, yyyy_mm)

1110
# Create directory if needed
try:
    os.makedirs(full_dir, exist_ok=True)
except Exception as e:
1115
    messagebox.showerror(
        "Directory Error",
        f"Could not create directory {full_dir}: {str(e)}"
    )
    return

1120
# Set filename with full path
full_path = os.path.join(full_dir, self.current_filename + ".txt")
self.daq.set_filename(full_path)
self.file_path_var.set(f"File will be saved to:\n{full_path}")

1125
# Show filename in UI
self.filenameVar.set(self.current_filename)

# Use effective duration (with 5s buffer)
1130
self.maxDuration = settings.effective_run_duration

# Get valve schedule from UI
settings.valve_schedule = self._get_valve_schedule()

1135
# Set initial valve
self.currentValve = self.initialValveVar.get()
self._setValveState(self.currentValve)

```

```

# Clear any existing swap jobs
1140 for job_id in self.swap_job_ids:
        self.root.after_cancel(job_id)
self.swap_job_ids = []

# Schedule all valve swaps
1145 for swap_time, valve_target in settings.valve_schedule:
        if swap_time > 0 and swap_time < self.maxDuration:
            job_id = self.root.after(
                int(swap_time * 1000),
                lambda v=valve_target: self._setValveState(v)
1150             )
            self.swap_job_ids.append(job_id)

self.xData.clear()
self.yData.clear()
1155 self.line.set_data([], [])

self.startTime = time.perf_counter()
self.recording = True
self.daq.start()

1160 self.startBtn.config(state="disabled")
self.stopBtn.config(state="normal")

def stopRecording(self):
1165     if not self.recording:
        return

self.recording = False

```

```

self.daq.stop()

1170
    # Cancel all swap jobs
    for job_id in self.swap_job_ids:
        self.root.after_cancel(job_id)
    self.swap_job_ids = []

1175
    self.startBtn.config(state="normal")
    self.stopBtn.config(state="disabled")

    # Clear filename after short delay to show it was saved
1180    self.root.after(2000, lambda: self.filenameVar.set(""))

#

# Main update loop
1185 #

def updateLoop(self):
    while not self.dataQueue.empty():
        t_rel, v = self.dataQueue.get_nowait()
        1190        self.xData.append(t_rel)
        self.yData.append(v)

    if self.xData:
        elapsed = self.xData[-1]
        1195        remaining = max(0.0, self.maxDuration - elapsed)

        self.timeVar.set(f'{elapsed:.4f}')
        self.remainingVar.set(f'{remaining:.4f}')
        self.signalVar.set(f'{self.yData[-1]:.4f}')

```

```

1200         self.line.set_data(self.xData, self.yData)

        xmin = self.xData[0]
        xmax = self.xData[-1]
1205     pad_x = max(1e-6, (xmax - xmin) * 0.02)
        self.ax.set_xlim(xmin - pad_x, xmax + pad_x)

        if self.autoscaleVar.get():
            ymin = min(self.yData)
1210            ymax = max(self.yData)
            pad_y = max(1e-6, (ymax - ymin) * 0.05)
            self.ax.set_ylim(ymin - pad_y, ymax + pad_y)
        else:
            lims = self._manualYLimits()
1215            if lims:
                self.ax.set_ylim(lims)

        self.fig.canvas.draw_idle()

1220        if self.recording and elapsed >= self.maxDuration:
            self.stopRecording()

        self.jobId = self.root.after(self.blockMS, self.updateLoop)

1225        #

```

---

```

        # Utility helpers
        #

```

---

```

1230     def _manualYLimits(self):

```

```

try:
    ymin = float(self.yMinVar.get())
    ymax = float(self.yMaxVar.get())
    if ymin >= ymax:
1235         raise ValueError
    return ymin, ymax
except ValueError:
    return None

1240 def _safe_float(self, tk_var: tk.StringVar, default: float) -> float:
    try:
        return float(tk_var.get())
    except ValueError:
        return default

1245 # Manual override buttons
def toggleValveA(self):
    self._setValveState("A")

1250 def toggleValveB(self):
    self._setValveState("B")

# Clean shutdown
def closeWindow(self):
1255     if self.recording:
        self.stopRecording()

    if self.jobId:
        self.root.after_cancel(self.jobId)

1260     for job_id in self.swap_job_ids:

```



```

        if job_id:
            self.root.after_cancel(job_id)

1265         if self.auto_run_job:
            self.root.after_cancel(self.auto_run_job)

        self.root.destroy()

1270     # Stand-alone entry point
    def main():
        root = tk.Tk()
        Display(root)
1275     root.mainloop()

    if __name__ == "__main__":
        main()

1280

Settings.py

from __future__ import annotations
from dataclasses import dataclass, field
from typing import Dict, Any, List, Tuple
1285 import os

@dataclass
class Settings:
    # Board configuration
1290     ai_board_number: int = 0 # Analog input board number
    dio_board_number: int = 0 # Digital I/O board number (for valves)

```

```

ai_channel: int = 0 # Analog input channel

# Acquisition parameters
1295 sampling_frequency: int = 10_000 # Hz, e.g. 10_000 for 10 kHz
      block_size: int = 1_000 # samples grabbed per driver call
      run_duration: float = 595.0 # seconds, total length of a run (595 for 10 min interval)

# Misc / operator info
1300 operator_initials: str = "NULL" # appears in data-file names
      save_directory: str = field(default=os.getcwd())

# Auto-run parameters
      auto_run: bool = False # Enable auto-run feature
1305 auto_run_interval: int = 600 # Seconds between runs (default 10 minutes)

# Valve scheduling - now a list of (time, valve) pairs
      valve_schedule: List[Tuple[float, str]] = field(default_factory=lambda: [
          (15.0, "B") # Default: swap to B at 15s
1310 ])

# Properties for synchronization
      @property
      def effective_run_duration(self) -> float:
1315         """Run duration minus 5s buffer"""
         return max(0, self.run_duration - 5.0)

# Helpers
      def validate(self) -> None:
1320         """Raise ValueError if any field is outside a sane range."""
         if not (0 <= self.ai_board_number <= 15):
             raise ValueError("AI board number must be between 0 and 15 (inclusive)")

```

```

if not (0 <= self.dio_board_number <= 15):
    raise ValueError("DIO board number must be between 0 and 15 (inclusive)")
1325 if not (0 <= self.ai_channel <= 15):
    raise ValueError("AI channel must be between 0 and 15 (inclusive)")
if self.sampling_frequency <= 0:
    raise ValueError("sampling_frequency must be positive")
if self.block_size <= 0:
1330     raise ValueError("block_size must be positive")
if self.run_duration <= 0:
    raise ValueError("run_duration must be positive")
for time, valve in self.valve_schedule:
    if time < 0:
1335         raise ValueError(f"valve time cannot be negative")
    if valve not in ("A", "B"):
        raise ValueError(f"valve must be 'A' or 'B'")
if self.auto_run_interval <= 0:
    raise ValueError("auto_run_interval must be positive")
1340
# Easy-to-read dump (handy for logging)
def as_dict(self) -> Dict[str, Any]:
    """Return a plain dict of the current settings."""
    return {
1345         "ai_board_number": self.ai_board_number,
        "dio_board_number": self.dio_board_number,
        "ai_channel": self.ai_channel,
        "sampling_frequency": self.sampling_frequency,
        "block_size": self.block_size,
1350         "run_duration": self.run_duration,
        "operator_initials": self.operator_initials,
        "auto_run": self.auto_run,
        "auto_run_interval": self.auto_run_interval,
    }

```

```

        "valve_schedule": list(self.valve_schedule),
1355     }

    def __str__(self) -> str:
        items = [f"{k}: {v}" for k, v in self.as_dict().items()]
        return "\n".join(items)

1360

# Global singleton – import once, everywhere
settings = Settings()

1365 # Validate immediately so typos are caught on launch
settings.validate()

```

### **USB1408FS.py**

```

from Display import main as run_gui

1370

if __name__ == "__main__":
    # Launch the Tkinter interface
    run_gui()

```

### **1375 Valves.py**

```

from mcculw import ul
from mcculw.enums import DigitalPortType
from time import sleep

1380 from Settings import settings

class Valves:

```

```

def __init__(self):
    self.board_num = settings.dio_board_number
1385 self._hardware_available = False

    try:
        # Try to access the board to verify it exists
        ul.get_board_name(self.board_num)
1390 ul.d_config_port(self.board_num, DigitalPortType.FIRSTPORTA, 1)
        self._hardware_available = True
    except Exception as e:
        print(f'Warning: Digital I/O board {self.board_num} not found. Valve controls will be simulated.')
        self._hardware_available = False
1395

# Function to switch to Position A (open Valve A, close Valve B)
def set_valve_position_a(self) -> None:
    if not self._hardware_available:
        print("Simulating valve A open")
1400 return

    try:
        ul.d_bit_out(self.board_num, DigitalPortType.FIRSTPORTA, 0, 0) # Valve A ON
        ul.d_bit_out(self.board_num, DigitalPortType.FIRSTPORTA, 1, 1) # Valve B OFF
1405 except Exception as e:
        print(f'Error setting valve A: {str(e)}")

# Function to switch to Position B (open Valve B, close Valve A)
def set_valve_position_b(self) -> None:
1410 if not self._hardware_available:
        print("Simulating valve B open")
        return

```

```

try:
1415     ul.d_bit_out(self.board_num, DigitalPortType.FIRSTPORTA, 0, 1) # Valve A OFF
        ul.d_bit_out(self.board_num, DigitalPortType.FIRSTPORTA, 1, 0) # Valve B ON
except Exception as e:
    print(f'Error setting valve B: {str(e)}')

1420
def testValves():
    testValve = Valves()
    testValve.set_valve_position_a()
    sleep(3)
1425     testValve.set_valve_position_b()

# Enable this to test valves
# testValves()

```

## 1430 **Measurement Computing's USB-1608FS**

### **DataAcquisition.py**

```

# DataAcquisition.py
import numpy as np
from mcculw import ul
1435 from mcculw.enums import ULRange
    from mcculw.ul import ULError
    import ctypes as ct
    import threading, queue, time
    from datetime import datetime
1440 import os

from Settings import settings

```

```

1445 class DataAcquisition:
    blockSize = 100
    samplingFrequency = 10_000 # Hz

    def __init__(self):
1450     # Board-specific settings (updated to use settings)
        self.board_num = settings.ai_board_number
        self.channel = settings.ai_channel
        self.ai_range = ULRange.BIP10VOLTS
        self._hardware_available = False

1455     try:
        # Try to access the board to verify it exists
        ul.get_board_name(self.board_num)
        self._hardware_available = True

1460     except ULError:
        print(f"Warning: Analog input board {self.board_num} not found. Running in simulation mode.")
        self._hardware_available = False

        # Pre-allocate one-block buffer
1465     self._buf = (ct.c_uint16 * self.blockSize)()

        # Run bookkeeping
        self.data: list[tuple[float, float]] = []

1470     # initial file name
        self.filename = None

        # Threading helpers

```

```

self._queue: queue.Queue | None = None
1475 self._thread: threading.Thread | None = None
self._running = threading.Event()

def set_filename(self, filename):
    self.filename = filename

1480
# Public control surface
def attach_queue(self, q: queue.Queue) -> None:
    """GUI supplies a queue to receive (t_rel, volts)."""
    self._queue = q

1485
def start(self) -> None:
    if self._thread and self._thread.is_alive():
        return
    self._running.set()
1490 self._thread = threading.Thread(target=self._worker, daemon=True)
self._thread.start()

def stop(self, join_timeout: float = 1.0) -> None:
    self._running.clear()
1495 if self._thread:
    self._thread.join(timeout=join_timeout)
    self._thread = None
self.writeData(self.data) # auto-save
self.data = [] # clear for next run

1500
# Background worker — runs in its own thread
def _worker(self) -> None:
    t0 = time.perf_counter()
    while self._running.is_set():

```



```

1505     volts = self.getSignalData()
        if volts is None:
            continue # skip bad scan, keep running

        t_rel = time.perf_counter() - t0
1510     epoch1904 = self.getTimeData()
        self.recordData(epoch1904, volts)

        if self._queue:
            try:
1515         self._queue.put_nowait((t_rel, volts))
            except queue.Full: # drop oldest if GUI lags
                _ = self._queue.get_nowait()
                self._queue.put_nowait((t_rel, volts))
        # a_in_scan blocks  $\approx$  blockSize/samplingFrequency
1520     # so no extra sleep is needed

# Low-level helpers
def getSignalData(self) -> float | None:
    if not self._hardware_available:
1525         # Simulate a sine wave when hardware isn't available
        return 2.5 + 2.5 * np.sin(time.perf_counter() * 2 * np.pi * 0.1)

    try:
        ul.a_in_scan(self.board_num,
1530         self.channel, self.channel,
            self.blockSize, self.samplingFrequency,
            self.ai_range, self._buf, 0)

        counts = np.ctypeslib.as_array(self._buf).mean()
1535     return float(ul.to_eng_units(self.board_num, self.ai_range, int(counts)))

```

```

except ULError as e:
    print("UL error:", e.errorcode, e.message)
    return None

1540 def getTimeData(self) -> float:
    return (datetime.now() - datetime(1904, 1, 1)).total_seconds()

def recordData(self, epoch1904: float, volts: float) -> None:
    self.data.append((epoch1904, volts))

1545 # File I/O

def writeData(self, data: list[tuple[float, float]]) -> None:
    if not data or not self.filename:
        return

1550 try:
    # Get directory path and ensure it exists
    dir_path = os.path.dirname(self.filename)
    if dir_path: # Only try to create if there is a directory component
        os.makedirs(dir_path, exist_ok=True)

1555 # Write the data file
    with open(self.filename, "w", encoding="utf-8") as f:
        for epoch, v in data:
            # Format: "[time since Jan 1st 1904] TAB [Signal up to 4 decimal places]"
            f.write(f'{epoch:.4f}\t{v:.4f}\n')

        print(f'Successfully saved {len(data)} rows to {self.filename}')

1565 except PermissionError as e:
    print(f'Error: Permission denied when writing to {self.filename}: {str(e)}')

```

```

except OSError as e:
    print(f'Error writing to {self.filename}: {str(e)}')
except Exception as e:
1570     print(f'Unexpected error saving data: {str(e)}')

```

## Display.py

```

▪   import time
    import queue
1575   import tkinter as tk
    from tkinter import ttk, messagebox, filedialog
    import os
    from datetime import datetime, timedelta
    import math

1580   import matplotlib

    matplotlib.use("TkAgg")
    from matplotlib.backends.backend_tkagg import FigureCanvasTkAgg
1585   import matplotlib.pyplot as plt

    from DataAcquisition import DataAcquisition
    from Valves import Valves
    from Settings import settings

1590

    class Display:
        """Real-time GUI with variable valve-swap schedules, X/Y autoscaling, and auto-run."""

1595         OPEN_CLR = "#90EE90"
        CLOSED_CLR = "#D3D3D3"

```

```
#
```

---

```
1600 # Construction
```

```
#
```

---

```
def __init__(self, root: tk.Tk):
```

```
    self.root = root
```

```
1605 self.root.title("Real-Time Signal Monitor")
```

```
    # Create notebook for tabs
```

```
    self.notebook = ttk.Notebook(self.root)
```

```
    self.notebook.pack(fill=tk.BOTH, expand=True, padx=10, pady=10)
```

```
1610
```

```
    # Create control tab
```

```
    self.control_tab = ttk.Frame(self.notebook)
```

```
    self.notebook.add(self.control_tab, text="Control")
```

```
1615
```

```
    # Create config tab
```

```
    self.config_tab = ttk.Frame(self.notebook)
```

```
    self.notebook.add(self.config_tab, text="Configuration")
```

```
    self.daq = DataAcquisition()
```

```
1620
```

```
    self.dataQueue = queue.Queue()
```

```
    self.daq.attach_queue(self.dataQueue)
```

```
    self.blockMS = max(
```

```
        1,
```

```
1625         round(1000 * self.daq.blockSize / self.daq.samplingFrequency),
```

```
    )
```

```

# Run-state
self.recording = False
1630 self.maxDuration = settings.effective_run_duration
self.currentValve = "A"
self.swap_job_ids = [] # List to store all swap job IDs

# Auto-run state
1635 self.auto_run_job = None
self.next_run_time = None

# Initialize valves after settings
self.valves = Valves()
1640 if not hasattr(self.daq, '_hardware_available') or not self.daq._hardware_available:
    messagebox.showwarning("Hardware Not Found",
                           f"Analog input board {settings.ai_board_number} not found. Running in
simulation mode.")

1645 if not hasattr(self.valves, '_hardware_available') or not self.valves._hardware_available:
    messagebox.showwarning("Hardware Not Found",
                           f"Digital I/O board {settings.dio_board_number} not found. Valve controls will be
simulated.")

1650 # Build GUI
self._build_widgets()

self.jobId = self.root.after(self.blockMS, self.updateLoop)
self.root.protocol("WM_DELETE_WINDOW", self.closeWindow)

1655 # Start auto-run scheduler if enabled
if settings.auto_run:
    self._start_auto_run_scheduler()

```

```

1660      #


---


      # GUI layout
      #


---


1665  def _build_widgets(self):
      # Build configuration tab first
      self._build_config_tab()

      # Build control tab
1670  self._build_control_tab()

  def _build_config_tab(self):
      """Build the configuration tab"""
      config_frm = ttk.LabelFrame(self.config_tab, text="Board Configuration", padding=10)
1675  config_frm.pack(fill=tk.BOTH, expand=True, padx=10, pady=10)

      # AI Board
      ai_frm = ttk.Frame(config_frm)
      ai_frm.pack(fill=tk.X, pady=5)
1680  ttk.Label(ai_frm, text="AI Board Number:").pack(side=tk.LEFT, padx=(0, 10))
      self.ai_board_var = tk.IntVar(value=settings.ai_board_number)
      ai_board_spin = ttk.Spinbox(ai_frm, from_=0, to=15, width=5,
                                  textvariable=self.ai_board_var)
      ai_board_spin.pack(side=tk.LEFT)

1685  # DIO Board
      dio_frm = ttk.Frame(config_frm)
      dio_frm.pack(fill=tk.X, pady=5)
      ttk.Label(dio_frm, text="DIO Board Number:").pack(side=tk.LEFT, padx=(0, 10))

```

```

1690         self.dio_board_var = tk.IntVar(value=settings.dio_board_number)
        dio_board_spin = ttk.Spinbox(dio_frm, from_=0, to=15, width=5,
                                     textvariable=self.dio_board_var)
        dio_board_spin.pack(side=tk.LEFT)

1695         # AI Channel
        chan_frm = ttk.Frame(config_frm)
        chan_frm.pack(fill=tk.X, pady=5)
        ttk.Label(chan_frm, text="AI Channel:").pack(side=tk.LEFT, padx=(0, 10))
        self.ai_channel_var = tk.IntVar(value=settings.ai_channel)
1700         ai_channel_spin = ttk.Spinbox(chan_frm, from_=0, to=15, width=5,
                                     textvariable=self.ai_channel_var)
        ai_channel_spin.pack(side=tk.LEFT)

        # Apply Button
1705         btn_frm = ttk.Frame(config_frm)
        btn_frm.pack(fill=tk.X, pady=(20, 5))
        apply_btn = ttk.Button(btn_frm, text="Apply Configuration",
                               command=self._apply_config)
        apply_btn.pack(pady=10)

1710         # Status message
        self.config_status = tk.StringVar(value="")
        ttk.Label(config_frm, textvariable=self.config_status, foreground="blue").pack()

1715         def _build_control_tab(self):
            """Build the main control tab"""
            # Top bar
            top = ttk.Frame(self.control_tab, padding=(10, 5))
            top.pack(fill=tk.X)
1720

```

```

1725     ttk.Label(top, text="Operator Initials:").grid(row=0, column=0, sticky="w")
        self.initialsVar = tk.StringVar()
        ttk.Entry(top, width=5, textvariable=self.initialsVar).grid(
            row=0,
            column=1,
            padx=(2, 15),
        )

        self.startBtn = ttk.Button(top, text="Start", command=self.startRecording)
1730     self.startBtn.grid(row=0, column=2, padx=(10, 2))

        self.stopBtn = ttk.Button(top, text="Stop", command=self.stopRecording, state="disabled")
        self.stopBtn.grid(row=0, column=3)

1735     ttk.Label(top, text="File:").grid(row=0, column=4, padx=(10, 2))
        self.filenameVar = tk.StringVar(value="")
        self.filenameLabel = ttk.Label(top, textvariable=self.filenameVar, foreground="blue")
        self.filenameLabel.grid(row=0, column=5, sticky="w")

1740     ttk.Separator(self.control_tab, orient="horizontal").pack(fill=tk.X, pady=4)

        # Main frame
        main = ttk.Frame(self.control_tab)
        main.pack(fill=tk.X, padx=10)

1745     info = ttk.Frame(main)
        info.pack(side=tk.LEFT, expand=True)

        # New: Save Directory selection

1750     dir_frm = ttk.Frame(info)
        dir_frm.grid(row=0, column=0, columnspan=6, sticky="we", pady=(0, 5))

```



```

1755 ttk.Label(dir_frm, text="Save Directory:").pack(side=tk.LEFT, padx=(0, 5))
self.save_dir_var = tk.StringVar(value=settings.save_directory)
dir_entry = ttk.Entry(dir_frm, textvariable=self.save_dir_var, width=40)
dir_entry.pack(side=tk.LEFT, fill=tk.X, expand=True)
ttk.Button(
    dir_frm,
    text="Browse",
1760    width=8,
    command=self._select_directory
).pack(side=tk.LEFT, padx=(5, 0))

# New: File path display
1765 self.file_path_var = tk.StringVar(value="")
ttk.Label(
    info,
    textvariable=self.file_path_var,
    foreground="green",
1770    wraplength=500
).grid(row=1, column=0, columnspan=6, sticky="w", pady=(0, 5))

# Live readouts
ttk.Label(info, text="Time Elapsed (s):").grid(row=2, column=0, sticky="w")
1775 self.timeVar = tk.StringVar(value="0.0000")
ttk.Label(info, textvariable=self.timeVar).grid(row=2, column=1, padx=(4, 20))

ttk.Label(info, text="Current Signal (V):").grid(row=2, column=2, sticky="w")
self.signalVar = tk.StringVar(value="0.0000")
1780 ttk.Label(info, textvariable=self.signalVar).grid(row=2, column=3, padx=(4, 20))

ttk.Label(info, text="Time Remaining (s):").grid(row=2, column=4, sticky="w")

```

```

self.remainingVar = tk.StringVar(value="0.0000")
1785   ttk.Label(info, textvariable=self.remainingVar).grid(row=2, column=5)

# Run-duration row
dur = ttk.Frame(info)
dur.grid(row=3, column=0, columnspan=6, sticky="w", pady=(6, 0))

1790   ttk.Label(dur, text="Run Duration (s):").pack(side=tk.LEFT, padx=(0, 2))
self.durationVar = tk.StringVar(value=str(settings.run_duration))
self.durationEntry = ttk.Entry(dur, width=7, textvariable=self.durationVar)
self.durationEntry.pack(side=tk.LEFT)
self.durationEntry.bind("<FocusOut>", self._update_duration)
1795   self.durationEntry.bind("<Return>", self._update_duration)

ttk.Label(dur, text="Presets:").pack(side=tk.LEFT, padx=(10, 2))
preset_btns = [
    ("2 min", 120),
1800     ("5 min", 300),
    ("10 min", 600)
]
for text, sec in preset_btns:
    1805     ttk.Button(
        dur,
        text=text,
        width=7,
        command=lambda s=sec: self._set_duration(s)
    ).pack(side=tk.LEFT, padx=(0, 2))

1810
# Valve schedule controls
valve_schedule_frm = ttk.LabelFrame(info, text="Valve Schedule")
valve_schedule_frm.grid(row=4, column=0, columnspan=6, sticky="we", pady=(10, 5), padx=5)

```

```

1815         # Initial valve
        initial_frm = ttk.Frame(valve_schedule_frm)
        initial_frm.pack(fill=tk.X, padx=5, pady=(5, 0))
        ttk.Label(initial_frm, text="Initial Valve:").pack(side=tk.LEFT, padx=(0, 5))
        self.initialValveVar = tk.StringVar(value="A")
1820         ttk.Radiobutton(initial_frm, text="A", variable=self.initialValveVar,
        value="A").pack(side=tk.LEFT)
        ttk.Radiobutton(initial_frm, text="B", variable=self.initialValveVar,
        value="B").pack(side=tk.LEFT)

1825         # Valve swap table
        swap_frm = ttk.Frame(valve_schedule_frm)
        swap_frm.pack(fill=tk.X, padx=5, pady=5)

        # Table header
1830         header = ttk.Frame(swap_frm)
        header.pack(fill=tk.X, pady=(0, 5))
        ttk.Label(header, text="Swap #", width=8).pack(side=tk.LEFT)
        ttk.Label(header, text="Time (s)", width=8).pack(side=tk.LEFT, padx=5)
        ttk.Label(header, text="Valve", width=8).pack(side=tk.LEFT, padx=5)
1835         ttk.Label(header, text="Action", width=8).pack(side=tk.LEFT)

        # Container for swap rows
        self.swap_rows_frame = ttk.Frame(swap_frm)
        self.swap_rows_frame.pack(fill=tk.X)

1840         # Add/remove controls
        ctrl_frm = ttk.Frame(valve_schedule_frm)
        ctrl_frm.pack(fill=tk.X, padx=5, pady=(0, 5))
        ttk.Button(ctrl_frm, text="+ Add Swap", command=self._add_swap_row).pack(side=tk.LEFT)

```

```

1845         ttk.Button(ctrl_frm, text="- Remove Last", command=self._remove_last_swap).pack(side=tk.LEFT,
padx=5)

        # Populate with existing schedule
        self.swap_vars = []
1850     for time, valve in settings.valve_schedule:
        self._add_swap_row(time, valve)

        # Auto-run row
        auto_run_f = ttk.Frame(info)
1855     auto_run_f.grid(row=5, column=0, columnspan=6, sticky="w", pady=(10, 0))

        self.autoRunVar = tk.BooleanVar(value=settings.auto_run)
        ttk.Checkbutton(
            auto_run_f,
1860         text="Auto-run every",
            variable=self.autoRunVar,
            command=self._toggle_auto_run
        ).pack(side=tk.LEFT)

1865     # Interval entry
        self.autoIntVar = tk.StringVar(value=str(settings.auto_run_interval))
        self.autoIntEntry = ttk.Entry(auto_run_f, width=5, textvariable=self.autoIntVar)
        self.autoIntEntry.pack(side=tk.LEFT)
        self.autoIntEntry.bind("<FocusOut>", self._update_auto_interval)
1870     self.autoIntEntry.bind("<Return>", self._update_auto_interval)

        ttk.Label(auto_run_f, text="seconds").pack(side=tk.LEFT, padx=(0, 2))

        # Next run display
1875     self.nextRunVar = tk.StringVar(value="Next run: --:--:--")

```

```

tkk.Label(auto_run_f, textvariable=self.nextRunVar).pack(side=tk.LEFT, padx=(10, 0))

# Y-axis controls
yctrl = ttk.Frame(info)
1880 yctrl.grid(row=6, column=0, columnspan=6, sticky="w", pady=(6, 0))

self.autoscaleVar = tk.BooleanVar(value=True)
tkk.Checkbutton(
    yctrl,
1885     text="Autoscale Y",
    variable=self.autoscaleVar,
    command=self._toggleAutoscale,
).pack(side=tk.LEFT)

1890 tkk.Label(yctrl, text="Y min:").pack(side=tk.LEFT, padx=(10, 2))
self.yMinVar = tk.StringVar(value="0")
self.yMinEntry = ttk.Entry(yctrl, width=7, textvariable=self.yMinVar, state="disabled")
self.yMinEntry.pack(side=tk.LEFT)

1895 tkk.Label(yctrl, text="Y max:").pack(side=tk.LEFT, padx=(6, 2))
self.yMaxVar = tk.StringVar(value="1")
self.yMaxEntry = ttk.Entry(yctrl, width=7, textvariable=self.yMaxVar, state="disabled")
self.yMaxEntry.pack(side=tk.LEFT)

1900 # Manual valve buttons
valve_f = ttk.Frame(main, padding=(20, 0))
valve_f.pack(side=tk.RIGHT, anchor="ne")

self.buttonA = tk.Button(valve_f, text="Open A", width=10, bg=self.CLOSED_CLR,
1905 command=self.toggleValveA)
self.buttonA.pack(pady=(0, 5))

```

```

        self.buttonB = tk.Button(valve_f, text="Open B", width=10, bg=self.CLOSED_CLR,
command=self.toggleValveB)
1910         self.buttonB.pack()

        # Matplotlib figure
        self.fig, self.ax = plt.subplots(figsize=(6, 4))
        self.ax.set_xlabel("Time (s)")
1915         self.ax.set_ylabel("Signal (V)")

        self.line, = self.ax.plot([], [], lw=1.3)

        FigureCanvasTkAgg(self.fig, master=self.control_tab).get_tk_widget().pack(fill=tk.BOTH,
1920         expand=True)

        self.xData = []
        self.yData = []

1925         #


---


        # Configuration methods
        #


---


1930         def _apply_config(self):
            """Apply new configuration settings"""
            try:
                if self.recording:
                    messagebox.showerror("Error", "Cannot change configuration while recording")
1935                 return

            # Validate inputs

```

```

1940     ai_board = int(self.ai_board_var.get())
        dio_board = int(self.dio_board_var.get())
        ai_channel = int(self.ai_channel_var.get())

        if not (0 <= ai_board <= 15):
            raise ValueError("AI board number must be 0-15")
        if not (0 <= dio_board <= 15):
1945             raise ValueError("DIO board number must be 0-15")
        if not (0 <= ai_channel <= 15):
            raise ValueError("AI channel must be 0-15")

        # Update settings
1950     settings.ai_board_number = ai_board
        settings.dio_board_number = dio_board
        settings.ai_channel = ai_channel

        # Reinitialize hardware
1955     self.valves = Valves()
        self.daq = DataAcquisition()
        self.daq.attach_queue(self.dataQueue)

        self.config_status.set("Configuration updated successfully")
1960     except ValueError as e:
        messagebox.showerror("Error", f"Invalid configuration: {str(e)}")

        #

```

---

```

1965     # Valve schedule management
        #

```

---

```

def _add_swap_row(self, time_val: float = 0.0, valve_val: str = "B"):

```

```

1970 """Add a new row to the valve schedule table"""
row = ttk.Frame(self.swap_rows_frame)
row.pack(fill=tk.X, pady=2)

# Swap number
swap_num = len(self.swap_vars) + 1
1975 ttk.Label(row, text=f"#{swap_num}", width=8).pack(side=tk.LEFT)

# Time entry
time_var = tk.StringVar(value=str(time_val))
time_ent = ttk.Entry(row, width=8, textvariable=time_var)
1980 time_ent.pack(side=tk.LEFT, padx=5)

# Valve selection
valve_var = tk.StringVar(value=valve_val)
valve_cmb = ttk.Combobox(row, width=8, textvariable=valve_var, state="readonly")
1985 valve_cmb['values'] = ("A", "B")
valve_cmb.pack(side=tk.LEFT, padx=5)

# Remove button
remove_btn = ttk.Button(row, text="Remove", width=8,
1990 command=lambda r=row: self._remove_swap_row(r))
remove_btn.pack(side=tk.LEFT)

# Store variables
self.swap_vars.append((time_var, valve_var, row))
1995

def _remove_swap_row(self, row):
    """Remove a specific row from the valve schedule"""
    # Find and remove the row from our list
    for i, (time_var, valve_var, row_widget) in enumerate(self.swap_vars):

```



```

2000         if row_widget == row:
                self.swap_vars.pop(i)
                row.destroy()
                break

2005     # Renumber remaining swaps
    for i, (_, row_widget) in enumerate(self.swap_vars):
        swap_num_label = row_widget.winfo_children()[0]
        swap_num_label.config(text=f"#{i + 1}")

2010 def _remove_last_swap(self):
        """Remove the last swap from the schedule"""
        if self.swap_vars:
            _, row = self.swap_vars.pop()
            row.destroy()

2015 def _get_valve_schedule(self) -> list[tuple[float, str]]:
        """Get the current valve schedule from the UI"""
        schedule = []
        for time_var, valve_var, _ in self.swap_vars:

2020             try:
                    time_val = float(time_var.get())
                    valve_val = valve_var.get()
                    if time_val >= 0 and valve_val in ("A", "B"):
                        schedule.append((time_val, valve_val))

2025             else:
                    messagebox.showerror("Invalid Input",
                                           f"Invalid valve schedule: time={time_val}, valve={valve_val}")
                    except ValueError:
                        messagebox.showerror("Invalid Input", "Time must be a number")

2030 return sorted(schedule, key=lambda x: x[0])

```

```
#
```

---

```
# Directory selection
```

```
#
```

---

```
def _select_directory(self):
    """Open directory dialog and update save path"""
    dir_path = filedialog.askdirectory(
        initialdir=self.save_dir_var.get(),
        title="Select Save Directory"
    )
    if dir_path:
        self.save_dir_var.set(dir_path)
        settings.save_directory = dir_path
```

```
#
```

---

```
# Duration and interval synchronization
```

```
#
```

---

```
def _set_duration(self, seconds: float):
    """Set duration without affecting auto-run interval"""
    settings.run_duration = seconds
    self.durationVar.set(str(seconds))
```

```
def _update_duration(self, event=None):
    """Update from GUI entry"""
    try:
        seconds = float(self.durationVar.get())
        settings.run_duration = seconds
```

```
except ValueError:
```

```
    pass
```

```
2065 def _update_auto_interval(self, event=None):
```

```
    """Update auto-run interval from GUI"""
```

```
    try:
```

```
        interval = int(self.autoIntVar.get())
```

```
        settings.auto_run_interval = interval
```

```
2070 except ValueError:
```

```
    pass
```

```
#
```

---

```
2075 # Auto-run methods
```

```
#
```

---

```
def _toggle_auto_run(self):
```

```
    settings.auto_run = self.autoRunVar.get()
```

```
2080 if settings.auto_run:
```

```
    # Update settings from GUI
```

```
    try:
```

```
        settings.auto_run_interval = int(self.autoIntVar.get())
```

```
    except ValueError:
```

```
2085         pass # Keep previous value
```

```
    self._start_auto_run_scheduler()
```

```
elif self.auto_run_job:
```

```
    self.root.after_cancel(self.auto_run_job)
```

```
    self.auto_run_job = None
```

```
2090 self.next_run_time = None
```

```
self.nextRunVar.set("Next run: --:--:--")
```

```

def _calculate_next_run(self):
    """Calculate next run time at exact second interval."""
    now = datetime.now()
    interval_seconds = settings.auto_run_interval

    # Calculate next time that is multiple of interval seconds
    current_seconds = now.hour * 3600 + now.minute * 60 + now.second
    remainder = current_seconds % interval_seconds

    if remainder == 0:
        # Already at interval, run immediately
        next_seconds = current_seconds
    else:
        next_seconds = current_seconds + interval_seconds - remainder

    # Convert seconds back to time
    next_hour = next_seconds // 3600
    next_minute = (next_seconds % 3600) // 60
    next_second = next_seconds % 60

    # Create next run time
    next_run = now.replace(hour=next_hour, minute=next_minute, second=next_second,
microsecond=0)

    # Handle day rollover
    if next_hour >= 24:
        next_run = next_run + timedelta(days=1)

    return next_run

def _start_auto_run_scheduler(self):

```

```

2125         if not settings.auto_run:
            return

        # Calculate next run time
        self.next_run_time = self._calculate_next_run()
        self.nextRunVar.set(f'Next run: {self.next_run_time.strftime("%H:%M:%S')}")

2130

        # Calculate delay in milliseconds
        now = datetime.now()
        delay_ms = int((self.next_run_time - now).total_seconds() * 1000)

2135

        # Schedule next run
        if self.auto_run_job:
            self.root.after_cancel(self.auto_run_job)
            self.auto_run_job = self.root.after(delay_ms, self._execute_auto_run)

2140    def _execute_auto_run(self):
        if not settings.auto_run:
            return

        # Start recording
2145        self.startRecording()

        # Schedule next run after current run completes
        self.auto_run_job = self.root.after(
            int(settings.auto_run_interval * 1000), # Use full interval
2150            self._start_auto_run_scheduler
        )

        #

```

---

```

2155     # Valve helpers
        #


---


        def _setValveState(self, valve: str):
            if valve == "A":
2160                 self.valves.set_valve_position_a()
                    self.buttonA.config(bg=self.OPEN_CLR)
                    self.buttonB.config(bg=self.CLOSED_CLR)
            else:
                self.valves.set_valve_position_b()
2165                 self.buttonB.config(bg=self.OPEN_CLR)
                    self.buttonA.config(bg=self.CLOSED_CLR)

            self.currentValve = valve

2170     #


---


        # Autoscale toggle
        #


---


2175     def _toggleAutoscale(self):
        state = "disabled" if self.autoscaleVar.get() else "normal"
        self.yMinEntry.config(state=state)
        self.yMaxEntry.config(state=state)

2180     #


---


        # Start / Stop
        #


---


2185     def startRecording(self):

```

```

if self.recording:
    return

# Set operator initials from GUI
2190 settings.operator_initials = self.initialsVar.get().strip() or "NULL"

# Generate filename for this run
initials = settings.operator_initials.upper()
stamp = datetime.now().strftime("%y%m%d_%H%M%S")
2195 self.current_filename = f"{initials}_{stamp}"

# Generate directory path
base_dir = self.save_dir_var.get()
yyyy_mm = datetime.now().strftime("%Y-%m")
2200 full_dir = os.path.join(base_dir, yyyy_mm)

# Create directory if needed
try:
    os.makedirs(full_dir, exist_ok=True)
2205 except Exception as e:
    messagebox.showerror(
        "Directory Error",
        f"Could not create directory {full_dir}: {str(e)}"
    )
2210 return

# Set filename with full path
full_path = os.path.join(full_dir, self.current_filename + ".txt")
self.daq.set_filename(full_path)
2215 self.file_path_var.set(f"File will be saved to:\n{full_path}")

```

```

# Show filename in UI
self.filenameVar.set(self.current_filename)

2220     # Use effective duration (with 5s buffer)
        self.maxDuration = settings.effective_run_duration

        # Get valve schedule from UI
        settings.valve_schedule = self._get_valve_schedule()

2225

        # Set initial valve
        self.currentValve = self.initialValveVar.get()
        self._setValveState(self.currentValve)

2230     # Clear any existing swap jobs
        for job_id in self.swap_job_ids:
            self.root.after_cancel(job_id)
        self.swap_job_ids = []

2235     # Schedule all valve swaps
        for swap_time, valve_target in settings.valve_schedule:
            if swap_time > 0 and swap_time < self.maxDuration:
                job_id = self.root.after(
                    int(swap_time * 1000),
2240                    lambda v=valve_target: self._setValveState(v)
                )
                self.swap_job_ids.append(job_id)

        self.xData.clear()

2245     self.yData.clear()
        self.line.set_data([], [])

```



```

        self.startTime = time.perf_counter()
        self.recording = True
2250     self.daq.start()

        self.startBtn.config(state="disabled")
        self.stopBtn.config(state="normal")

2255     def stopRecording(self):
        if not self.recording:
            return

        self.recording = False
2260     self.daq.stop()

        # Cancel all swap jobs
        for job_id in self.swap_job_ids:
            self.root.after_cancel(job_id)
2265     self.swap_job_ids = []

        self.startBtn.config(state="normal")
        self.stopBtn.config(state="disabled")

2270     # Clear filename after short delay to show it was saved
        self.root.after(2000, lambda: self.filenameVar.set(""))

        #

```

---

```

2275     # Main update loop
        #

```

---

```

    def updateLoop(self):

```

```

while not self.dataQueue.empty():
2280     t_rel, v = self.dataQueue.get_nowait()
        self.xData.append(t_rel)
        self.yData.append(v)

if self.xData:
2285     elapsed = self.xData[-1]
        remaining = max(0.0, self.maxDuration - elapsed)

        self.timeVar.set(f'{elapsed:.4f}')
        self.remainingVar.set(f'{remaining:.4f}')
2290     self.signalVar.set(f'{self.yData[-1]:.4f}')

        self.line.set_data(self.xData, self.yData)

        xmin = self.xData[0]
2295     xmax = self.xData[-1]
        pad_x = max(1e-6, (xmax - xmin) * 0.02)
        self.ax.set_xlim(xmin - pad_x, xmax + pad_x)

        if self.autoscaleVar.get():
2300             ymin = min(self.yData)
                    ymax = max(self.yData)
                    pad_y = max(1e-6, (ymax - ymin) * 0.05)
                    self.ax.set_ylim(ymin - pad_y, ymax + pad_y)
        else:
2305             lims = self._manualYLimits()
                    if lims:
                            self.ax.set_ylim(lims)

        self.fig.canvas.draw_idle()

```

```

2310         if self.recording and elapsed >= self.maxDuration:
            self.stopRecording()

        self.jobId = self.root.after(self.blockMS, self.updateLoop)

2315     #

```

---

```

    # Utility helpers
    #

```

---

```

2320 def _manualYLimits(self):
    try:
        ymin = float(self.yMinVar.get())
        ymax = float(self.yMaxVar.get())
2325     if ymin >= ymax:
        raise ValueError
        return ymin, ymax
    except ValueError:
        return None

2330 def _safe_float(self, tk_var: tk.StringVar, default: float) -> float:
    try:
        return float(tk_var.get())
    except ValueError:
2335     return default

    # Manual override buttons
    def toggleValveA(self):
        self._setValveState("A")

```

---

```

2340

```

```
def toggleValveB(self):  
    self._setValveState("B")
```

```
# Clean shutdown
```

2345

```
def closeWindow(self):
```

```
    if self.recording:
```

```
        self.stopRecording()
```

```
    if self.jobId:
```

2350

```
        self.root.after_cancel(self.jobId)
```

```
    for job_id in self.swap_job_ids:
```

```
        if job_id:
```

```
            self.root.after_cancel(job_id)
```

2355

```
    if self.auto_run_job:
```

```
        self.root.after_cancel(self.auto_run_job)
```

```
    self.root.destroy()
```

2360

```
# Stand-alone entry point
```

```
def main():
```

```
    root = tk.Tk()
```

2365

```
    Display(root)
```

```
    root.mainloop()
```

```
if __name__ == "__main__":
```

2370

```
    main()
```

## Settings.py

```
from __future__ import annotations
from dataclasses import dataclass, field
2375 from typing import Dict, Any, List, Tuple
import os

@dataclass
class Settings:
2380     # Board configuration
    ai_board_number: int = 0 # Analog input board number
    dio_board_number: int = 0 # Digital I/O board number (for valves)
    ai_channel: int = 0 # Analog input channel

2385     # Acquisition parameters
    sampling_frequency: int = 10_000 # Hz, e.g. 10_000 for 10 kHz
    block_size: int = 1_000 # samples grabbed per driver call
    run_duration: float = 600.0 # seconds, total length of a run (595 for 10 min interval)

2390     # Misc / operator info
    operator_initials: str = "NULL" # appears in data-file names
    save_directory: str = field(default=os.getcwd())

    # Auto-run parameters
2395     auto_run: bool = False # Enable auto-run feature
    auto_run_interval: int = 600 # Seconds between runs (default 10 minutes)

    # Valve scheduling - now a list of (time, valve) pairs
    valve_schedule: List[Tuple[float, str]] = field(default_factory=lambda: [
2400         (15.0, "B") # Default: swap to B at 15s
    ])
])
```

```

# Properties for synchronization
@property
2405 def effective_run_duration(self) -> float:
    """Run duration minus 5s buffer"""
    return max(0, self.run_duration - 5.0)

# Helpers
2410 def validate(self) -> None:
    """Raise ValueError if any field is outside a sane range."""
    if not (0 <= self.ai_board_number <= 15):
        raise ValueError("AI board number must be between 0 and 15 (inclusive)")
    if not (0 <= self.dio_board_number <= 15):
2415     raise ValueError("DIO board number must be between 0 and 15 (inclusive)")
    if not (0 <= self.ai_channel <= 15):
        raise ValueError("AI channel must be between 0 and 15 (inclusive)")
    if self.sampling_frequency <= 0:
        raise ValueError("sampling_frequency must be positive")
2420 if self.block_size <= 0:
        raise ValueError("block_size must be positive")
    if self.run_duration <= 0:
        raise ValueError("run_duration must be positive")
    for time, valve in self.valve_schedule:
2425     if time < 0:
        raise ValueError(f"valve time cannot be negative")
        if valve not in ("A", "B"):
            raise ValueError(f"valve must be 'A' or 'B'")
    if self.auto_run_interval <= 0:
2430     raise ValueError("auto_run_interval must be positive")

# Easy-to-read dump (handy for logging)

```

```

def as_dict(self) -> Dict[str, Any]:
    """Return a plain dict of the current settings."""
2435     return {
        "ai_board_number": self.ai_board_number,
        "dio_board_number": self.dio_board_number,
        "ai_channel": self.ai_channel,
        "sampling_frequency": self.sampling_frequency,
2440     "block_size": self.block_size,
        "run_duration": self.run_duration,
        "operator_initials": self.operator_initials,
        "auto_run": self.auto_run,
        "auto_run_interval": self.auto_run_interval,
2445     "valve_schedule": list(self.valve_schedule),
    }

def __str__(self) -> str:
    items = [f"{k}: {v}" for k, v in self.as_dict().items()]
2450     return "\n".join(items)

# Global singleton – import once, everywhere
settings = Settings()
2455

# Validate immediately so typos are caught on launch
settings.validate()

```

### **USB1608FS.py**

```

2460 from Display import main as run_gui

if __name__ == "__main__":

```

```
# Launch the Tkinter interface
```

```
run_gui()
```

2465

### **Valves.py**

```
from mcculw import ul
```

```
from mcculw.enums import DigitalPortType
```

```
from time import sleep
```

2470

```
from Settings import settings
```

```
class Valves:
```

2475

```
    def __init__(self):
```

```
        self.board_num = settings.dio_board_number
```

```
        self._hardware_available = False
```

```
        try:
```

2480

```
            # Try to access the board to verify it exists
```

```
            ul.get_board_name(self.board_num)
```

```
            # Configure all digital I/O bits as outputs
```

```
            ul.d_config_port(self.board_num, DigitalPortType.AUXPORT, 1)
```

```
            self._hardware_available = True
```

2485

```
        except Exception as e:
```

```
            print(f'Warning: Digital I/O board {self.board_num} not found. Valve controls will be simulated.')
            self._hardware_available = False
```

```
    def _set_valve(self, a_state: int, b_state: int):
```

2490

```
        """Set both valve control lines to specified states"""
```

```
        if not self._hardware_available:
```

```
            return
```



```

try:
2495     # Set Position B control (DIO1)
        ul.d_bit_out(self.board_num, DigitalPortType.AUXPORT, 1, b_state)
        # Set Position A control (DIO3)
        ul.d_bit_out(self.board_num, DigitalPortType.AUXPORT, 3, a_state)

2500 except Exception as e:
        print(f'Error setting valve states: {str(e)}')

def set_valve_position_b(self) -> None:
    if not self._hardware_available:
2505         print("Simulating valve B open")
        return

    try:
        # Set A high, B low
2510         self._set_valve(a_state=1, b_state=0)
        print("Valve set to Position B")
    except Exception as e:
        print(f'Error setting valve B: {str(e)}')

2515 def set_valve_position_a(self) -> None:
    if not self._hardware_available:
        print("Simulating valve A open")
        return

2520 try:
        # Set B high, A low
        self._set_valve(a_state=0, b_state=1)
        print("Valve set to Position A")

```

```
except Exception as e:
```

```
2525     print(f'Error setting valve A: {str(e)}')
```

```
def testValves():
```

```
    testValve = Valves()
```

```
    testValve.board_num = 0
```

```
2530    ul.d_bit_out(0, DigitalPortType.AUXPORT, 1, 1)
```

```
    sleep(5)
```

```
    ul.d_bit_out(0, DigitalPortType.AUXPORT, 1, 0)
```

```
# Uncomment the line below to run the test
```

```
2535 # testValves()
```

## **National Instruments' USB-6008 and USB-6009**

### **ConfigWindow.py**

```
import tkinter as tk
```

```
2540 from tkinter import ttk
```

```
class ConfigWindow(tk.Toplevel):
```

```
    def __init__(self, parent, daq, channel_config, valve_config):
```

```
2545        super().__init__(parent)
```

```
        self.title("DAQ Configuration")
```

```
        self.daq = daq
```

```
        self.channel_config = channel_config
```

```
        self.valve_config = valve_config
```

```
2550        self.parent = parent
```

```
# Create notebook for tabs
```

```
self.notebook = ttk.Notebook(self)
self.notebook.pack(fill='both', expand=True, padx=10, pady=10)
```

2555

```
# Analog Channels Tab
self.analog_tab = ttk.Frame(self.notebook)
self.notebook.add(self.analog_tab, text="Analog Channels")
```

2560

```
# Device configuration
ttk.Label(self.analog_tab, text="Device Name:").grid(row=0, column=0, padx=5, pady=5)
self.device_var = tk.StringVar(value=self.daq.device_name)
ttk.Entry(self.analog_tab, textvariable=self.device_var).grid(row=0, column=1, padx=5, pady=5)
```

2565

```
# Channel mapping
ttk.Label(self.analog_tab, text="Controller").grid(row=1, column=0)
ttk.Label(self.analog_tab, text="Output Channel").grid(row=1, column=1)
ttk.Label(self.analog_tab, text="Input Channel").grid(row=1, column=2)
```

2570

```
self.ao_vars = []
self.ai_vars = []

for i, config in enumerate(self.channel_config):
    ttk.Label(self.analog_tab, text=f"Controller {i + 1}").grid(row=i + 2, column=0, padx=5, pady=5)
```

2575

```
    ao_var = tk.StringVar(value=config['ao'])
    ai_var = tk.StringVar(value=config['ai'])
```

2580

```
    ttk.Entry(self.analog_tab, textvariable=ao_var, width=8).grid(row=i + 2, column=1, padx=5, pady=5)
    ttk.Entry(self.analog_tab, textvariable=ai_var, width=8).grid(row=i + 2, column=2, padx=5, pady=5)

self.ao_vars.append(ao_var)
self.ai_vars.append(ai_var)
```

```

2585     # Digital Channels Tab
self.digital_tab = ttk.Frame(self.notebook)
self.notebook.add(self.digital_tab, text="Digital Channels")

    # Valve configuration table
2590     ttk.Label(self.digital_tab, text="Valve").grid(row=0, column=0, padx=5, pady=5)
        ttk.Label(self.digital_tab, text="Port/Line").grid(row=0, column=1, padx=5, pady=5)

self.valve_vars = []
for i, valve in enumerate(self.valve_config):
2595     ttk.Label(self.digital_tab, text=valve['name']).grid(row=i + 1, column=0, padx=5, pady=5)
        port_var = tk.StringVar(value=valve['port_line'])
        ttk.Entry(self.digital_tab, textvariable=port_var).grid(row=i + 1, column=1, padx=5, pady=5)
        self.valve_vars.append(port_var)

2600     # Save button
        ttk.Button(self, text="Save Configuration", command=self.save_config).pack(pady=10)

def save_config(self):
    """Save configuration to main application"""
2605     self.daq.set_device_name(self.device_var.get())

    for i in range(len(self.channel_config)):
        self.channel_config[i]['ao'] = self.ao_vars[i].get()
        self.channel_config[i]['ai'] = self.ai_vars[i].get()

2610     # Save valve config
    for i in range(len(self.valve_config)):
        self.valve_config[i]['port_line'] = self.valve_vars[i].get()

```

```
2615     self.parent.update_channel_labels()
        self.parent.update_valve_config()
        self.destroy()
```

### **DAQController.py**

```
2620 import nidaqmx

class DAQController:
    def __init__(self, device_name="Dev2"):
        self.device_name = device_name
2625     self.digital_states = {} # Track valve states

    def set_device_name(self, device_name):
        self.device_name = device_name

2630     def write_voltage(self, channel, voltage):
        """Write voltage to analog output channel (clamped to 0-5V)"""
        clamped_voltage = max(0.0, min(5.0, voltage))

        with nidaqmx.Task() as task:
2635             task.ao_channels.add_ao_voltage_chan(
                f"{self.device_name}/{channel}",
                min_val=0.0,
                max_val=5.0
            )
2640             task.write(clamped_voltage)

    def read_voltage(self, channel):
        """Read voltage from analog input channel"""
        with nidaqmx.Task() as task:
```

```
2645     task.ai_channels.add_ai_voltage_chan(f'{self.device_name}/{channel}')
        return task.read()
```

```
def write_digital(self, port_line, state):
    """Write digital output (on/off) to a specific port/line"""
```

```
2650     with nidaqmx.Task() as task:
        task.do_channels.add_do_chan(f'{self.device_name}/{port_line}')
        task.write(bool(state))
        # Update state tracking
        self.digital_states[port_line] = bool(state)
```

```
2655
def read_digital_state(self, port_line):
    """Read last set digital state"""
    return self.digital_states.get(port_line, False)
```

## 2660 **Display.py**

```
    import tkinter as tk
    from tkinter import ttk, messagebox, Menu
    import time
    from datetime import datetime, timedelta
2665    from Flowrate import MFCManager
    from DAQController import DAQController
    from ConfigWindow import ConfigWindow
    from ValveControlFrame import ValveControlFrame
    from ValveScheduler import ValveScheduler
```

2670

```
class MFCControlFrame(tk.LabelFrame):
    def __init__(self, parent, index, daq, mfc_manager, channel_config, *args, **kwargs):
        super().__init__(parent, *args, **kwargs)
```

```

2675     self.daq = daq
        self.mfc_manager = mfc_manager
        self.index = index
        self.channel_config = channel_config

2680     # Channel info labels
        self.channel_info = tk.StringVar()
        ttk.Label(self, textvariable=self.channel_info, font=("Arial", 8)).grid(
            row=0, column=0, columnspan=4, sticky="w", padx=5
        )

2685     # MFC selection
        ttk.Label(self, text="MFC Type:").grid(row=1, column=0, padx=5, pady=5, sticky="e")
        self.mfc_var = tk.StringVar()
        self.mfc_dropdown = ttk.Combobox(self, textvariable=self.mfc_var, state="readonly", width=12)
2690     self.mfc_dropdown['values'] = self.mfc_manager.get_all_mfc_names()
        self.mfc_dropdown.grid(row=1, column=1, padx=5, pady=5, columnspan=3, sticky="w")

        # Set flow section
        ttk.Label(self, text="Set Flow:").grid(row=2, column=0, padx=5, pady=5, sticky="e")
2695     self.flow_var = tk.StringVar()
        self.flow_entry = ttk.Entry(self, textvariable=self.flow_var, width=8)
        self.flow_entry.grid(row=2, column=1, padx=5, pady=5, sticky="w")

        # Set flow unit display
2700     self.set_unit_var = tk.StringVar(value="SCCM")
        ttk.Label(self, textvariable=self.set_unit_var, width=6).grid(row=2, column=2, padx=5, pady=5,
            sticky="w")

        # Set button
2705     self.set_btn = ttk.Button(self, text="Set", command=self.set_flow, width=6)

```

```
self.set_btn.grid(row=2, column=3, padx=5, pady=5, sticky="w")
```

```
# Actual flow section
```

```
ttk.Label(self, text="Actual Flow:").grid(row=3, column=0, padx=5, pady=5, sticky="e")
```

```
2710 self.actual_flow_var = tk.StringVar(value="0.0")
```

```
ttk.Label(self, textvariable=self.actual_flow_var, width=8).grid(row=3, column=1, padx=5, pady=5,  
sticky="w")
```

```
# Actual flow unit display
```

```
2715 self.actual_unit_var = tk.StringVar(value="SCCM")
```

```
ttk.Label(self, textvariable=self.actual_unit_var).grid(row=3, column=2, padx=5, pady=5,  
sticky="w")
```

```
# Scaling information
```

```
2720 self.scaling_info = tk.StringVar()
```

```
ttk.Label(self, textvariable=self.scaling_info, font=("Arial", 8)).grid(  
    row=4, column=0, columnspan=4, sticky="w", padx=5  
)
```

```
2725 # Initialize
```

```
if self.mfc_dropdown['values']:  
    self.mfc_var.set(self.mfc_dropdown['values'][0])  
    self.update_unit_display()  
    self.update_scaling_info()
```

```
2730
```

```
# Bind MFC selection change
```

```
self.mfc_var.trace_add("write", self.on_mfc_change)
```

```
# Update channel labels
```

```
2735 self.update_channel_info()
```



```
def on_mfc_change(self, *args):
```

```
    self.update_unit_display()
```

```
    self.update_scaling_info()
```

2740

```
def update_scaling_info(self):
```

```
    """Update scaling information display"""
```

```
    mfc = self.get_current_mfc()
```

```
    if mfc:
```

2745

```
        self.scaling_info.set(f"5V = {mfc.max_flow} {mfc.unit}, 0V = 0 {mfc.unit}")
```

```
def update_unit_display(self):
```

```
    """Update unit displays based on MFC selection"""
```

```
    mfc = self.get_current_mfc()
```

2750

```
    if mfc:
```

```
        unit = mfc.unit
```

```
        self.set_unit_var.set(unit)
```

```
        self.actual_unit_var.set(unit)
```

2755

```
def update_channel_info(self):
```

```
    """Update channel information display"""
```

```
    ao = self.channel_config[self.index]['ao']
```

```
    ai = self.channel_config[self.index]['ai']
```

```
    self.channel_info.set(f"Output: {ao} | Input: {ai}")
```

2760

```
def get_current_mfc(self):
```

```
    return self.mfc_manager.get_mfc(self.mfc_var.get())
```

```
def set_flow(self):
```

2765

```
    try:
```

```
        mfc = self.get_current_mfc()
```

```
        if not mfc:
```

```
        messagebox.showerror("Selection Error", "No MFC selected")
```

```
        return
```

2770

```
        flow = float(self.flow_var.get())
```

```
        voltage = mfc.flow_to_voltage(flow)
```

```
        ao_channel = self.channel_config[self.index]['ao']
```

```
        self.daq.write_voltage(ao_channel, voltage)
```

2775

```
    except (ValueError, AttributeError) as e:
```

```
        messagebox.showerror("Input Error", f"Invalid flow value: {e}")
```

```
    except Exception as e:
```

```
        messagebox.showerror("Error", f"Failed to set flow: {str(e)}")
```

2780

```
    def update_reading(self):
```

```
        try:
```

```
            mfc = self.get_current_mfc()
```

```
            if not mfc:
```

```
                return
```

2785

```
            ai_channel = self.channel_config[self.index]['ai']
```

```
            voltage = self.daq.read_voltage(ai_channel)
```

```
            flow = mfc.voltage_to_flow(voltage)
```

```
            self.actual_flow_var.set(f"{flow:.2f}")
```

2790

```
    except Exception as e:
```

```
        # Fail silently for read errors to avoid spamming
```

```
        pass
```

2795

```
class ScheduledRunTab(ttk.Frame):
```

```
    def __init__(self, parent, daq, valve_config, *args, **kwargs):
```

```
        super().__init__(parent, *args, **kwargs)
```

```
        self.daq = daq
```

```

self.valve_config = valve_config
2800 self.swap_job_ids = []
self.recording = False
self.auto_run_job = None
self.next_run_time = None
self.position_job = None

2805

# Configure grid for columns
for i in range(4):
    self.columnconfigure(i, weight=1, uniform="valve_cols")

2810

# Valve position display (top)
self.position_frame = ttk.LabelFrame(self, text="Current Valve Positions")
self.position_frame.grid(row=0, column=0, columnspan=4, sticky="we", padx=5, pady=5)

self.valve_position_vars = []

2815
for i in range(4):
    frame = ttk.Frame(self.position_frame)
    frame.pack(side=tk.LEFT, padx=10, pady=5)
    ttk.Label(frame, text=f"Valve {i + 1}:" ).pack(side=tk.LEFT)
    pos_var = tk.StringVar(value="OFF")
    2820    ttk.Label(frame, textvariable=pos_var, width=5).pack(side=tk.LEFT)
    self.valve_position_vars.append(pos_var)

# Run controls frame (middle)
self.control_frame = ttk.LabelFrame(self, text="Run Controls", padding=10)
2825 self.control_frame.grid(row=1, column=0, columnspan=4, sticky="we", padx=5, pady=10)

# Run duration
ttk.Label(self.control_frame, text="Run Duration (s):").grid(row=0, column=0, padx=(0, 5))
self.duration_var = tk.StringVar(value="60")

```

```

2830         ttk.Entry(self.control_frame, width=8, textvariable=self.duration_var).grid(row=0, column=1)

        # Start/Stop buttons
        self.start_btn = ttk.Button(self.control_frame, text="Start Run", command=self.start_recording)
        self.start_btn.grid(row=0, column=2, padx=10)

2835
        self.stop_btn = ttk.Button(self.control_frame, text="Stop Run", command=self.stop_recording,
state="disabled")
        self.stop_btn.grid(row=0, column=3)

2840
        # Auto-run controls
        auto_frame = ttk.Frame(self.control_frame)
        auto_frame.grid(row=0, column=4, padx=(20, 0))

        self.auto_run_var = tk.BooleanVar(value=False)
2845         ttk.Checkbutton(auto_frame, text="Auto-run every", variable=self.auto_run_var,
                        command=self.toggle_auto_run).pack(side=tk.LEFT)

        self.interval_var = tk.StringVar(value="300")
        ttk.Entry(auto_frame, width=5, textvariable=self.interval_var).pack(side=tk.LEFT, padx=5)
2850         ttk.Label(auto_frame, text="seconds").pack(side=tk.LEFT)

        self.next_run_var = tk.StringVar(value="Next run: --:--:--")
        ttk.Label(auto_frame, textvariable=self.next_run_var).pack(side=tk.LEFT, padx=(10, 0))

2855
        # Valve schedulers (bottom)
        self.valve_schedulers = []
        for i in range(4):
            scheduler = ValveScheduler(
                self, i, daq, valve_config,
2860                 padding=10,

```

```

        relief="groove"
    )
    scheduler.grid(row=2, column=i, padx=5, pady=5, sticky="nsew")
    self.valve_schedulers.append(scheduler)

```

2865

```

def toggle_auto_run(self):
    if self.auto_run_var.get():
        self.start_auto_run_scheduler()
    elif self.auto_run_job:
2870         self.master.after_cancel(self.auto_run_job)
        self.auto_run_job = None
        self.next_run_time = None
        self.next_run_var.set("Next run: --:--:--")

```

2870

2875

```

def calculate_next_run(self):
    """Calculate next run time at exact second interval."""
    now = datetime.now()
    try:
        interval_seconds = int(self.interval_var.get())
    except ValueError:
2880         interval_seconds = 300

```

2880

```

    current_seconds = now.hour * 3600 + now.minute * 60 + now.second
    remainder = current_seconds % interval_seconds

```

2885

```

    if remainder == 0:
        next_seconds = current_seconds
    else:
        next_seconds = current_seconds + interval_seconds - remainder

```

2890

```

    next_hour = next_seconds // 3600

```

```
next_minute = (next_seconds % 3600) // 60
```

```
next_second = next_seconds % 60
```

```
2895 next_run = now.replace(hour=next_hour, minute=next_minute,  
                        second=next_second, microsecond=0)
```

```
if next_hour >= 24:
```

```
    next_run = next_run + timedelta(days=1)
```

```
2900
```

```
    return next_run
```

```
def start_auto_run_scheduler(self):
```

```
    if not self.auto_run_var.get():
```

```
2905
```

```
        return
```

```
self.next_run_time = self.calculate_next_run()
```

```
self.next_run_var.set(f'Next run: {self.next_run_time.strftime("%H:%M:%S')}')
```

```
2910
```

```
now = datetime.now()
```

```
delay_ms = int((self.next_run_time - now).total_seconds() * 1000)
```

```
if self.auto_run_job:
```

```
    self.master.after_cancel(self.auto_run_job)
```

```
2915
```

```
self.auto_run_job = self.master.after(delay_ms, self.execute_auto_run)
```

```
def execute_auto_run(self):
```

```
    if not self.auto_run_var.get():
```

```
        return
```

```
2920
```

```
self.start_recording()
```

```
self.auto_run_job = self.master.after(
```

```

        int(self.interval_var.get()) * 1000,
        self.start_auto_run_scheduler
2925    )

def start_recording(self):
    if self.recording:
        return

2930    self.recording = True
    self.start_btn.config(state="disabled")
    self.stop_btn.config(state="normal")

2935    # Set initial states for all valves
    for scheduler in self.valve_schedulers:
        scheduler.set_initial_state()

    # Schedule valve swaps
2940    for scheduler in self.valve_schedulers:
        scheduler.schedule_actions(self.master)

    # Schedule run end
    try:
2945        duration = float(self.duration_var.get())
        job_id = self.master.after(
            int(duration * 1000),
            self.stop_recording
        )

2950        self.swap_job_ids.append(job_id)
    except ValueError:
        messagebox.showerror("Invalid Duration", "Please enter a valid number for run duration")

```

```

# Start updating valve positions
2955 self.update_valve_positions()

def update_valve_positions(self):
    """Update valve position display"""
    for i, scheduler in enumerate(self.valve_schedulers):
2960         self.valve_position_vars[i].set("ON" if scheduler.current_state else "OFF")

    # Continue updating if recording
    if self.recording:
        self.position_job = self.after(500, self.update_valve_positions)
2965

def stop_recording(self):
    if not self.recording:
        return

2970     self.recording = False

    # Cancel all swap jobs
    for job_id in self.swap_job_ids:
        self.master.after_cancel(job_id)
2975     self.swap_job_ids = []

    # Cancel valve schedules
    for scheduler in self.valve_schedulers:
        scheduler.cancel_schedules()
2980         scheduler.turn_off()

    # Cancel position updates
    if self.position_job:
        self.after_cancel(self.position_job)

```



2985

```
self.start_btn.config(state="normal")
self.stop_btn.config(state="disabled")
```

```
# Final position update
```

2990

```
self.update_valve_positions()
```

```
class MainApp(tk.Tk):
```

```
    def __init__(self):
```

2995

```
        super().__init__()
        self.title("MFC & Valve Control System")
        self.geometry("1000x700")
```

```
# Initialize managers
```

3000

```
self.mfc_manager = MFCManager()
self.daq = DAQController()
```

```
# Default channel configuration
```

```
self.channel_config = [
```

3005

```
    {'ao': 'ao0', 'ai': 'ai0'},
    {'ao': 'ao1', 'ai': 'ai1'},
    {'ao': 'ao2', 'ai': 'ai2'},
    {'ao': 'ao3', 'ai': 'ai3'}
]
```

3010

```
# Default valve configuration
```

```
self.valve_config = [
    {"name": "Valve 1", "port_line": "port1/line0"},
    {"name": "Valve 2", "port_line": "port1/line1"},
    {"name": "Valve 3", "port_line": "port1/line2"},
]
```

3015

```
        {"name": "Valve 4", "port_line": "port1/line3"},  
    ]
```

```
# Add available MFCs with output range 5.0V
```

```
3020 self.populate_mfcs()
```

```
# Create menu
```

```
self.create_menu()
```

```
3025 # Create notebook (tabs)
```

```
self.notebook = ttk.Notebook(self)
```

```
self.notebook.pack(fill='both', expand=True, padx=10, pady=10)
```

```
# Tab 1: MFC Control
```

```
3030 self.mfc_tab = ttk.Frame(self.notebook)
```

```
self.notebook.add(self.mfc_tab, text="MFC Control")
```

```
# Create MFC control frames
```

```
self.control_frames = []
```

```
3035 for i in range(4):
```

```
    frame = MFCControlFrame(  
        self.mfc_tab, i, self.daq, self.mfc_manager, self.channel_config,  
        text=f"MFC Controller {i + 1}", padx=10, pady=10  
    )
```

```
3040 frame.grid(row=i // 2, column=i % 2, padx=10, pady=10, sticky="nsew")
```

```
self.control_frames.append(frame)
```

```
# Configure grid weights for MFC tab
```

```
for i in range(2):
```

```
3045 self.mfc_tab.rowconfigure(i, weight=1)
```

```
self.mfc_tab.columnconfigure(i, weight=1)
```

```

# Tab 2: Valve Control
self.valve_tab = ttk.Frame(self.notebook)
3050 self.notebook.add(self.valve_tab, text="Valve Control")

# Create valve control frame
self.valve_frame = ValveControlFrame(
    self.valve_tab, self.daq, self.valve_config,
3055 text="Manual Valve Controls", padx=20, pady=20
)
self.valve_frame.pack(fill='both', expand=True, padx=20, pady=20)

# Tab 3: Scheduled Runs
3060 self.schedule_tab = ttk.Frame(self.notebook)
self.notebook.add(self.schedule_tab, text="Scheduled Runs")

# Create scheduled run frame
self.schedule_frame = ScheduledRunTab(
3065 self.schedule_tab, self.daq, self.valve_config,
padding=10
)
self.schedule_frame.pack(fill='both', expand=True)

3070 # Setup periodic updates for MFC readings
self.update_interval = 1000 # ms
self.update_readings()

def create_menu(self):
3075 """Create the menu bar"""
menubar = Menu(self)

```

```

config_menu = Menu(menubar, tearoff=0)
config_menu.add_command(label="Device Configuration", command=self.open_config)
3080 menubar.add_cascade(label="Configuration", menu=config_menu)

self.config(menu=menubar)

def open_config(self):
3085     """Open the configuration window"""
    ConfigWindow(self, self.daq, self.channel_config, self.valve_config)

def update_channel_labels(self):
    """Update channel info in all control frames"""
3090     for frame in self.control_frames:
        frame.update_channel_info()

def update_valve_config(self):
    """Update valve configuration in frames"""
3095     self.valve_frame.update_valve_ports()
    self.schedule_frame.valve_config = self.valve_config
    for i, scheduler in enumerate(self.schedule_frame.valve_schedulers):
        scheduler.port_line = self.valve_config[i]['port_line']

3100 def populate_mfcs(self):
    # Add all MFC types with output range 5.0V
    mfc_specs = [
        ("30 SLPM", 30, 5.0),
        ("15 SLPM", 15, 5.0),
3105     ("5 SLPM", 5, 5.0),
        ("1 SLPM", 1, 5.0),
        ("500 SCCM", 500, 5.0),
        ("100 SCCM", 100, 5.0),

```

```

        ("20 SCCM", 20, 5.0),
3110        ("10 SCCM", 10, 5.0)
    ]
    for name, max_flow, output_range in mfc_specs:
        self.mfc_manager.add_mfc(name, max_flow, output_range)

3115    def update_readings(self):
        for frame in self.control_frames:
            frame.update_reading()
        self.after(self.update_interval, self.update_readings)

3120    Flowrate.py

class MFC:
    def __init__(self, name, max_flow, output_range=5.0):
        self.name = name
        self.max_flow = max_flow
3125        self.unit = "SLPM" if "SLPM" in name else "SCCM"
        self.output_range = output_range # Voltage range for feedback signal

    def flow_to_voltage(self, flow_rate):
        """Convert flow rate to voltage (0-5V scale) based on MFC capacity"""
3130        if self.max_flow <= 0:
            return 0.0

        # Calculate voltage proportionally to max flow
        voltage = (flow_rate / self.max_flow) * 5.0

3135        # Clamp between 0-5V to prevent out-of-range errors
        return max(0.0, min(5.0, voltage))

```

```

def voltage_to_flow(self, voltage):
3140     """Convert voltage to flow rate based on MFC capacity and output range"""
    if self.max_flow <= 0:
        return 0.0
    # Scale based on MFC output range
    raw_value = (voltage / self.output_range) * self.max_flow
3145
    # voltage to flow rate not reading correct values? lets calibrate it.
    calibration_constant = (-0.2681 * self.max_flow) - 0.1454

    calibrated_value = raw_value - calibration_constant
3150
    return calibrated_value

class MFCManager:
    def __init__(self):
3155         self.mfcs = {}

    def add_mfc(self, name, max_flow, output_range=5.0):
        self.mfcs[name] = MFC(name, max_flow, output_range)

3160    def get_mfc(self, name):
        return self.mfcs.get(name)

    def get_all_mfc_names(self):
        return list(self.mfcs.keys())
3165

```

## NI DAQ.py

```

from Display import MainApp

```

```

if __name__ == "__main__":
3170     app = MainApp()
        app.mainloop()

```

### ValveControlFrame.py

```

import tkinter as tk
3175 from tkinter import ttk, messagebox

class ValveControlFrame(tk.LabelFrame):
    def __init__(self, parent, daq, valve_config, *args, **kwargs):
3180         super().__init__(parent, *args, **kwargs)
        self.daq = daq
        self.valve_config = valve_config
        self.valve_states = {}
        self.on_buttons = {}
3185         self.off_buttons = {}

        # Title
        ttk.Label(self, text="Valve Control", font=("Arial", 12, "bold")).grid(
            row=0, column=0, columnspan=4, pady=10
3190        )

        # Create regular buttons (not ttk) for full color control
        for i, valve in enumerate(self.valve_config):
            # Valve name
3195             ttk.Label(self, text=valve["name"]).grid(row=i + 1, column=0, padx=10, pady=5, sticky="w")

            # ON button (regular tk.Button)
            on_btn = tk.Button(

```

```

        self,
3200     text="ON",
        width=6,
        bg="SystemButtonFace", # Default color
        activebackground="SystemButtonFace",
        command=lambda v=valve["port_line"]: self.set_valve(v, True)
3205 )
    on_btn.grid(row=i + 1, column=1, padx=5, pady=5)
    self.on_buttons[valve["port_line"]] = on_btn

    # OFF button (regular tk.Button)
3210 off_btn = tk.Button(
        self,
        text="OFF",
        width=6,
        bg="SystemButtonFace", # Default color
3215     activebackground="SystemButtonFace",
        command=lambda v=valve["port_line"]: self.set_valve(v, False)
    )
    off_btn.grid(row=i + 1, column=2, padx=5, pady=5)
    self.off_buttons[valve["port_line"]] = off_btn

3220
    # Store state indicator
    self.valve_states[valve["port_line"]] = tk.StringVar(value="OFF")
    state_label = ttk.Label(self, textvariable=self.valve_states[valve["port_line"]], width=8)
    state_label.grid(row=i + 1, column=3, padx=5, pady=5)

3225
    # Set initial state to OFF
    self.set_valve(valve["port_line"], False)

def set_valve(self, port_line, state):

```



```

3230     try:
        self.daq.write_digital(port_line, state)
        self.valve_states[port_line].set("ON" if state else "OFF")

        # Update button colors directly
3235     if state:
        self.on_buttons[port_line].config(bg="#39FF14", activebackground="#39FF14") # Neon green
        self.off_buttons[port_line].config(bg="SystemButtonFace", activebackground="SystemButtonFace")
    else:
        self.on_buttons[port_line].config(bg="SystemButtonFace", activebackground="SystemButtonFace")
3240     self.off_buttons[port_line].config(bg="#FF5F1F", activebackground="#FF5F1F") # Neon orange

    except Exception as e:
        messagebox.showerror("Valve Error", f"Failed to control valve: {str(e)}")

3245 def update_valve_ports(self):
    """Update valve ports after configuration change"""
    for i, valve in enumerate(self.valve_config):
        port_line = valve['port_line']
        state = self.daq.read_digital_state(port_line)
3250     self.valve_states[port_line].set("ON" if state else "OFF")

        # Update button colors
        if state:
            self.on_buttons[port_line].config(bg="#39FF14", activebackground="#39FF14")
3255     self.off_buttons[port_line].config(bg="SystemButtonFace", activebackground="SystemButtonFace")
        else:
            self.on_buttons[port_line].config(bg="SystemButtonFace", activebackground="SystemButtonFace")
            self.off_buttons[port_line].config(bg="#FF5F1F", activebackground="#FF5F1F")

```

## 3260 **ValveScheduler.py**

```
import tkinter as tk
from tkinter import ttk
```

```
3265 class ValveScheduler(ttk.LabelFrame):
    def __init__(self, parent, valve_index, daq, valve_config, *args, **kwargs):
        super().__init__(parent, *args, **kwargs)
        self.daq = daq
        self.valve_index = valve_index
3270 self.valve_config = valve_config
        self.port_line = valve_config[valve_index]['port_line']
        self.swap_job_ids = []
        self.current_state = False # Track current valve state

3275 # Configure grid for column layout
        self.columnconfigure(0, weight=1)

        # Valve label
        ttk.Label(self, text=f"Valve {valve_index + 1} Schedule", font=("Arial", 10, "bold")).grid(
3280     row=0, column=0, padx=5, pady=5, sticky="w"
        )

        # Initial state
        ttk.Label(self, text="Initial State:").grid(row=1, column=0, sticky="w", padx=5)
3285 self.initial_state_var = tk.StringVar(value="OFF")
        initial_frame = ttk.Frame(self)
        initial_frame.grid(row=2, column=0, sticky="w", padx=5, pady=(0, 10))
        ttk.Radiobutton(initial_frame, text="OFF", variable=self.initial_state_var,
            value="OFF").pack(side=tk.LEFT)
```

```

3290     ttk.Radiobutton(initial_frame, text="ON", variable=self.initial_state_var,
        value="ON").pack(side=tk.LEFT, padx=(10, 0))

    # Swap schedule header
    header = ttk.Frame(self)
3295     header.grid(row=3, column=0, sticky="we", padx=5)
    ttk.Label(header, text="Time (s)", width=8).pack(side=tk.LEFT)
    ttk.Label(header, text="Action", width=8).pack(side=tk.LEFT, padx=5)
    ttk.Label(header, text="Remove", width=8).pack(side=tk.RIGHT)

3300     # Container for swap rows
    self.swap_rows_frame = ttk.Frame(self)
    self.swap_rows_frame.grid(row=4, column=0, sticky="we", padx=5, pady=5)

    # Add/remove buttons
3305     btn_frame = ttk.Frame(self)
    btn_frame.grid(row=5, column=0, sticky="w", padx=5, pady=(0, 10))
    ttk.Button(btn_frame, text="+ Add Swap", command=self.add_swap_row).pack(side=tk.LEFT)
    ttk.Button(btn_frame, text="- Remove Last", command=self.remove_last_swap).pack(side=tk.LEFT,
    padx=5)

3310     # Store swap variables
    self.swap_vars = []

    # Add one initial row
3315     self.add_swap_row()

    def add_swap_row(self):
        """Add a new row to the valve schedule table"""
        row = ttk.Frame(self.swap_rows_frame)
3320     row.pack(fill=tk.X, pady=2)

```

```

# Time entry
time_var = tk.StringVar(value="0.0")
time_ent = ttk.Entry(row, width=8, textvariable=time_var)
3325 time_ent.pack(side=tk.LEFT)

# Action selection
action_var = tk.StringVar(value="ON")
action_cmb = ttk.Combobox(row, width=8, textvariable=action_var, state="readonly")
3330 action_cmb['values'] = ("ON", "OFF")
action_cmb.pack(side=tk.LEFT, padx=5)

# Remove button
remove_btn = ttk.Button(row, text="Remove", width=8, command=lambda r=row:
3335 self.remove_swap_row(r))
remove_btn.pack(side=tk.RIGHT)

# Store variables
self.swap_vars.append((time_var, action_var, row))
3340

def remove_swap_row(self, row):
    """Remove a specific row from the valve schedule"""
    for i, (time_var, action_var, row_widget) in enumerate(self.swap_vars):
        if row_widget == row:
            3345 self.swap_vars.pop(i)
            row.destroy()
            break

def remove_last_swap(self):
    3350 """Remove the last swap from the schedule"""
    if self.swap_vars:

```

```
_, _, row = self.swap_vars.pop()
row.destroy()
```

```
3355 def get_schedule(self):
    """Get the schedule for this valve"""
    schedule = []
    for time_var, action_var, _ in self.swap_vars:
        try:
3360         time_val = float(time_var.get())
            action_val = action_var.get()
            if time_val >= 0:
                schedule.append((time_val, action_val))
        except ValueError:
3365         pass # Skip invalid entries
    return sorted(schedule, key=lambda x: x[0])
```

```
def set_initial_state(self):
    """Set the initial state for this valve"""
3370     state = self.initial_state_var.get() == "ON"
    self.current_state = state
    self.daq.write_digital(self.port_line, state)
```

```
def schedule_actions(self, master):
3375     """Schedule all actions for this valve"""
    schedule = self.get_schedule()
    for time_val, action_val in schedule:
        state = action_val == "ON"
        job_id = master.after(
3380         int(time_val * 1000),
            lambda s=state: self.set_valve_state(s)
        )
```

```
self.swap_job_ids.append(job_id)
```

```
3385 def set_valve_state(self, state):  
    """Set valve state and track current state"""  
    self.current_state = state  
    self.daq.write_digital(self.port_line, state)  
  
3390 def cancel_schedules(self):  
    """Cancel all scheduled jobs for this valve"""  
    for job_id in self.swap_job_ids:  
        self.master.after_cancel(job_id)  
    self.swap_job_ids = []  
  
3395 def turn_off(self):  
    """Turn off this valve"""  
    self.current_state = False  
    self.daq.write_digital(self.port_line, False)  
  
3400
```

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