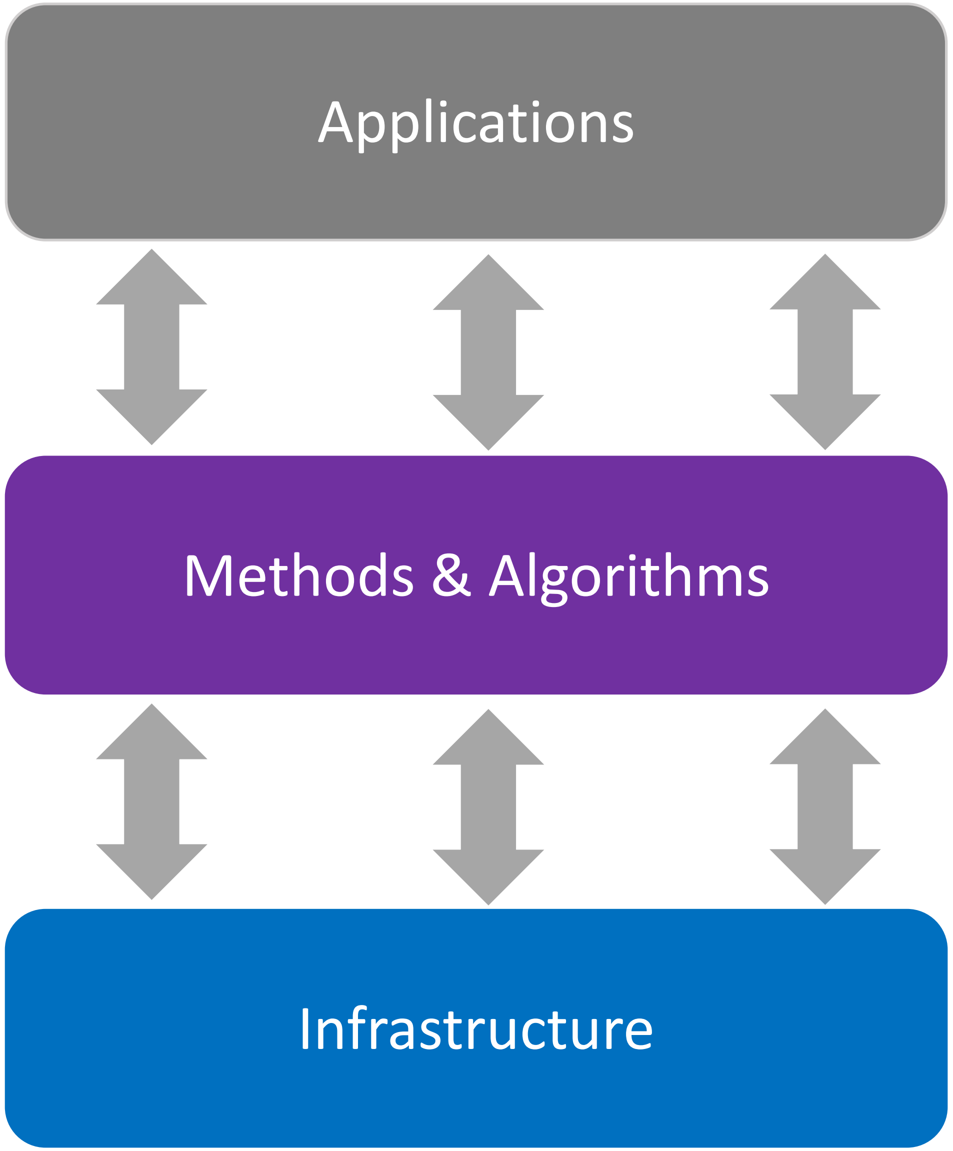
Data Science Department Research at Jefferson Lab

Dr. Malachi Schram

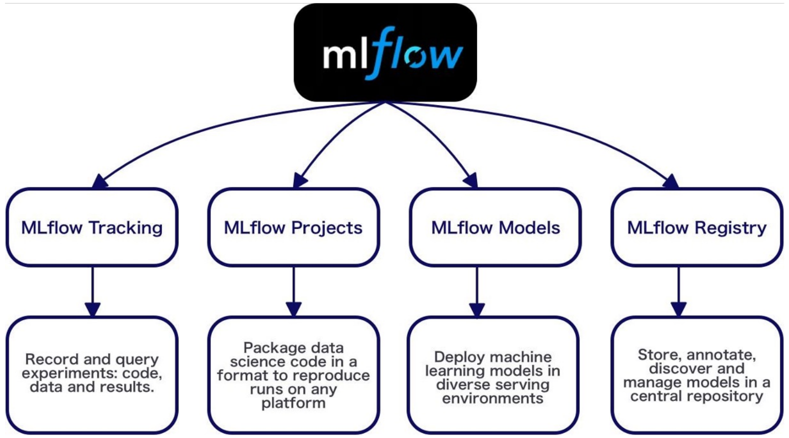
On behalf of the Data Science Department

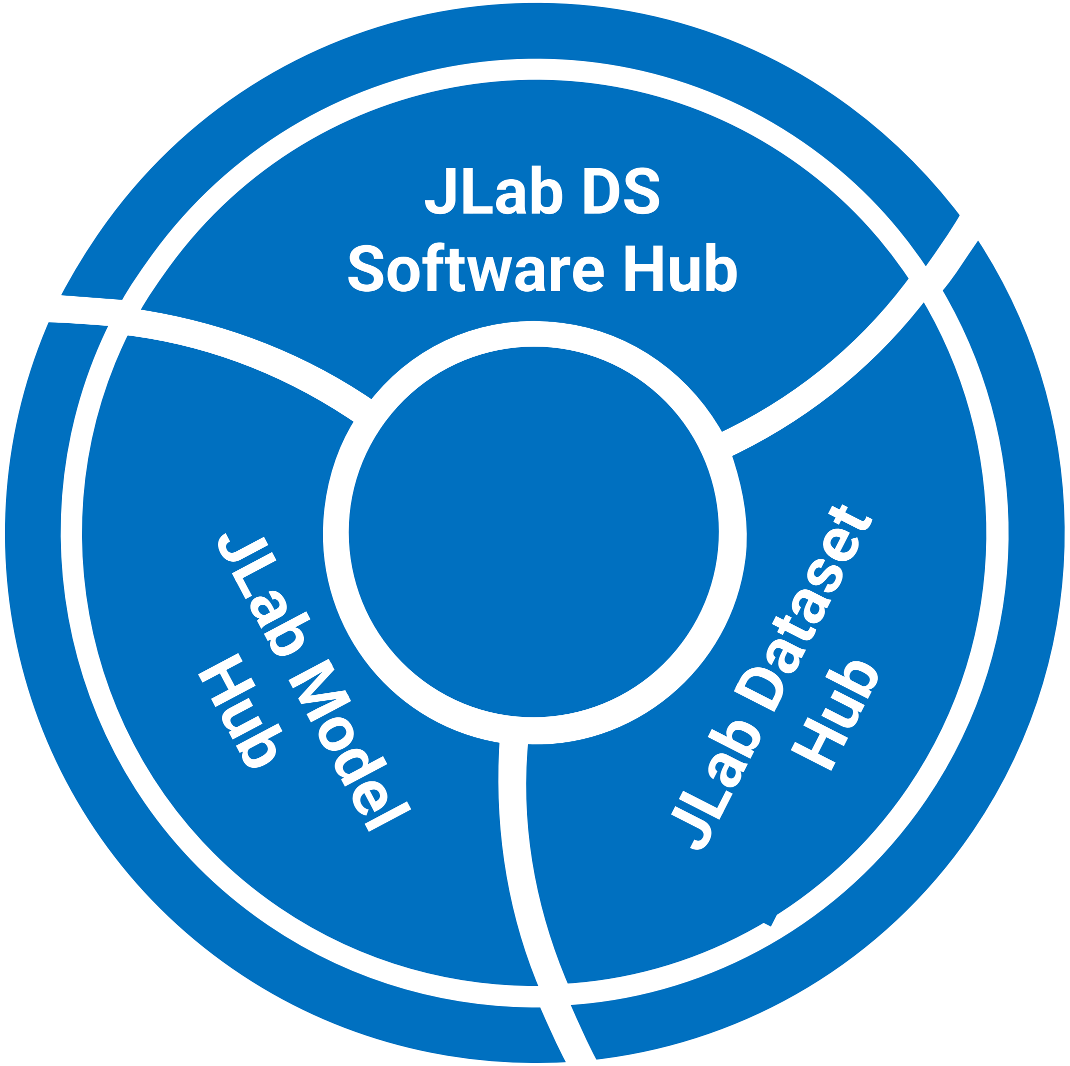
Data Science Pillars

- **<u>Applications</u>:**
  - Nuclear Physics
  - Advanced computing
  - Health & Climate
- **<u>Focused Methods & Algorithms</u>:**
  - Uncertainty Quantification
  - Interpretability and Explainability
  - Design & Control
- **<u>Infrastructure:</u>**
  - JLab ML & Data Hub
  - JLab Data Science software



Data Science Infrastructure





Data Science Methods & Algorithms

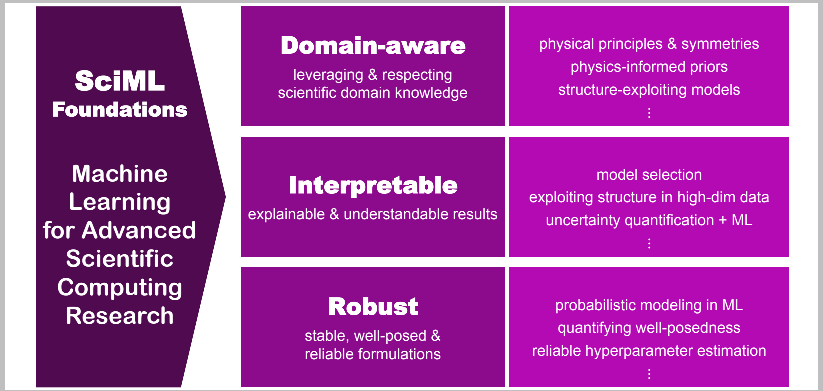


Figure 1: Foundational research themes of SciML must tackle the challenges of creating domain-aware, interpretable, and robust ML formulations, methods, and algorithms.

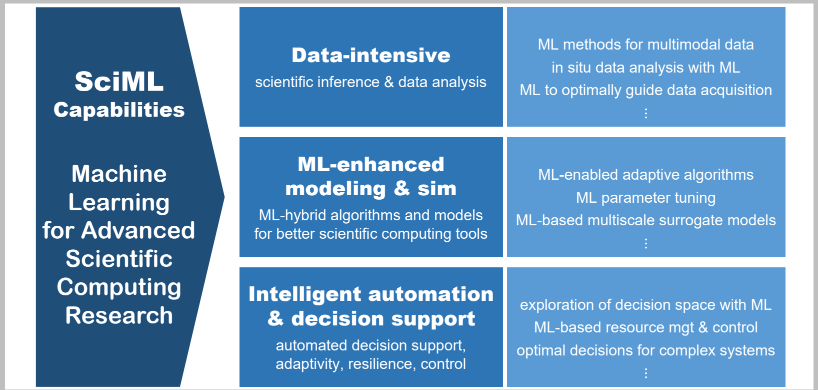
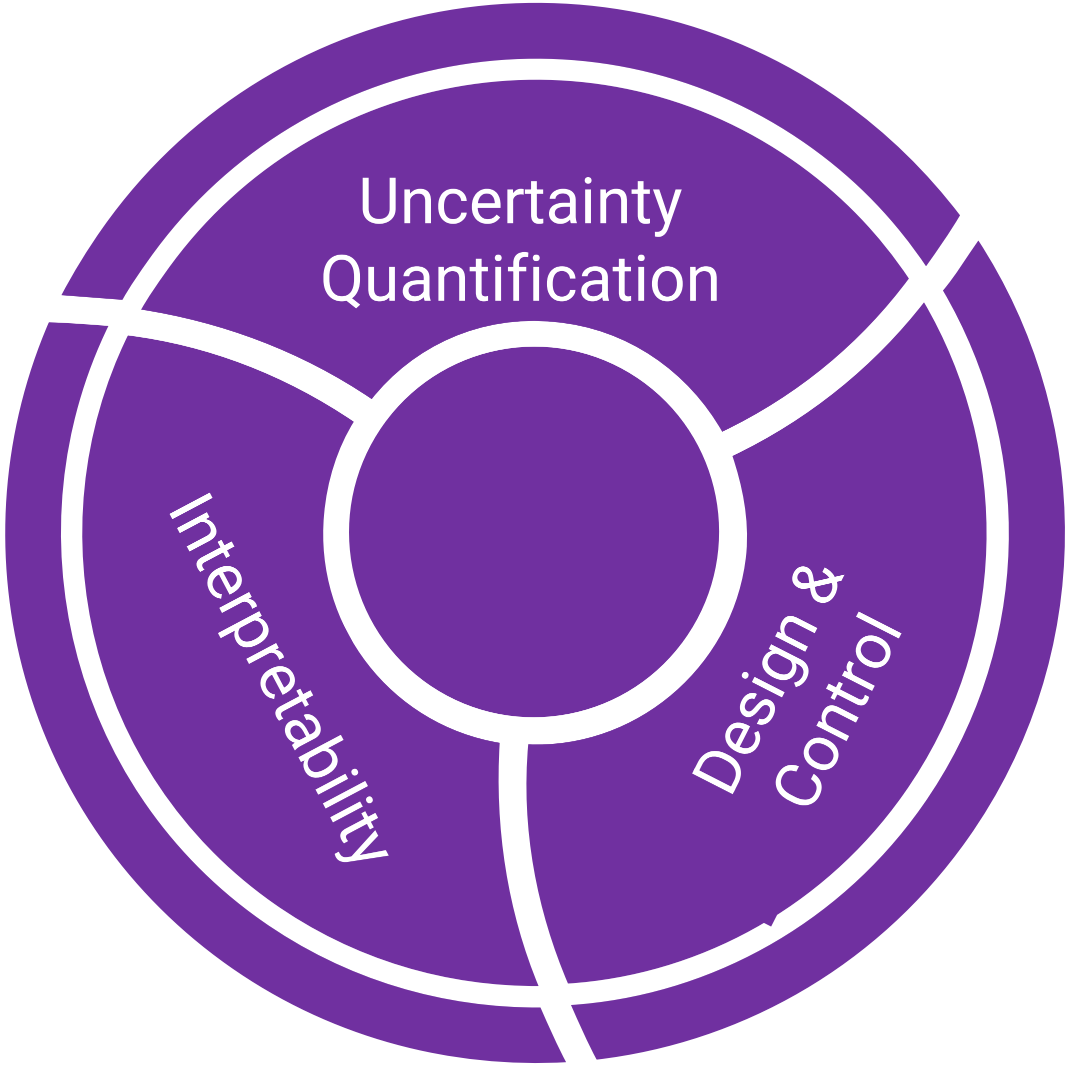


Figure 2: Opportunities for SciML impact arise in scientific inference and data analysis; in ML-enhanced modeling and simulation; in intelligent automation and decision support; and in related applications.

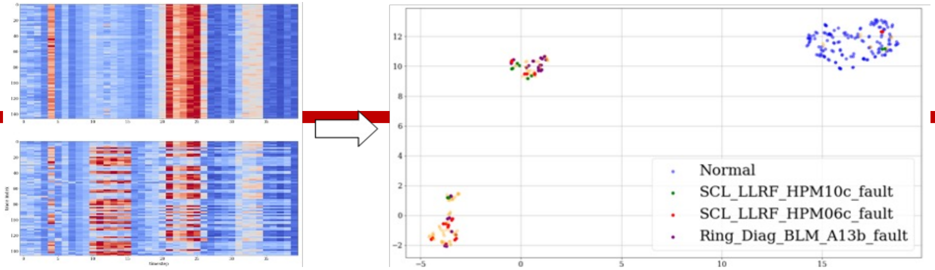


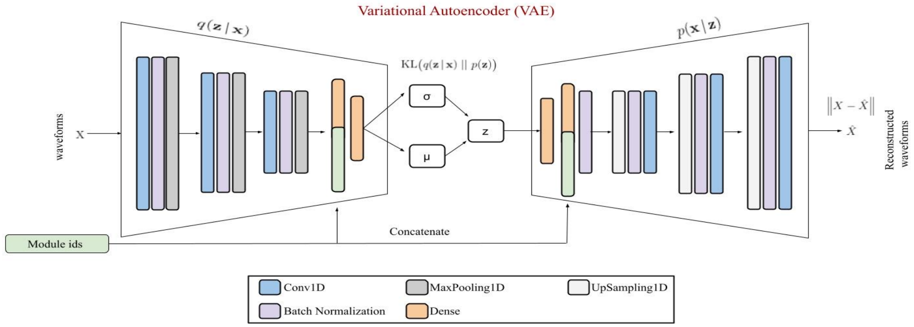
Applications in Experimental Halls

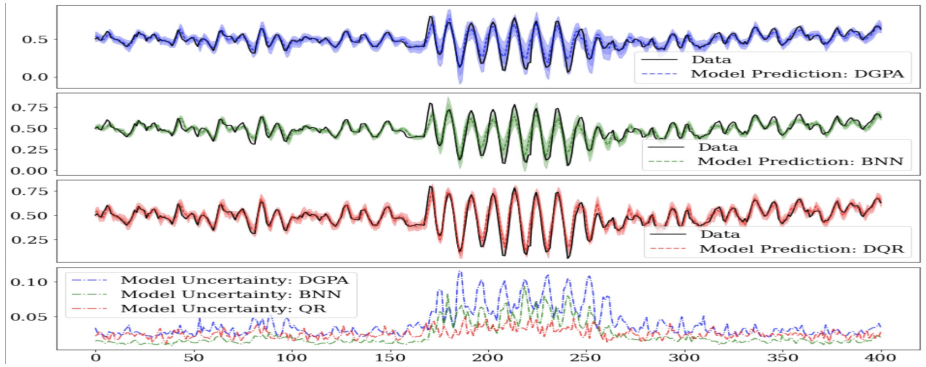
- Developing a JLab ML Hub to capture the workflow and artifacts
- Incorporating uncertainty quantification in ML models
  - Hall A:
    - Particle ID w/ UQ for SoLID
  - Hall B: Several discussions
  - Hall C: Working with Tanja Horn and Cristiano Fanelli to define effort
  - Hall D:
    - Gaussian Process method for AIEC controls
    - Develop some ML-based models for Particle ID for CPP
  - Hall E:
    - Contribute to AI4EIC workshops
    - Working to define a long term plan with Cristiano Fanelli (new bridge position at W&M)

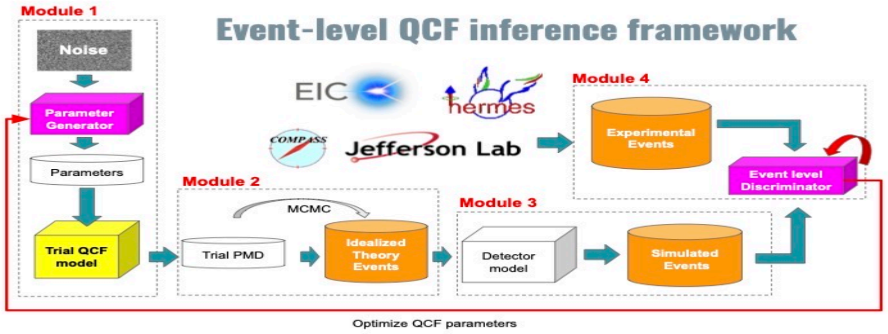
External Applications

- AI/ML for Spallation Neutron Source at ORNL:
  - Anomaly detection and fault prognostication
- Data-Driven Decision Control for Complex Systems (DnC2s):
  - Risk-averse reinforcement learning
  - Distance aware/preserving uncertainty quantification for ML-based regression
- Multi-objective RL for CEBAF
  - Accelerator and data science collaboration
- Hampton Roads Digital Twin:
  - Health and climate resiliency studies
- SciDAC project:
  - Theory, experiment, data science Integration









AI@DOE Executive Summary

- Top R&D priorities:
  1. Incorporate prior <u>knowledge</u> into AI systems
  2. Training for rare events
  3. <u>Explainability, interpretability and understanding</u>
  4. <u>Automation</u> and optimization -- self-driving labs, hypothesis generation
  5. Targeted algorithm development -- development focused on DOE missions
  6. Sustainable AI -- energy-efficient solutions (green AI)

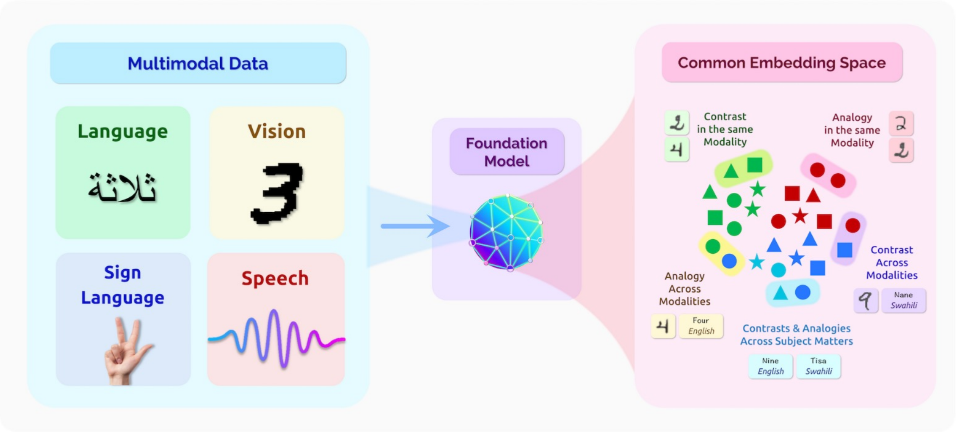
- Enablers:
  - Underlying <u>ecosystem</u> to enable AI R&D -- virtual AI user facility
  - Ethics framework to guide AI R&D – identify unexpected biases

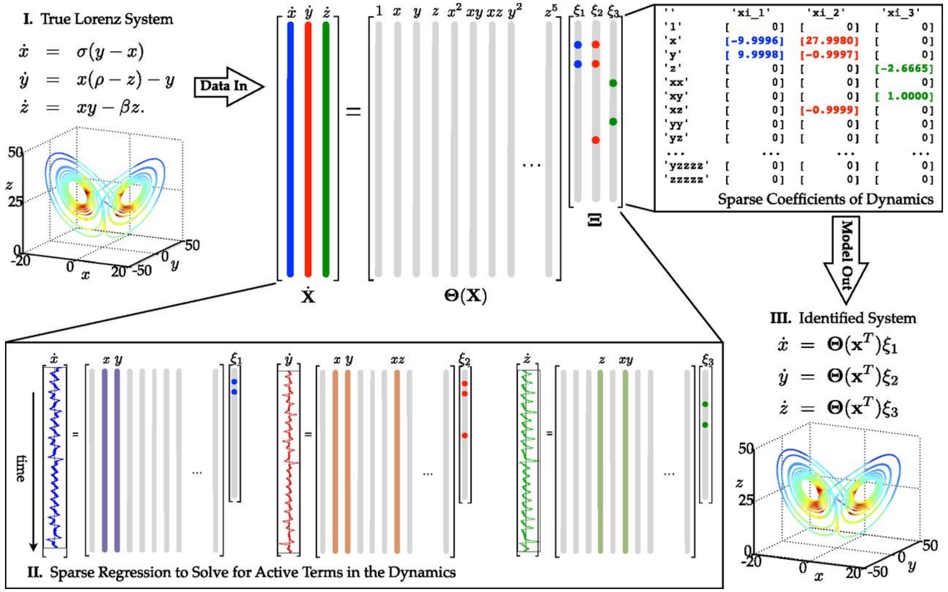
AI for Science and Security

- Three topical AI for Science & Security workshops recently held to discuss a long-term vision:
  1. June – AI Surrogates, AI for Complex Systems
  2. July – Properties and Inverse Design, Foundation Models
  3. August – Autonomous Discovery, AI for Programming
- Interesting themes:
  - Reinforcement learning for complex controls
  - ML-based surrogate models and digital twins
  - Uncertainty quantification (UQ), verification & validation (V&V), and guaranties
  - Building in physical constraints and relationships into the ML models
  - Integrating ML-based function surrogates with UQ & guaranties into code and simulations
  - Combined data and AI models management
  - Trustworthiness, robustness, and explainability

Ongoing and forward looking

- **Scalable Distributed Learning**
  - In order to efficiently train over from large dataset, the need for a distributed learning computing infrastructure will likely be required.
- **Uncertainty quantification for deep learning models**
  - Detailed study of uncertainty estimation techniques for AI/ML in NP applications as it relates to higher dimensionality and unique modalities.
  - Applications of UQ ML models on edge hardware (under constraint)
- **Computing co-design for AI/ML and NP**
  - AI/ML for NP is evolving and new techniques will be developed that might not perform optimally on existing hardware.
- **Techniques to advance scientific discovery**
  - Sparse Identification of Nonlinear Dynamical Systems (SINDy) is an algorithm to discover governing dynamical equations
- **Techniques for explicit physics knowledge integration**
  - Applications of automatic differentiation through known physics equations into the ML models
  - Low energy nuclear physics examples has shown some improved results
- **Foundations Models for NP**
  - A foundation model is any model that is trained on broad data (generally using self-supervision at scale) that can be adapted (e.g., fine-tuned) to a wide range of downstream tasks.





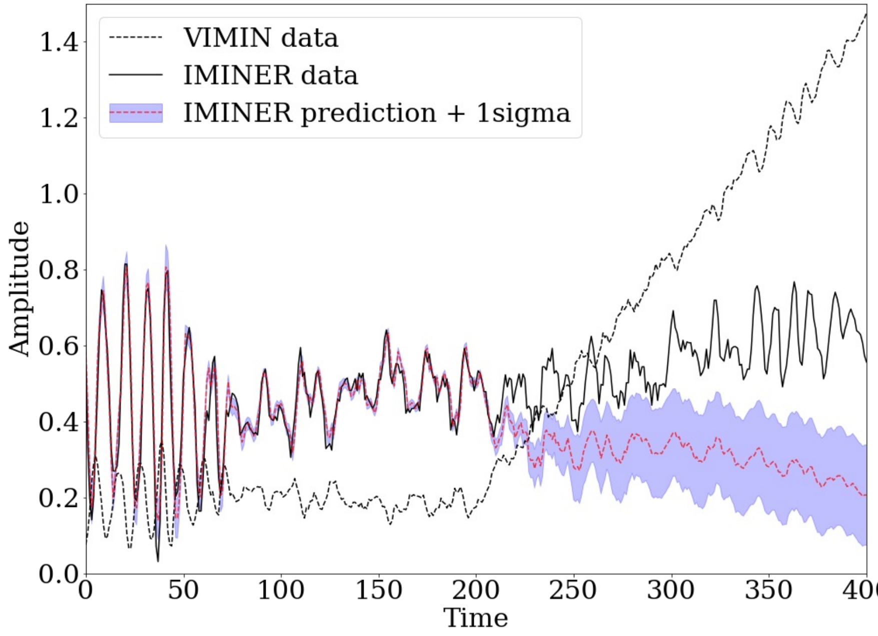
Jefferson Lab

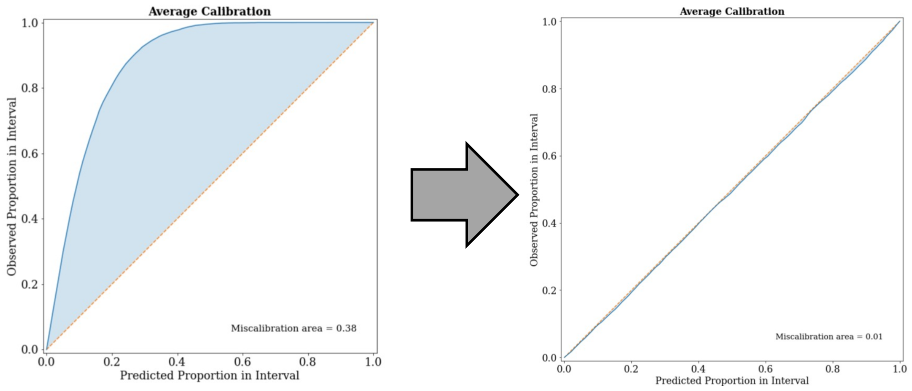
Thank you

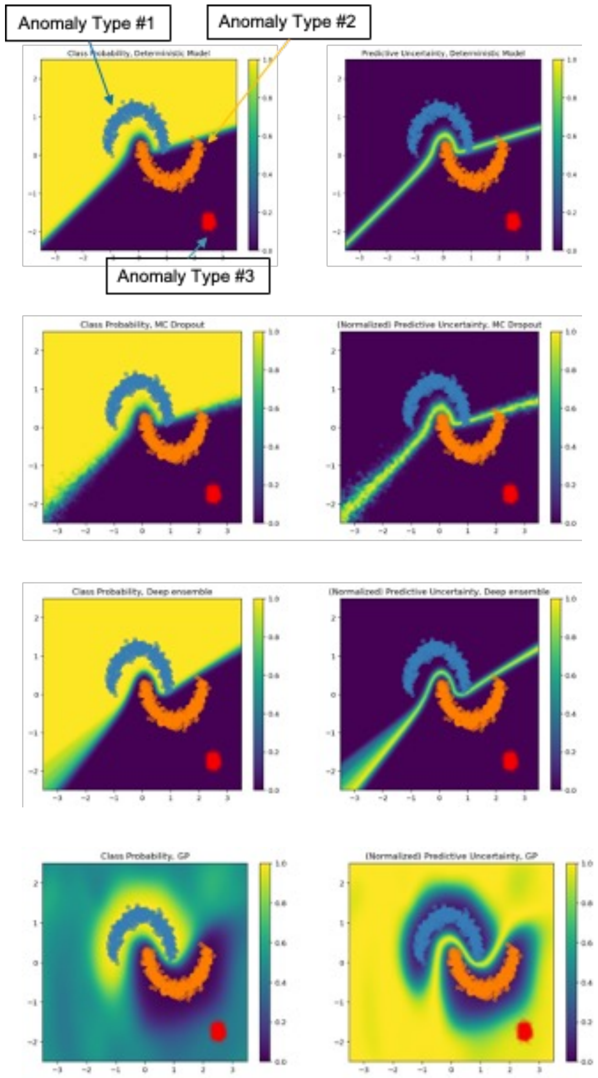
Extra

Uncertainty Quantification

- Understanding how to include UQ in deep ML models
  - Include OOD uncertainties
  - Auto-calibration
- Applications:
  - Data driven ML-based surrogate models
  - Real time controller
  - Anomaly detections
- Considerations for hardware constraints
  - Memory, Time, Performance trade-off







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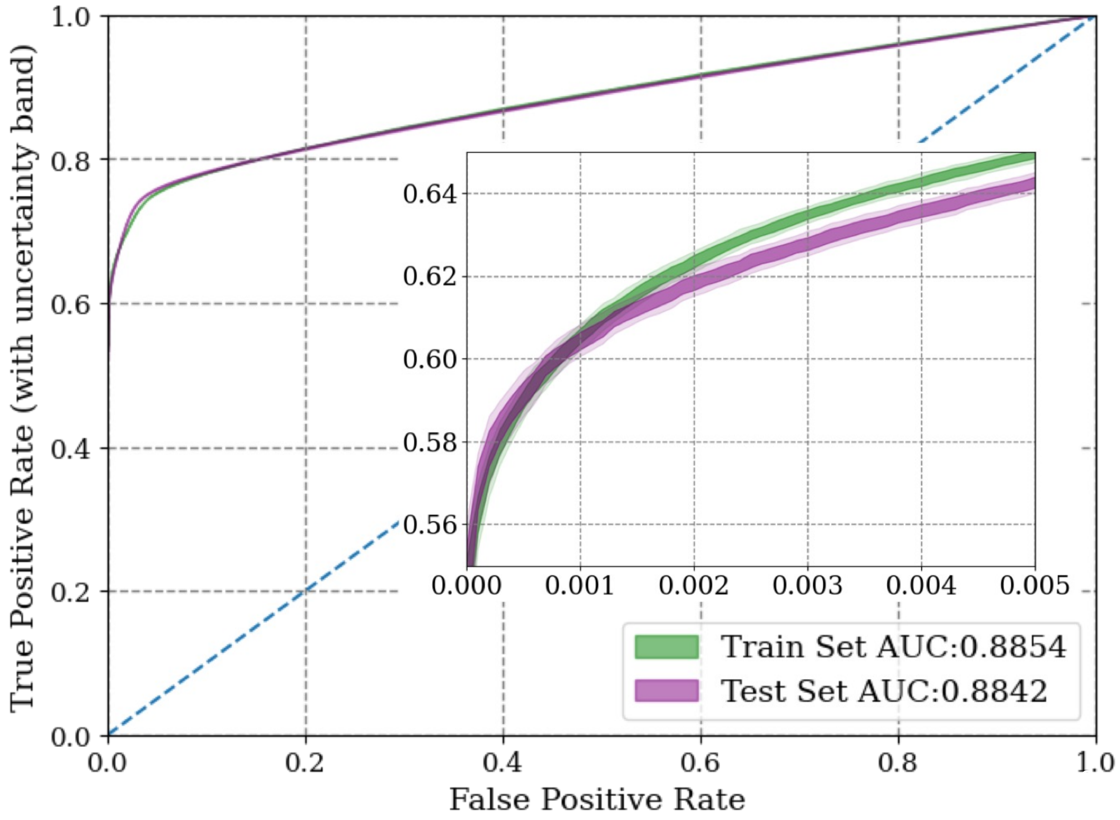
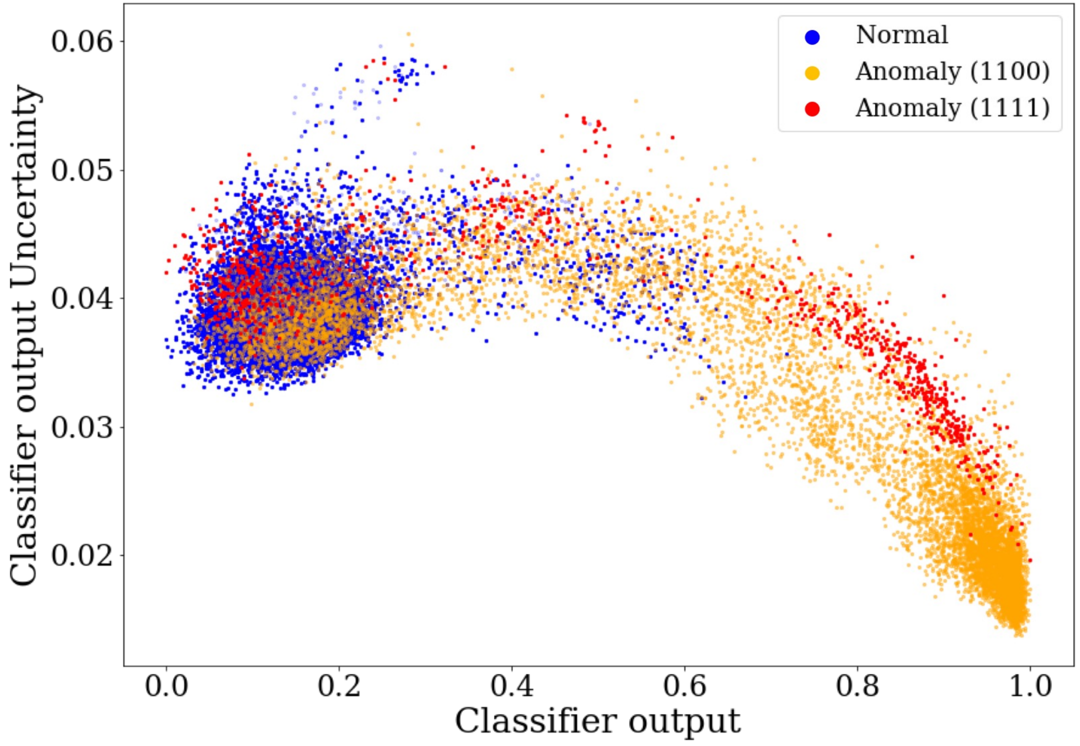
Uncertainty quantification for accelerator anomaly detection at SNS ORNL

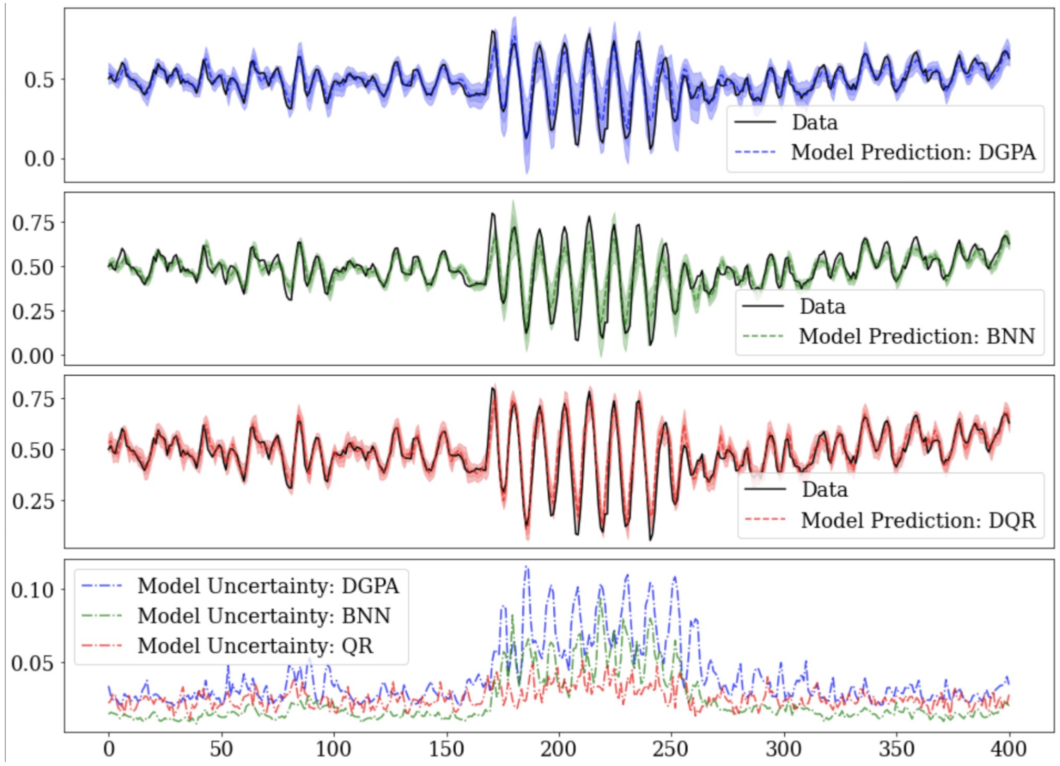
- Results from similarity model showed a ~4x improvement in performance over previously published results
- The ROC curve shows nearly the same level of performance (not optimized)
- We introduced an **out-of-domain anomaly**, labelled 1111 (red), the UQ-based model correctly identified the anomaly and indicated high uncertainty.

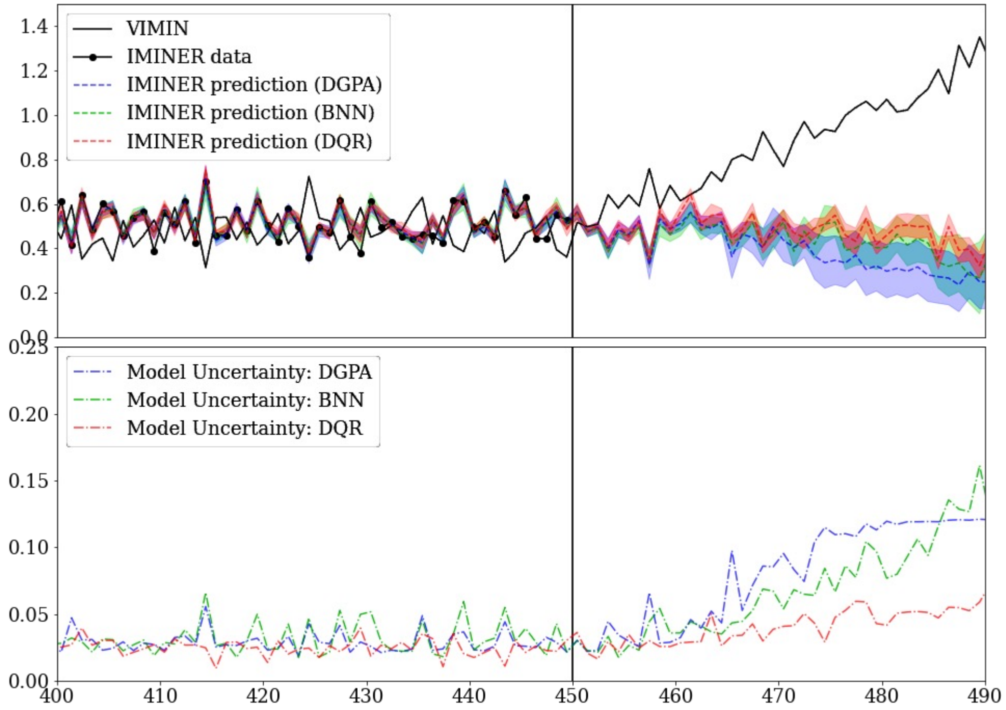




Uncertainty quantification for data driven ML-based surrogate models in risk averse control research

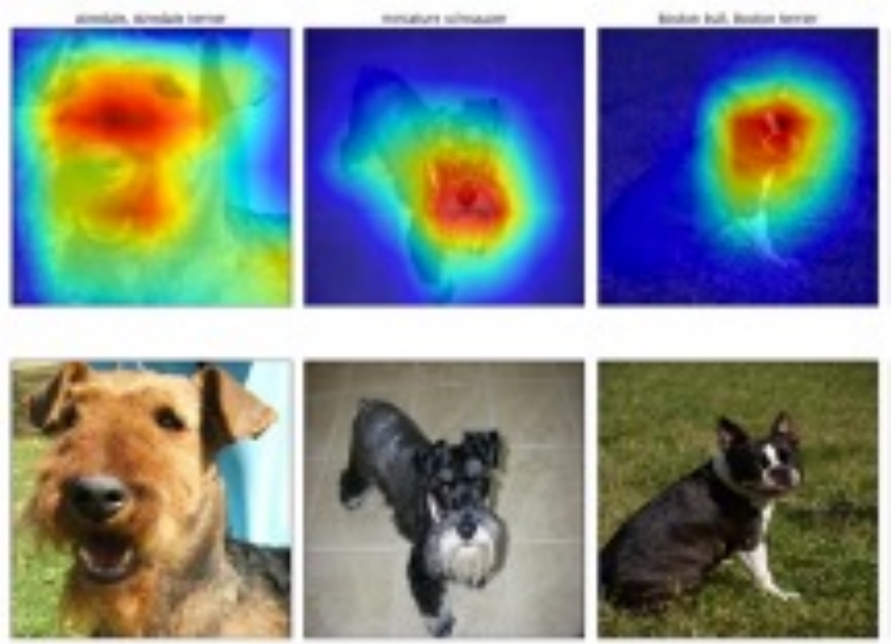
- Quantile regression method have great performance in training distribution and are calibrated by definition, however, they do not perform as well for OOD estimation
- BNN model provides does a better job to estimate OOD but require calibration
- DGPA model provide the best OOD estimation and is calibrated by design

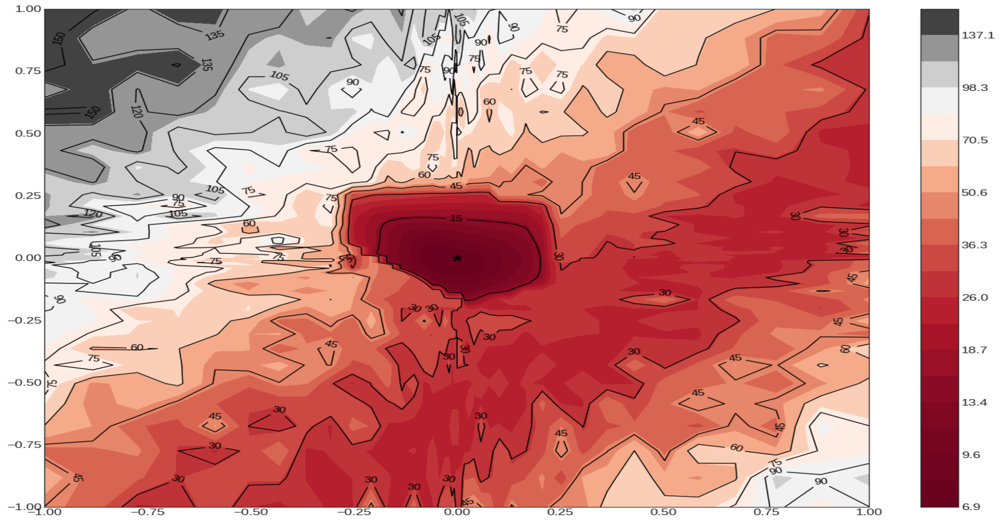




Interpretability, Explainability, and Robustness

- Applying and developing techniques to better understand model predictions and stability
- Gradient activation studies to understand what the model is focusing on
- Loss landscape analysis to better understand the model stability





Loss Landscape for FNAL system dynamic model

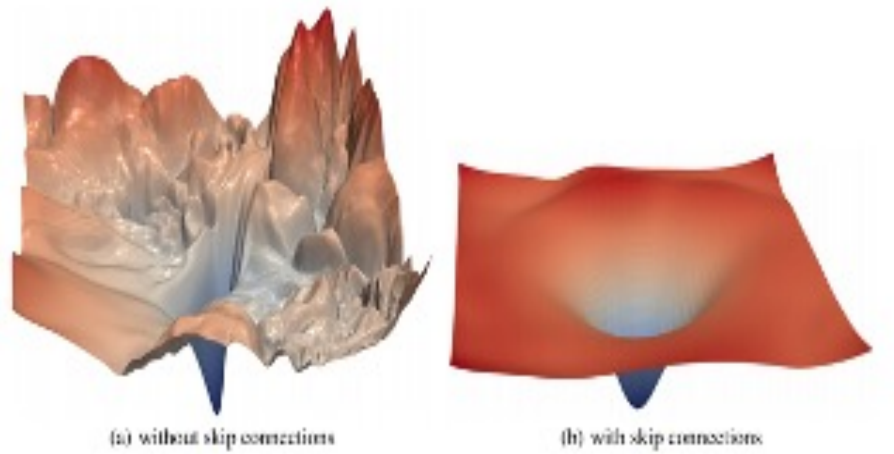
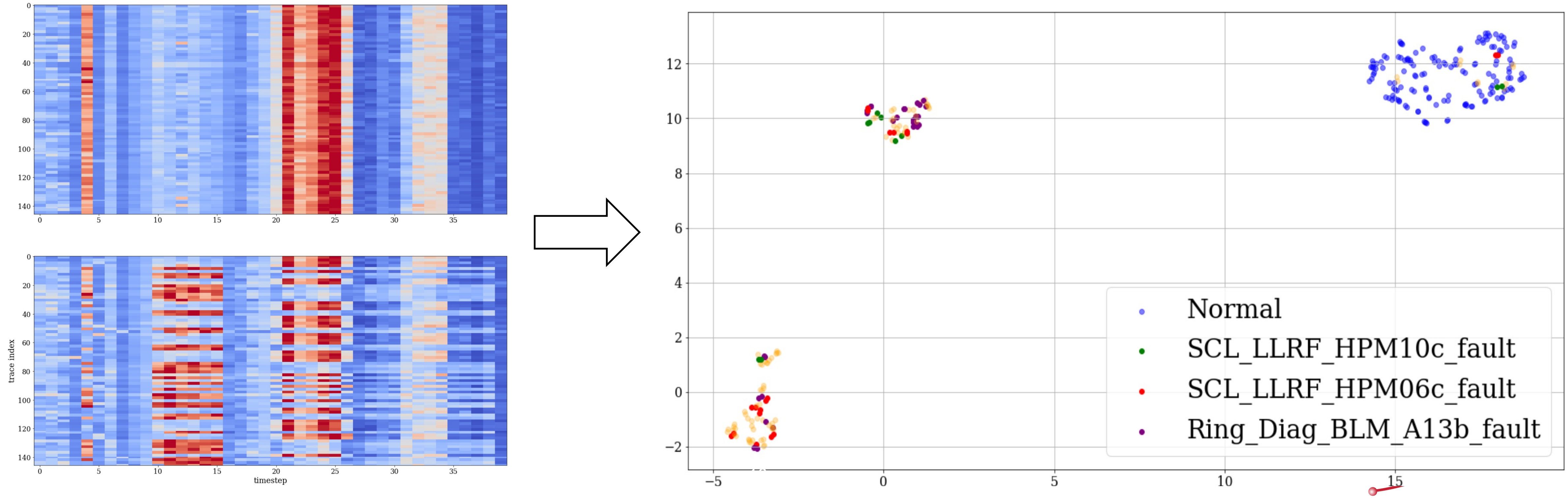


Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

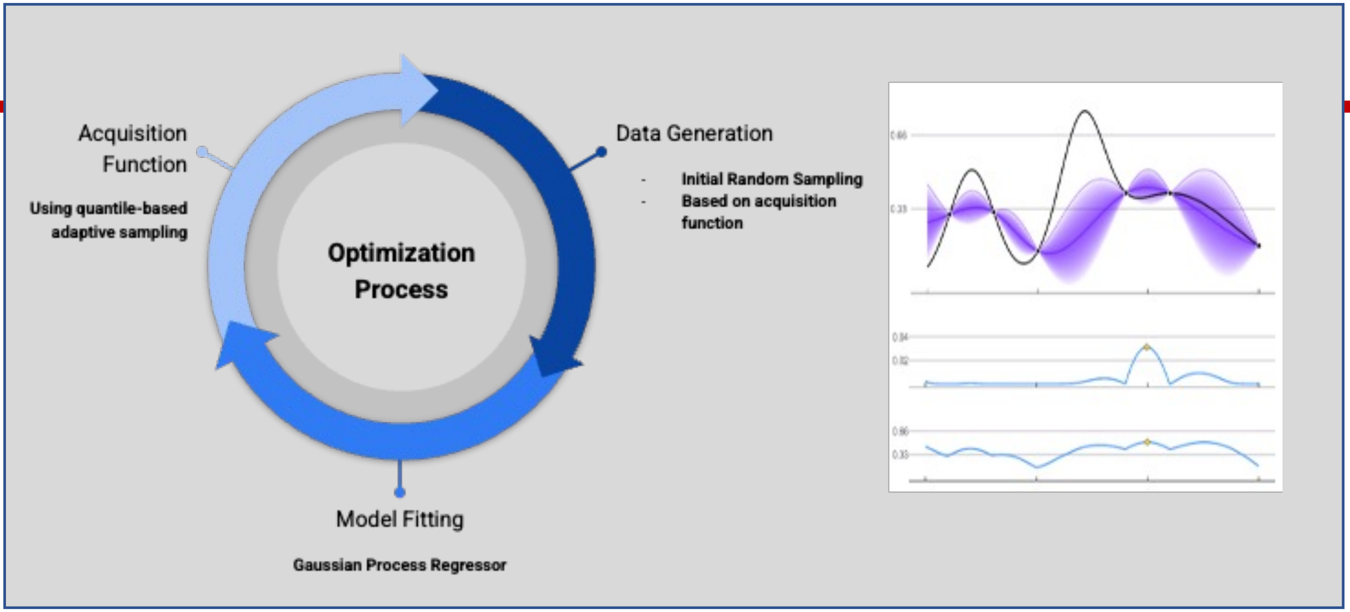
Activation Study and Fault Classifications at SNS ORNL

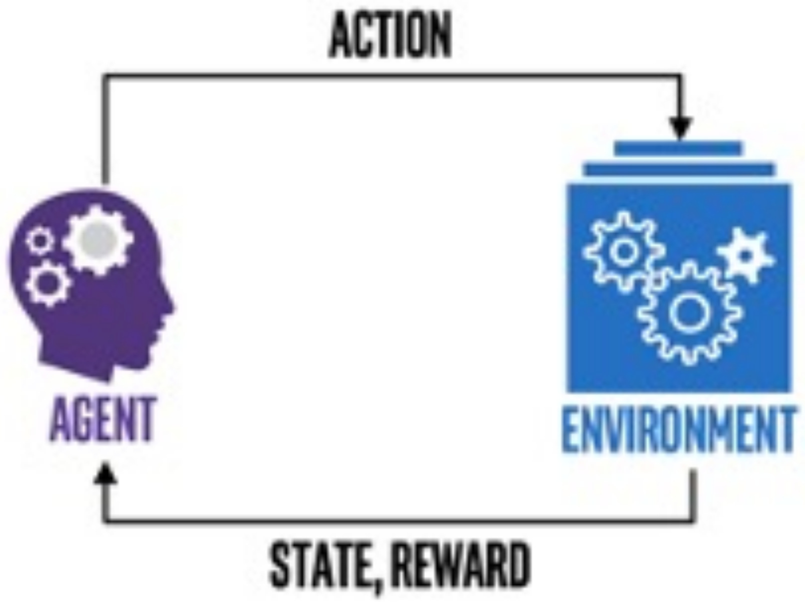
- Applied GradCAM analysis on trained ML-based model for errant beam prediction
- Identifies sections of the waveform most relevant for a particular decision from the model
- The GradCAM vectors are reduced to 2-dimensional space using clustering algorithm
- Clear clusters between normal and anomaly samples with some anomalies appearing in normal group
- The anomaly sub-clusters may belong to different equipment failures

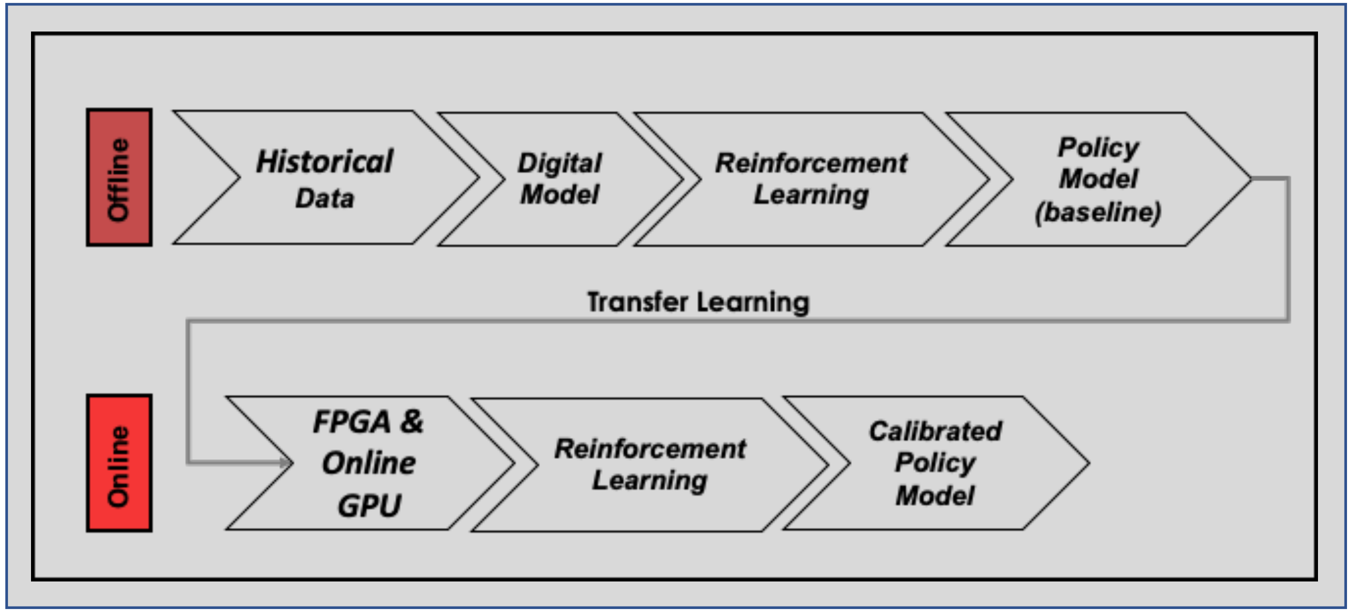


Design & Control

- Advance applications for design & control
- Bayesian Optimization
- Risk Averse and UQ aware Reinforcement Learning







Near real-time control and calibration for the GlueX CDC

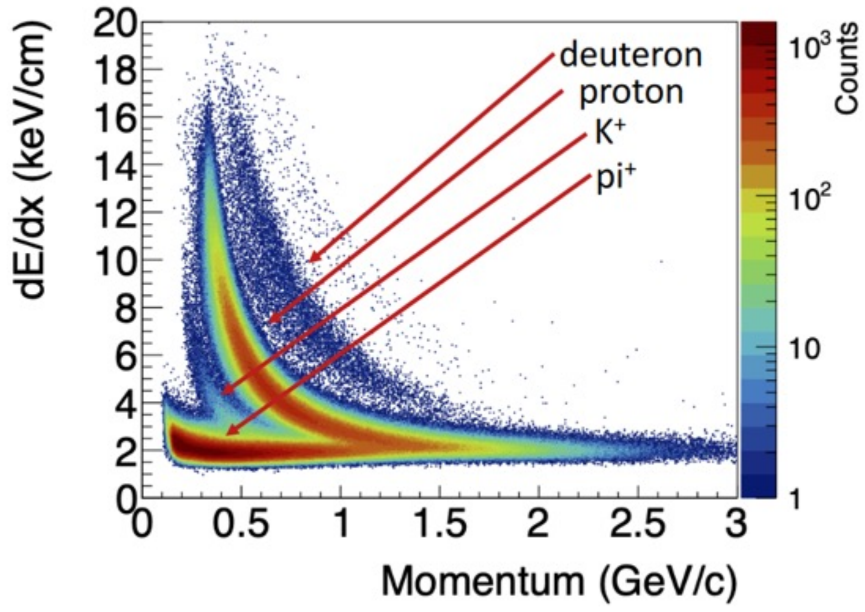
Accelerate the calibration from month(s) to minute(s).

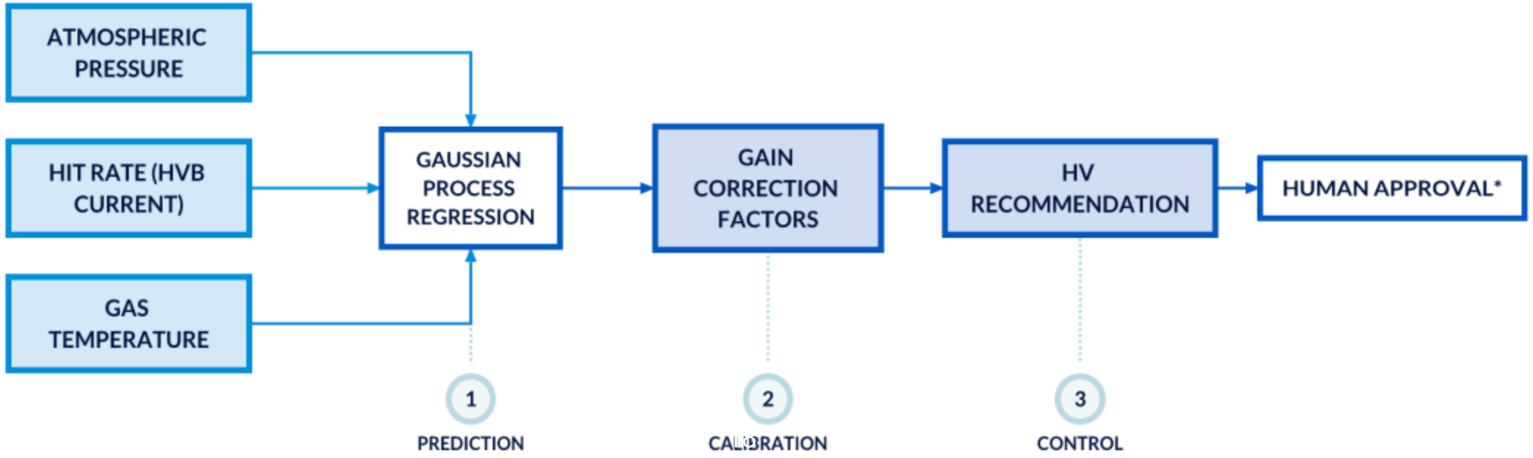
1. Gain Correction Factor: CDC Voltage Gain calibration
2. Time to Distance: track fitting calibration

Calibration is required to provide reliable PID for physics analysis

Considerations:

1. External environmental conditions (temperature, pressure)
2. Changing beam conditions (current)





Stabilizing Gain in the Central Drift Chamber

- **Peak heights from Gaussian Process side** of the CDC show dramatic reduction in pressure dependence compared to **constant HV**