# Towards Self-Driving Laboratories:

## AI Experimental Calibration and Control

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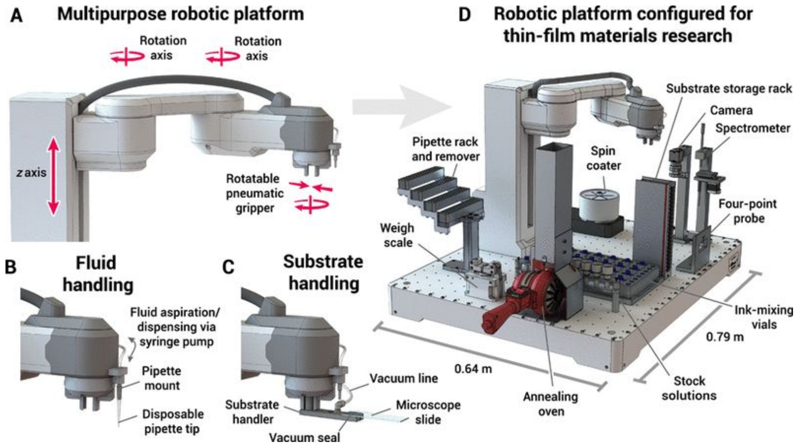
# Self-Driving Labs

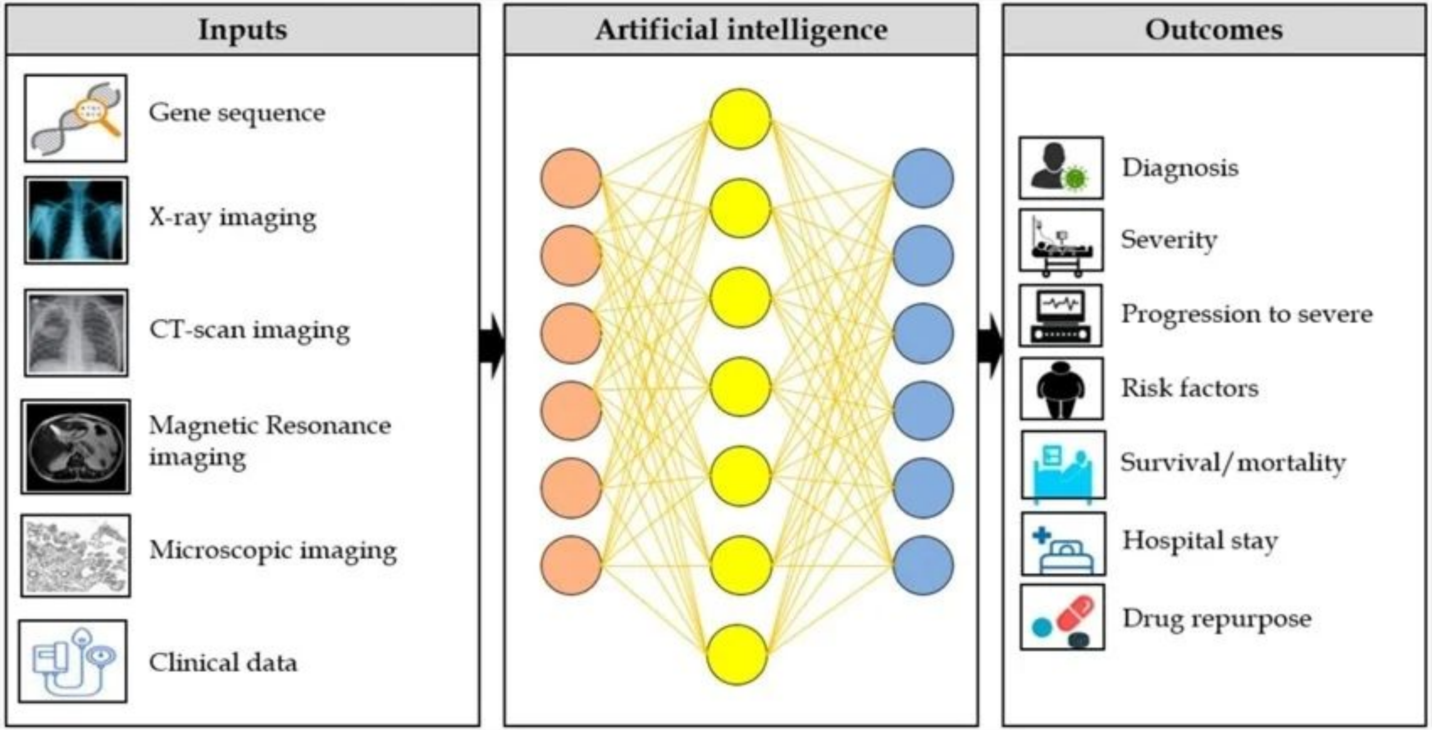
- Running experiments is a time consuming activity
  - Large amounts of time and expertise
  - Sometimes large amount of experiments to cover the parameter space




- Routine execution
  - Big steps in materials science, chemistry/biology
  - Tie-ins with robotics

# AI vs COVID

- https://www.news-medical.net/news/20210607/Using-AI-to-fight-COVID-19.aspx



# Self-Driving Labs

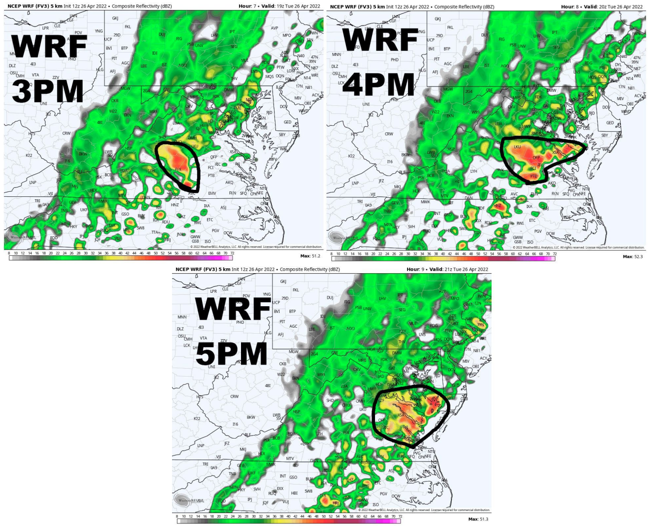
- AI can act as a **force multiplier**
  - Aid in the menial


- Single person shifts during covid
  - Monitoring
  - Routine actions

- Who wouldn't want untiring optimum?

# Self-Driving Labs

- Before we can do the analysis need to calibrate
  - Iterative and time consuming
    - Up to months depending on complexity
  - Impediment to analysis/publication
- Sometimes experts have to diligently watch environmental factors and intervene
  - Naomi late calls to the counting house to stop a run because of meteorological conditions



# Complex Interconnected Systems

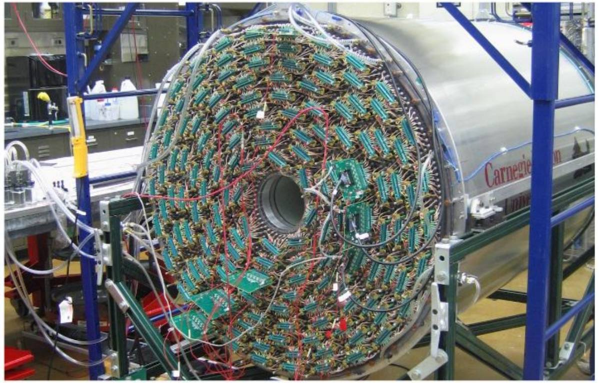
- Particle physics rely on very complex highly interconnected systems
  - Physics dependent on beam properties
    - Careful control of coupled magnets
  - Different detectors with specific goals
    - Tracking
    - Calorimetry
    - PID
  - Experimental setups select for kinematics
    - Angular
- All bundled with competing goals for physics

# Start Small

- Need to break it down:
  - **Low risk**
    - Recoverable
    - Abandonable
  - **Proveable**
    - Methods to show we are right
  - **Trustable**
    - Expected behavior
    - Needs to work alongside current systems
      - Paradigms don’t change immediately…

# Introducing the CDC

- 1.5 m long x 1.2 m diameter cylinder
- 3522 anode wires at 2125 V inside 1.6 cm diameter straws
- 50:50 Ar/$CO_2$ gas mix
- Used to detect and track charged particles with momenta p > 0.25 GeV/c
- **Requires two calibrations: chamber gain and time-to-distance**

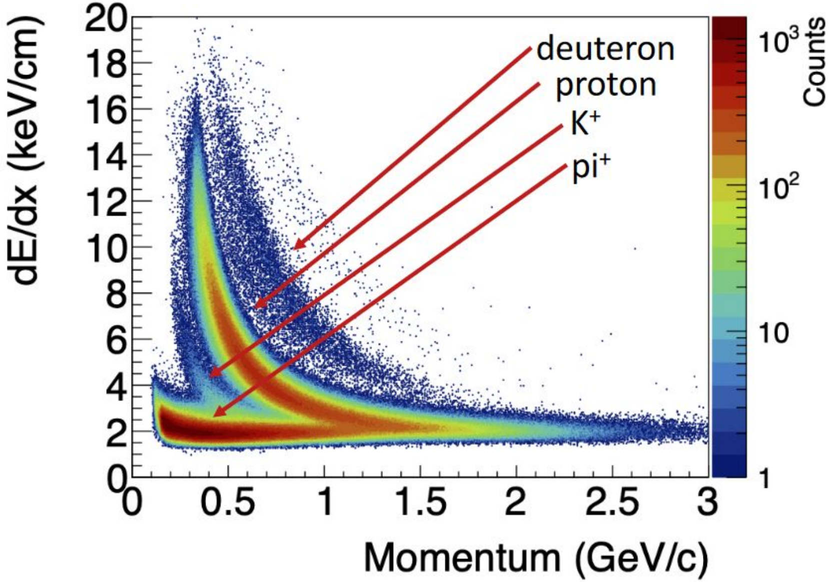


# Calibration AND Control

- Gain: affects PID selections in analysis
  - Sensitive to environmental conditions
  - Beam conditions change with the experiment
  - Gain correction factor obtained from Landau fit to amplitude

- Time to distance: track fitting, vertex and dE/dx resolution
  - Non-analytic fit function generates 6 unique calibration constants

- Calibration constants are generated per run

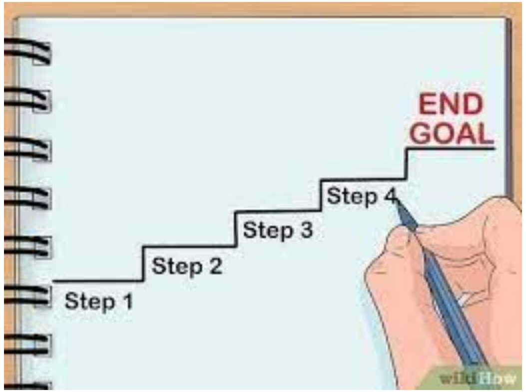


# Calibration AND Control

- Fairly simple controls
  - HV...and that is it
    - HV settings affect the gains and TtoD
- Potentially highly dimensional
  - Reconstructed tracks?
  - Beam properties?
  - Environmental conditions?
- Traditional method already exists
  - trusted

# The Plan

- Can AI even do “traditional” calibrations?
  - Can we understand the road?
    - Take in various input variables and produce the calibration value(s)
- Begin with supervised learning
  - Gains first
  - TtoD




- Leverage gains prediction for controls
  - Understood connection between HV and gains

# Gains

- Fairly simple
- Already knew that **pressure** is a primary driver
  - Related to board currents
  - PV=nRT
- Smaller dimensionality
  - One control
    - Assuming it works....

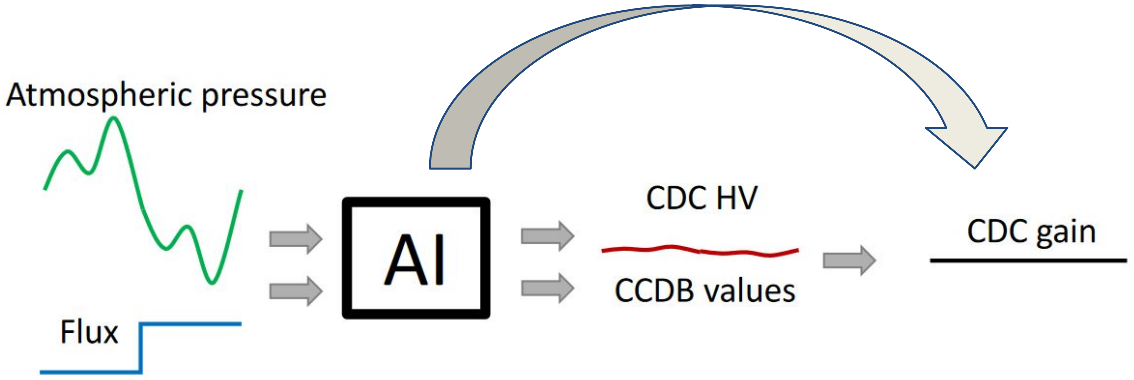
# Gains

## Conventional

- CDC operating voltage set at 2125 V
- Calibrations are fine tuned in an offline setting
- Current method is relatively slow, requires multiple iterations
- *Time scale to complete all calibrations is a few months*

## AI

- Maintain consistent detector response to changing environmental/experimental conditions by adjusting CDC HV
- Produce calibration constants online

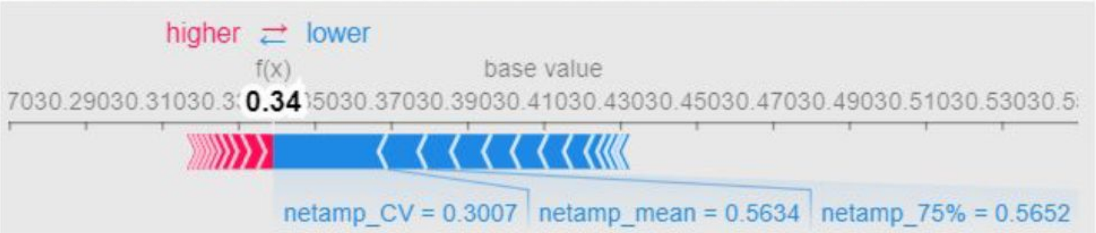


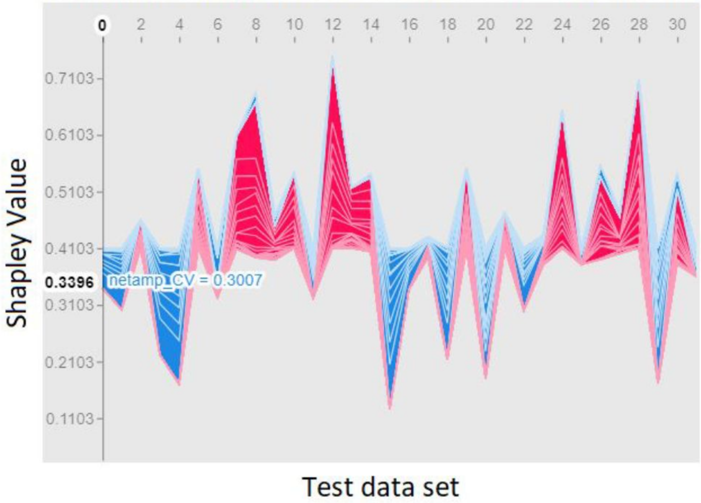
# Considerations

- An ML approach
  - How are we going to **train** the model?
    - What data do we need (see next slide)
  - Do we have the **needed data** for inference?
    - Is it formatted correctly?
  - How do we **integrate** it with current operations?
    - Want as little human input as necessary

# Feature Importance

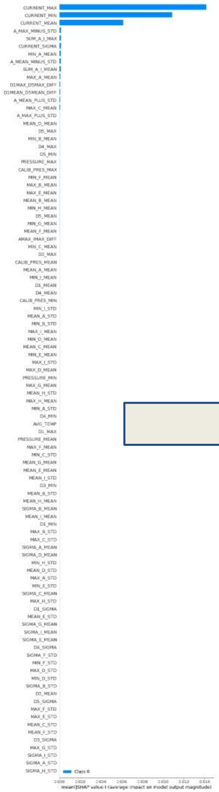
- Many different metrics to use
  - L1-regularization
    - Pro: simple
    - Con: small num variables linearly correlated
  - Shapely Values
  - Gini importance
  - Etc etc etc

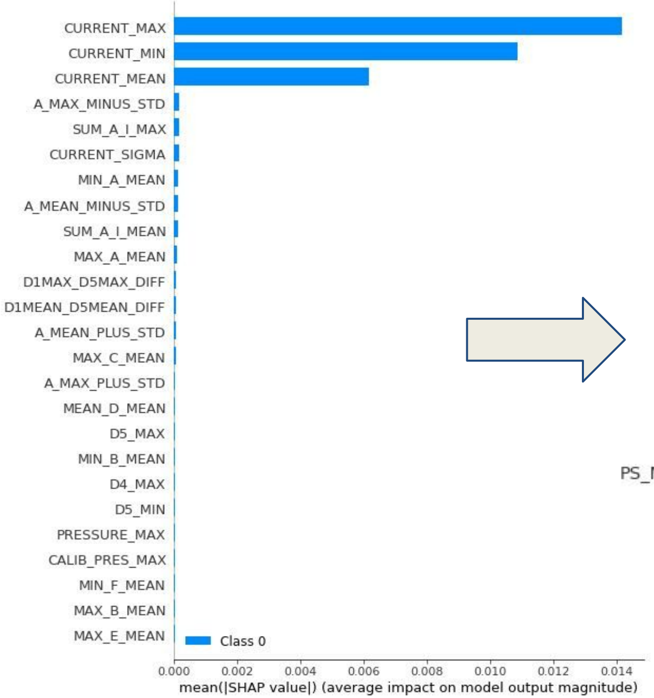


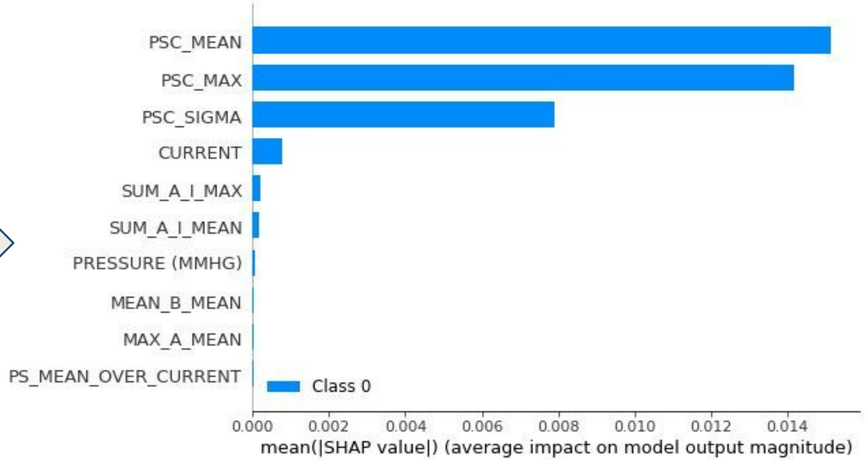



# Feature Importance

- What sticks?

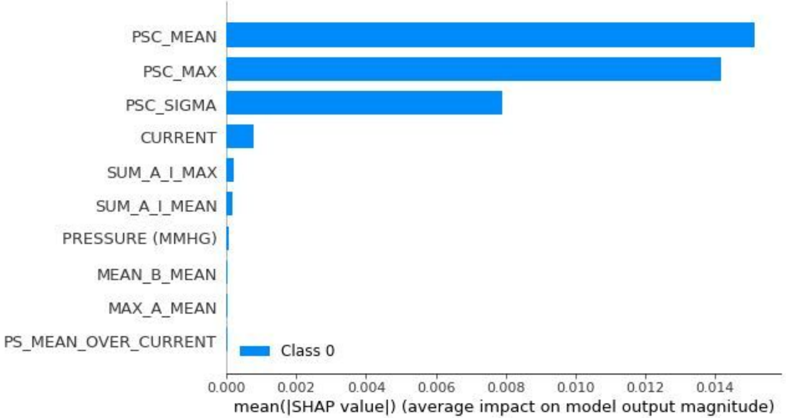




# Feature Importance

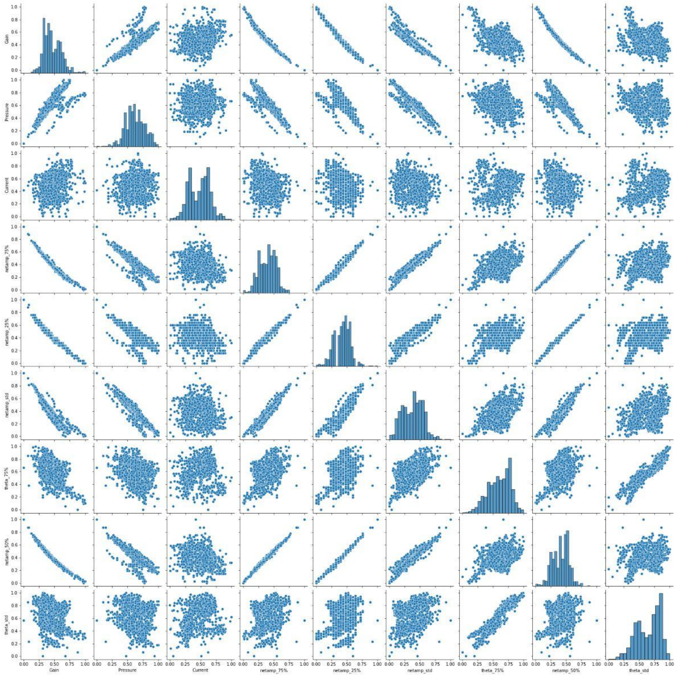
- Reconstruction takes a long time
  - Time based tracking ~90% of recon time
  - Less feasible for an online environment
    - For now............




- Best to do it with “EPICS only” data
  - Turns out completely doable

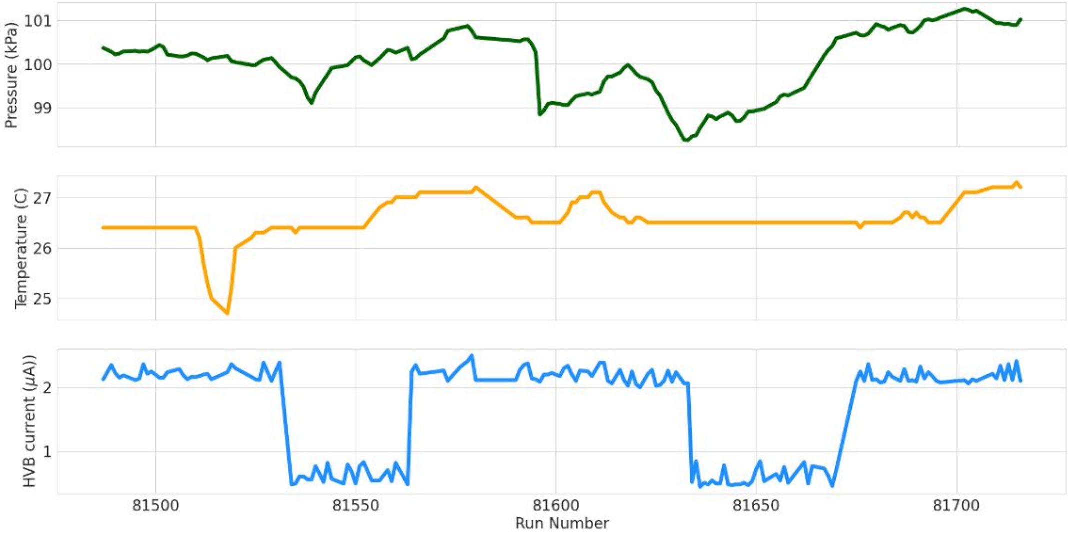
# Feature importance

- Are things correlated?
  - Silly to use both F and C if temperature is important
- Seek the minimal set of features
  - While still being robust
    - Some redundancy might be ok



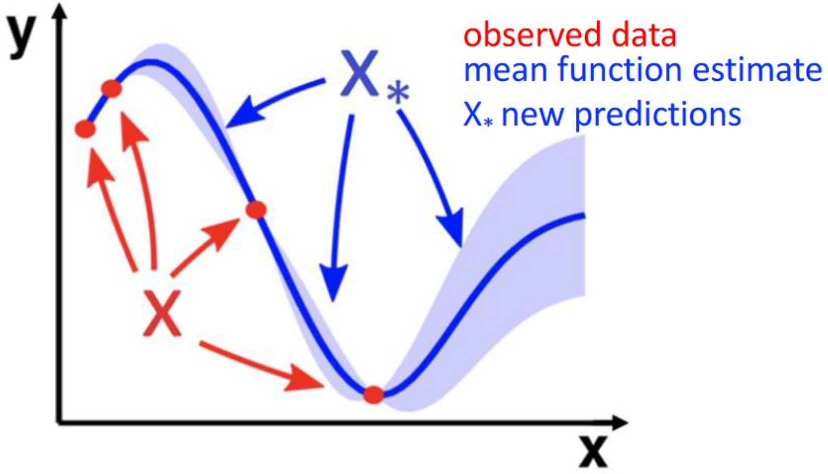
# Feature Importance

- Data extracted from Experimental Physics Industrial Controls System (EPICS)
- Initial features generated from:
  - Atmospheric pressure
  - Gas temperature
  - Current drawn from CDC HV boards
- Readily available during the experiment



# Gaussian Process

- Gaussian process model: probability distribution over possible functions that fit a set of points
- Suited to small data set:
    - 430 training runs
    - 106 testing runs
- Provides uncertainty quantification
- Implemented using SciKit Learn



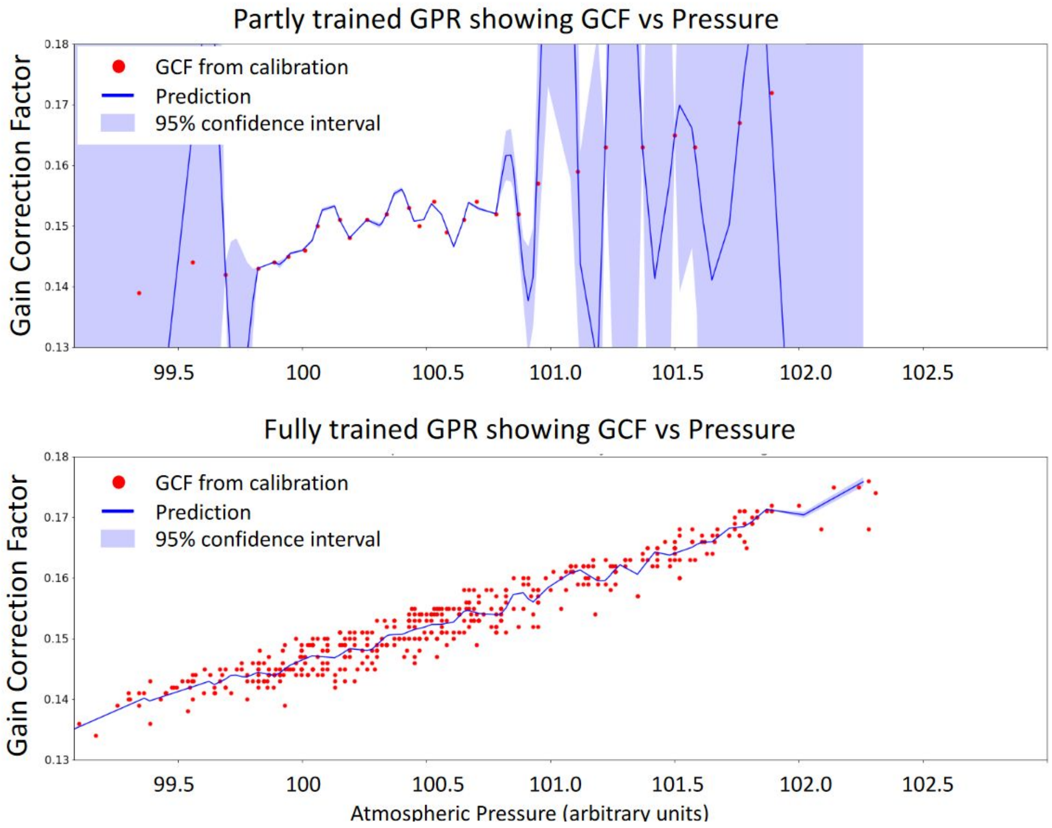
# Early Results

**Some methods don't generalize** well over datasets

Makes sense with the **discrete running conditions**

| Model | # Features | MAPE | MAX PE | ratio > 1% | ratio > 2% | ratio > 5% |
|---|---|---|---|---|---|---|
| Linear Regression | 11 | 1.3% | 19.1% | 97 / 164 | | |
| Linear Regression | 5 | 2.3% | 20.3% | 96 / 164 | 60 / 164 | 21 / 164 |
| Linear Regression (2020) | 11 | 0.72% | 2.0% | 30 / 106 | 1 / 106 | 0 / 106 |
| Linear Regression (2020) | 5 | 0.74% | 2.6% | 26 / 106 | 3 / 106 | 0 / 106 |
| MLP - 7 layers | 122 | 1.8% | 11.4% | 75 / 164 | | |
| MLP – 3 layers | 122 | 1.9% | 11.9% | 90 / 164 | | |
| MLP – 4 layers | 122 | 1.9% | 10.8% | 84 / 164 | 51 / 164 | 16 / 164 |
| GPR – 26 Features | 26 | 1.7% | 10.9% | 80 / 164 | 42 / 164 | 12 / 164 |
| GPR – 14 Features | 14 | 1.45% | 9.7% | 66 / 164 | 38 / 164 | 12 /164 |
| GPR – 11 Features | 11 | 1.5% | 10.1% | 72 / 164 | 37 / 164 | 12 / 164 |
| GPR – 5 Features | 5 | 1.5% | 9.1% | 70 / 164 | 37 / 164 | 10 /164 |
| GPR – 11 Features (2020) | 11 | 0.5% | 4.1% | 17 / 106 | 1 / 106 | 0 / 106 |
| GPR – 5 Features (2020) | 5 | 0.7% | 3.6% | 28/106 | 3 / 106 | 0 / 106 |
| RF – 82 Features | 82 | 1.7% | 18.5% | 83 / 164 | | |
| XGBoost – corr > 0.2 | 82 | 1.44% | 11.8% | 68 / 164 | | |
| XGBoost – corr > 0.3 | 71 | 1.55% | 11.2% | 71 / 164 | | |
| XGBoost – corr > 0.4 | 12 | 1.8% | 11.1% | 72 / 164 | | EPIC |
| XGBoost – All Features | 122 | 1.56% | 10.2% | 76 / 164 | | |

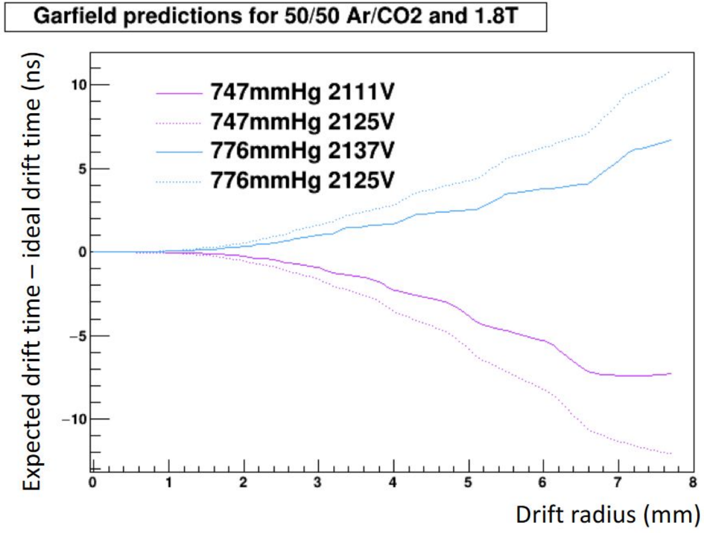
# GPR Model



Partly trained GPR showing GCF vs Pressure
Gain Correction Factor
GCF from calibration
Prediction
95% confidence interval
0.18
0.17
0.16
0.15
0.14
0.13
99.5
100
100.5
101.0
101.5
102.0
102.5
Fully trained GPR showing GCF vs Pressure
Gain Correction Factor
GCF from calibration
Prediction
95% confidence interval
0.18
0.17
0.16
0.15
0.14
0.13
99.5
100
100.5
101.0
101.5
102.0
102.5
Atmospheric Pressure (arbitrary units)

# Time to Distance

- CDC is a tracking detector
    - Interested in the <u>where</u> of particles
- Take the signals and through an understanding of how fast the electrons drift to the wires convert to distance
    - HV dependent
    - Gas dependent
        - Both mixture and PV=nRT



# Time to Distance

- Current calibration method produces 6 unique calibration constants from fit to data

$$d(t) = f_\delta\left(\frac{d_0(t)}{f_0}P + 1 - P\right)$$

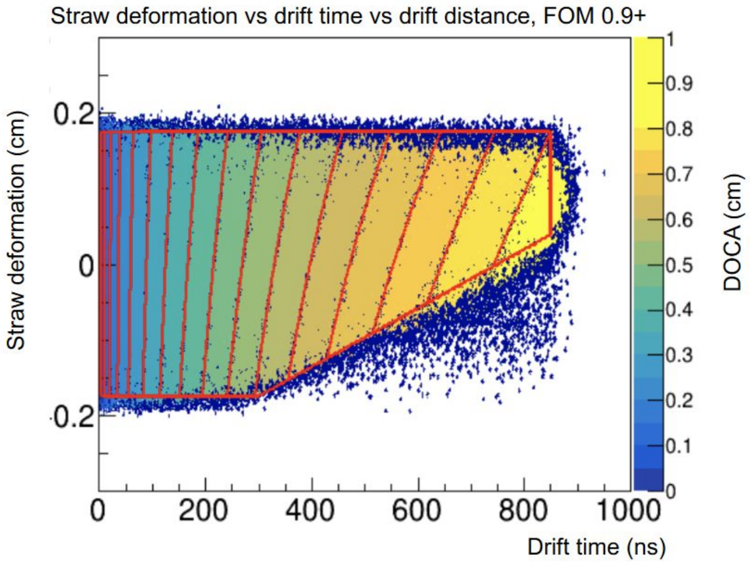
$$f_\delta = a\sqrt{t} + bt + ct^3$$

$$f_0 = a_1\sqrt{t} + b_1 t + c_1 t^3$$

$$a = a_1 + a_2|\delta|$$

$$b = b_1 + b_2|\delta|$$

$$c = c_1 + c_2|\delta|$$



# Difficulties

- **6 parameters**
  - a1, b1, c1, a2, b2, c2
    - Ambiguities in sign
- NN used **custom loss** to "bake in" functional forms
  - Sign shifting observed
- Switched to **GPR**
  - **Cascade**: use a1 to learn the next....those 2 to get the third
    - Errors
  - **One GPR per parameter**

# Results

## Model Results: PRELIMINARY

| | 2018 & 2020 Mean % $f_{Drift}$ Difference | 2018 & 2020 Max % $f_{Drift}$ Difference | 2020 Mean % $f_{Drift}$ Difference | 2020 Max % $f_{Drift}$ Difference |
|---|---|---|---|---|
| NN | 0.11% | 0.5% | 0.066% | 0.27% |
| GPR | 0.093% | 0.5% | 0.052% | 0.21% |

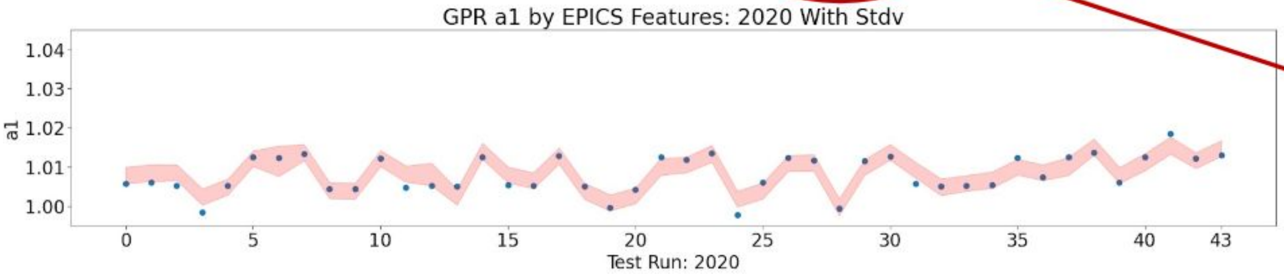
NN: 4 layers, 16 nodes per layer, sigmoid and tanh activation functions. 5 input features, 6 output values. Used double integral custom loss function.

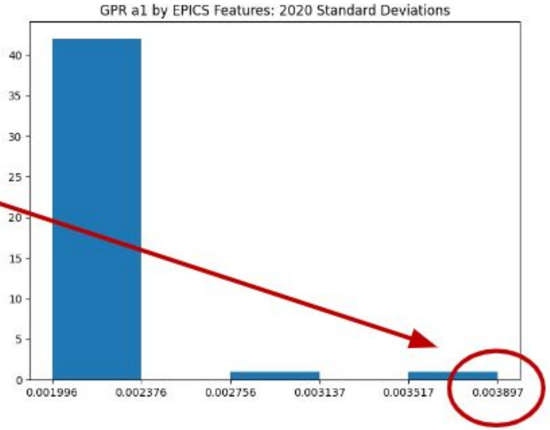
GPR: kernel = Radial Basis Function + WhiteNoise: tuned for each calibration constant. Six predictions: one for each calibration constant.

One can see that in addition to the uncertainty information, we also have more accurate predictions.

# Results

2020: Max Standard Deviation From GPR: 0.003897



# A Need(?) for Physics Measure

- The agreement with traditional methods is good
  - But leaves **unanswered questions**:
    - Why do we trust the traditional method?
    - How much difference is there in physics outcomes with error in gains?

- **Difficulties**
  - Not a singular value
  - Competing metric priorities

# Controls

- **What are our actions?**
  - CDC only has HV

- **How do we interact with the control?**
  - Turns out the CDC has an EPICS variable for the HV setpoint
    - If the voltage is on it will be set to the setpoint
    - Changing the setpoint changes the voltage
      - The rate of change is ~10V/s

# Goals

- **Modify V** to stabilize gains
  - Traditionally, the input variables are fluctuating, the V is held constant and the gains necessarily fluctuate
  - We can, in principle, fluctuate the V in response to the input variables and produce a stable gain

- Use cosmics to gain **confidence** before production
  - Higher stakes with beam on

# Towards Self-Calibrating Data

- Ultimately we would like to create a **smart detector system** which can adapt to its environment and **produce self-calibrated data**
  - Or at least reduce the iterations

- The system should be able to adequately **control the detector with no user input**
  - Maybe we'll put a human approval step in there to make people feel safe....or not

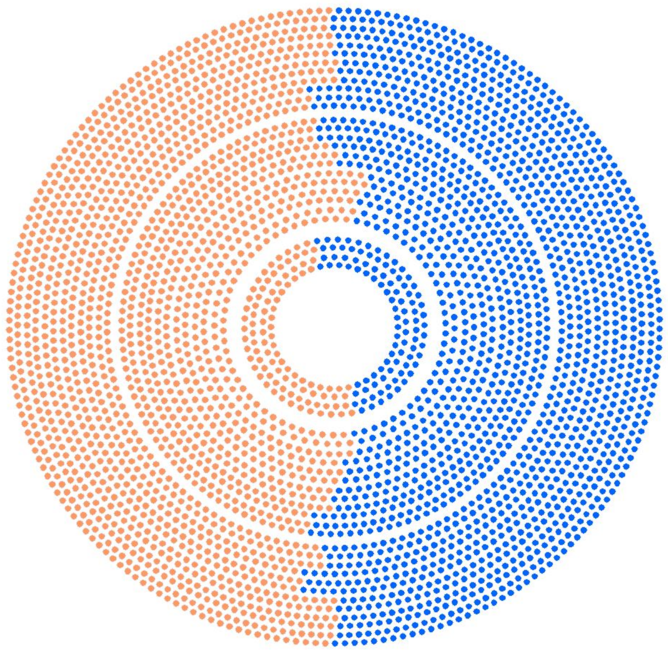
- Should be able to update "arbitrarily" fast
  - To facilitate a **change in paradigm**

# Cosmics Test

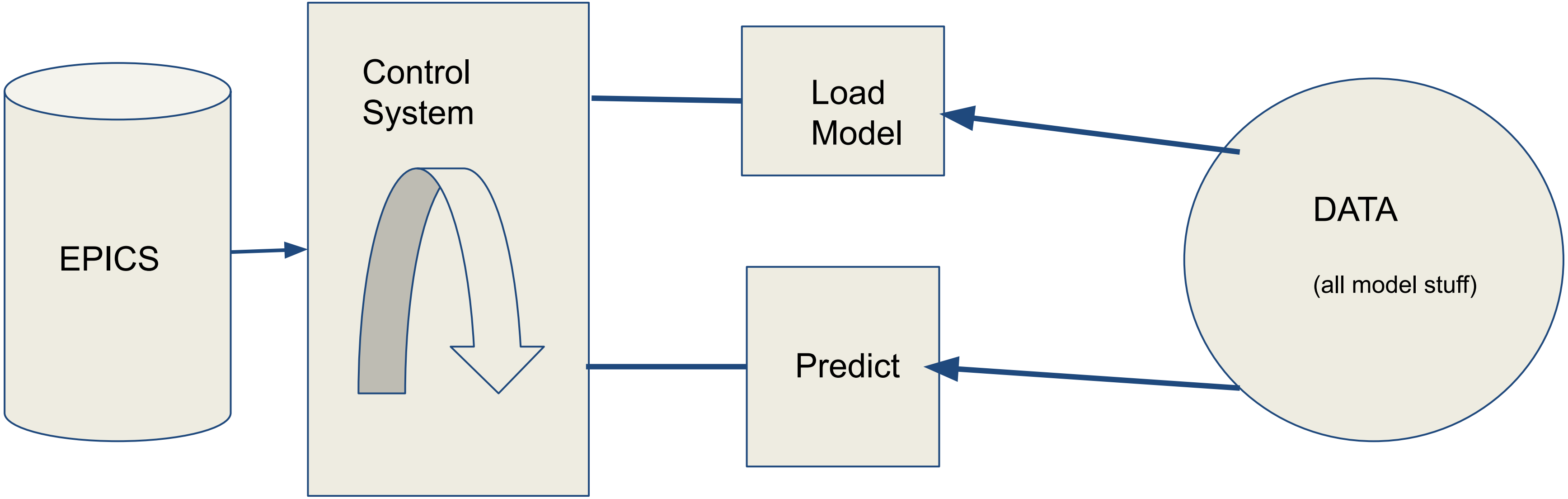
- Split the CDC into **2 halves**
  - Leave one side at a **fixed HV**
  - Let the **AI control the other**

- AI
  - Update the HV every 5 min
  - **Completely autonomous**

- Should see the AI system side's gains stabilized



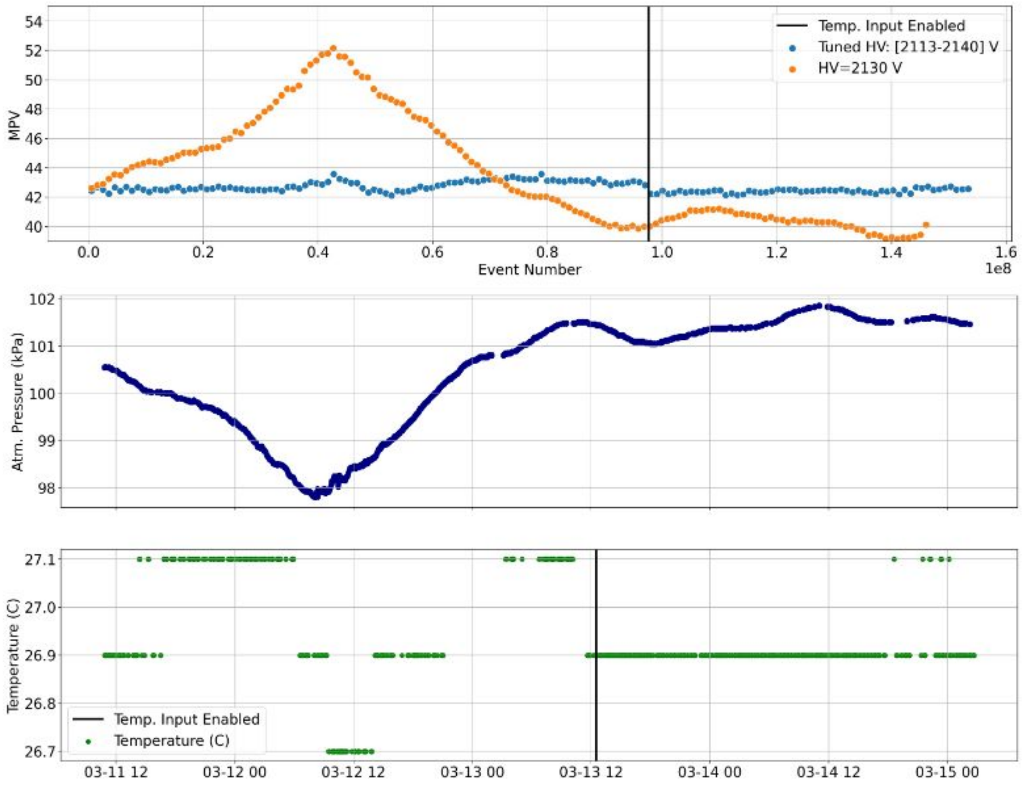
# Modular System



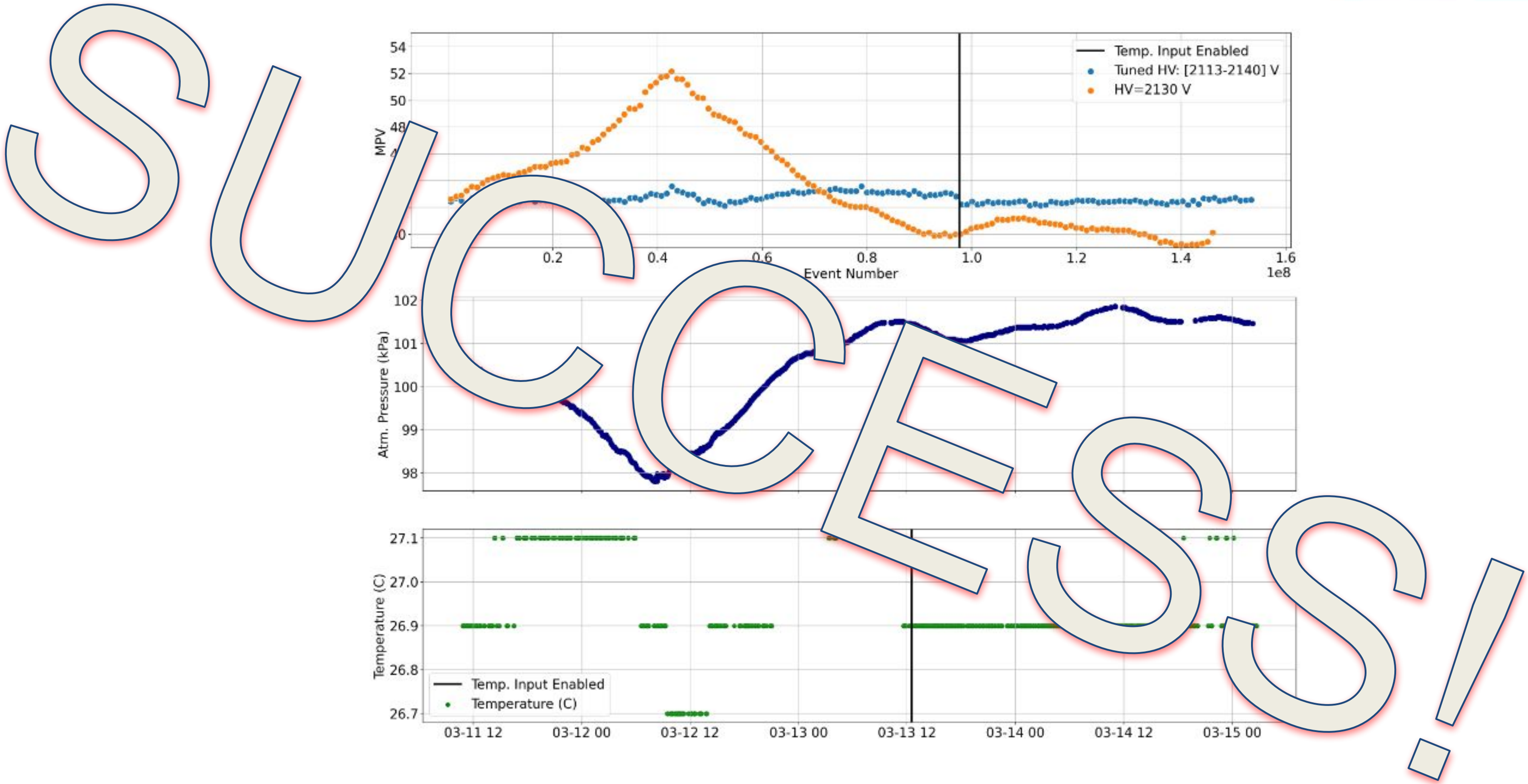
# The Controls System

- **On the fly configurable**
  - Once per control loop pass
    - Poll time
    - Recommend scale
    - Default values
    - Control mask
    - Look-back time
    - Other control parameters

# Cosmics Test Results



# Cosmics Test Results



# Next Steps

- Other systems
  - In and out of GlueX
    - **FDC** (another drift chamber)
    - **BCAL** (calorimeter)
    - **TOF** (downstream)

- <u>Interoperability</u>
  - Build a smart bridge between detector systems
    - Afterall, we want to optimize the physics results....

# Disrupt Data Taking

- Wait no!...do the opposite...**Change the paradigm!**

- Want to move to a mode of operation in which the idea of a "Run" is no more than a human construct
    - **More streaming read-out like**
    - Each event is perfectly calibrated and detectors can operate continuously in a changing experimental environment


- Perhaps the conditions themselves are optimized....
    - Perhaps the data is already reconstructed online....
        - Perhaps the paper is written for you....

# Towards Full Self-Driving

- Once the paradigm has changed we can move towards self driving
  - **Synergy with other AI tech**
    - E.g. Hydra

- Expert engagement at a high level
  - **Routine operations delegated to the machines** themselves

- Need protocol for **interoperability**
  - Operational data made for AI
  - Formatted for AI

# Beyond the Borders

- Set sights **beyond experimental border**
  - Accelerator connections
- What we really want to **optimize is the physics output**
  - Whatever that happens to be...
- Accelerators are a means to an end
  - **Tunings required for the physics**
  - **Detector configurations dependent on the beam properties**

- Imagine holistically managing both the experiment and beam

# Accelerator Work

- SLAC
    - GP models to optimize beam tunings
- SNS
    - Errant beam
    - Component degradation
- JLAB
    - RF cavity fault diagnosis

# Visions of the Future

- **Designing with AI for AI**
  - Bayesian optimization for detectors
- **Systems instrumented for AI**
  - Standard protocols for interoperability
- **Automated diagnostics**
  - Self-correcting
- **Self-documenting**
- **Quicker to physics**
  - Co-modeling?
    - Hypothesis generation