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Machine Learning Optimization Upstream and Downstream of the Accelerator: The Cases of VENUS and GRETA

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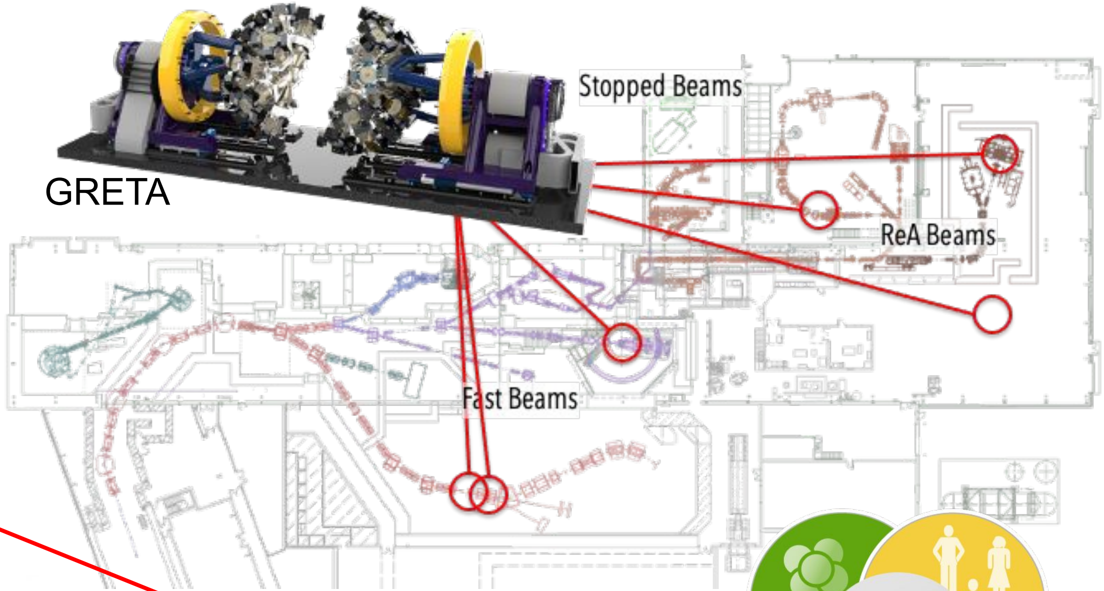
Nuclear Science Division, LBNL

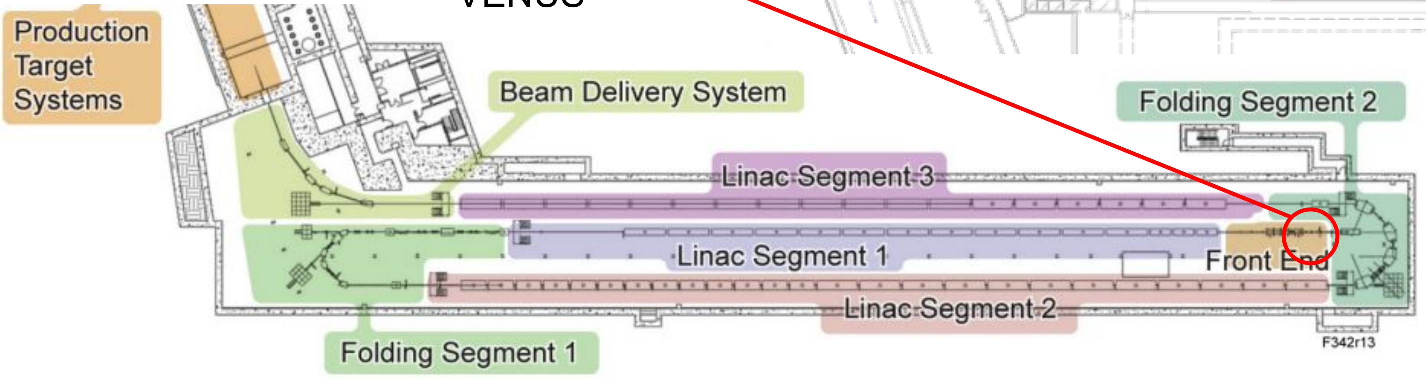
NP AI/ML PI Exchange Meeting - Wednesday, November 30, 2022

High-Level Overview

The connection to FRIB

VENUS



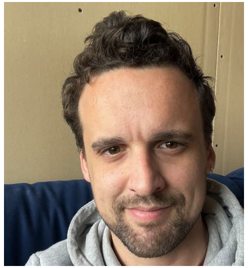


FRIB

Our Team

Marco Salathe
Senior Scientific Engineering Associate
Applied Nuclear Physics Program

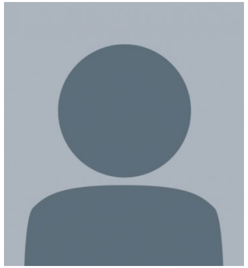
Damon Todd
Scientific Engineering Associate
88” Cyclotron



Victor Watson
Postdoctoral Researcher

Chris Campbell
Senior Scientific Engineering Associate
Nuclear Structure/GRETA Group

Yubin (Harvey) Hu
UC Berkeley
Computer Science & Physics
Class of 2023



Wenhan Sun
UC Berkeley
Computer Science, Physics and Math
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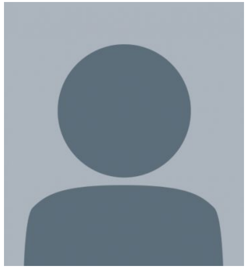
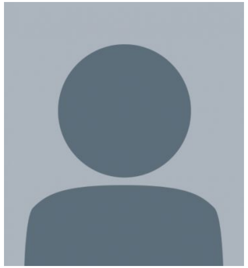


Julia Dreiling
Ohio State University
Data Analytics and Math
Class of 2024



Alex Kireeff
Carnegie Mellon University
Electrical Computer Engineering
Class of 2023

Overview and Goals

What are we doing?

The VENUS Ion Source

A Challenging Optimization Problem with High Potential Impact

- World's first fully-superconducting, third-generation electron cyclotron resonance (ECR) ion source (2004)
- Today is still one of the two highest-performing ECR ion sources in the world
- Prototype injector ion source for FRIB. **Near-identical copy being installed at FRIB**

A very impressive source:

- > 4.7 mA of O^{6+}, 20 mA He^{+}
- > 2 pμA of ^{48}Ca on target for BGS
- $^{197}Au^{61+}$ through cyclotron (> 2.3 GeV beams!)

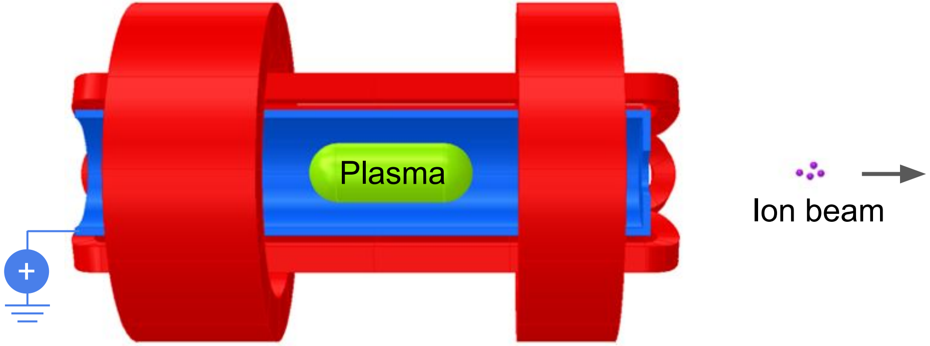
The VENUS Optimization Problem

A Challenging Optimization Problem with High Potential Impact

Control parameters include:

- Confining fields
- RF heating
- Plasma materials

~ 15-20 knobs



Diagnostics include:

- Beam current
- Charge state distribution
- Emittance
- Bremsstrahlung

What you really want to know:

- Plasma density distribution
- Electron energy distribution
- Particle lifetimes
- RF distribution

What you really want for operations:

- Maximum beam current at the desired charge state
- Operational stability and reproducibility
- Good emittance characteristics
- Low consumption of input material (efficient)

The VENUS Optimization Problem

A Challenging Optimization Problem with High Potential Impact

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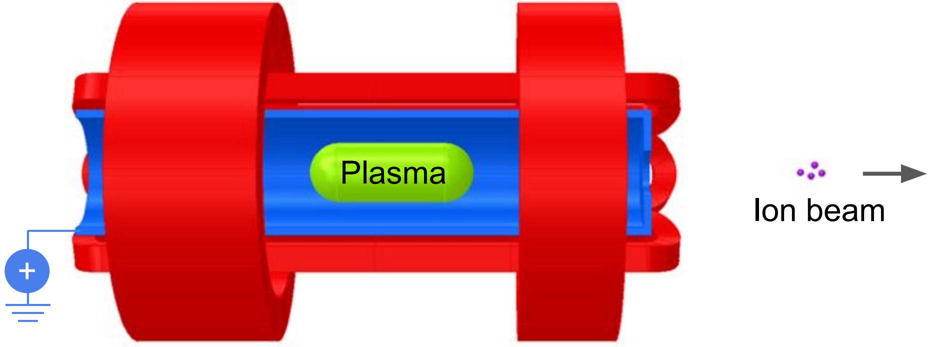


Diagnostics include:

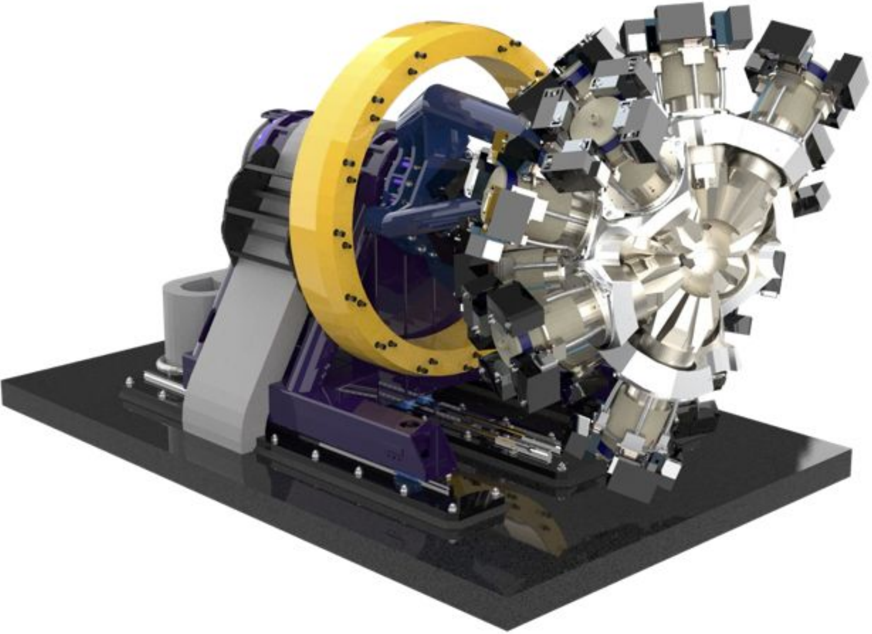
- Beam current
- Charge state distribution
- Emittance
- Bremsstrahlung

Goals of this Project:

- Consolidate diagnostic signals and setting readbacks into a consistent framework/database structure for application of efficient data processing
- Investigate automation of VENUS control parameters, or subsets for tuning
- Explore data correlations which may emerge and connections to the physics of the ion source
- Optimize tuning and other necessary procedures to enhance efficiency (e.g. of time, materials)

The Gamma-Ray Energy Tracking Array GRETA

A Large End-Station with 1000s of Parameters to Optimize for *every experiment*



- U.S. implementation of a gamma-ray tracking array
- Complete 4π solid angle coverage of active HPGe, consisting of 120 individual detector crystals, each with 37 electrical signals
- Gamma-ray tracking and Compton suppression is enabled by signal decomposition algorithm which localized gamma-ray scatter events to within ~mm3 volumes

GRETA will be the world-leading gamma-ray spectrometer once delivered to FRIB in early 2025, and will be an experimental work-horse for physics at FRIB.

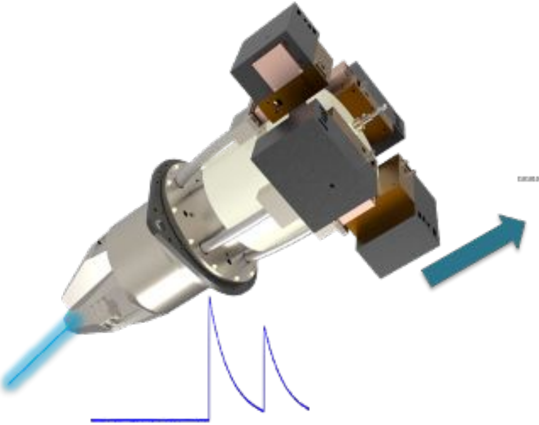
The GRETA Optimization Challenge

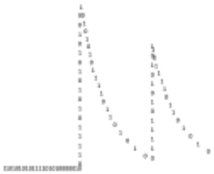
A Large End-Station with 1000s of Parameters to Optimize for *every experiment*

Simple control parameters include:

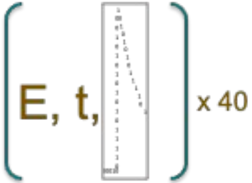
- 4-6+ energy filter parameters **per channel**
- 2+ calibration parameters **per channel**

~ 30k knobs ***just for energy spectra***

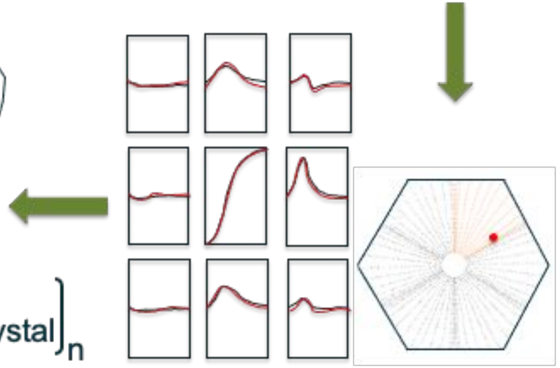




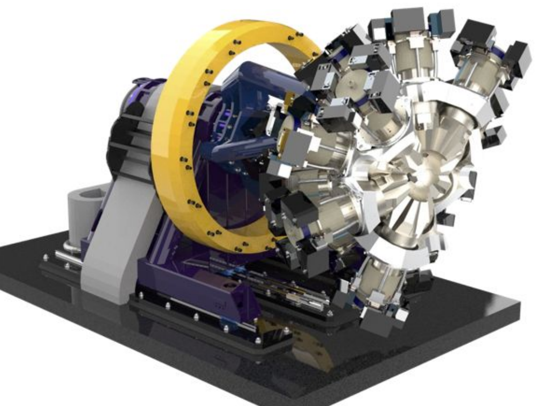
- Continuous 100MHz digitization of **40** preamplifier signals **per crystal**



- FPGA-based energy filters, event selection in response to physics triggers



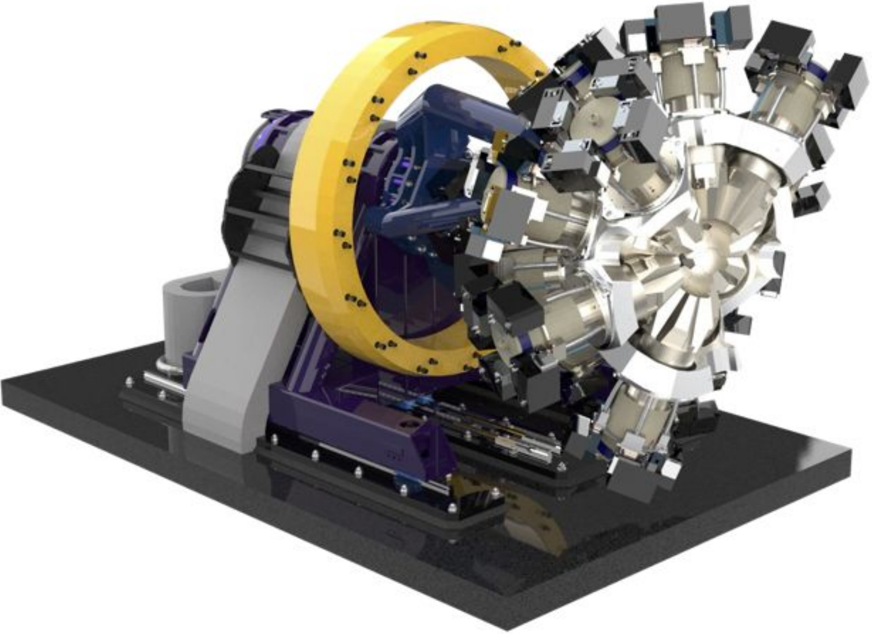
$$\left[E,\ t,\ (x,\ y,\ z)_{crystal}\right]_n$$



The GRETA challenge is optimizing consistently across the array to ensure every single channel is realizing its peak performance.

The GRETA Optimization Challenge

A Large End-Station with 1000s of Parameters to Optimize for *every experiment*



Goals of this Project:

- Consolidate diagnostic signals and setting readbacks into a consistent framework/database structure for application of efficient data processing
- Investigate automation of GRETA channel pipeline optimization (channel by channel energy filters and calibration)
- Explore potential for early fault detection specific to detector failures

Progress

How it’s going…

Progress on VENUS and GRETA

Overview Road Map

1. Data preparation and storage for VENUS
2. Data analytics and insights
3. Bayesian optimization for VENUS
4. Modeling VENUS with a neural network
5. Data preparation and sources for GRETA
6. Energy filter optimization

1 Data Preparation for VENUS

A case with limited data sources

- VENUS data sources are primarily via the PLC controls system
  - Magnet current settings, RF settings, bias supply voltages etc.
- Additional work was required to enable automation of less frequent measurements e.g. charge state distributions
- Future work will be extended to a new emittance scanning capability

- Data collection is now continuous at VENUS and populates a simple time-stamped indexed SQLite database from which data is readily pulled for analysis

1 Data Collection for VENUS

A case with limited data sources

- Data collection is now continuous at VENUS and populates a simple time-stamped indexed SQLite database from which data is readily pulled for analysis

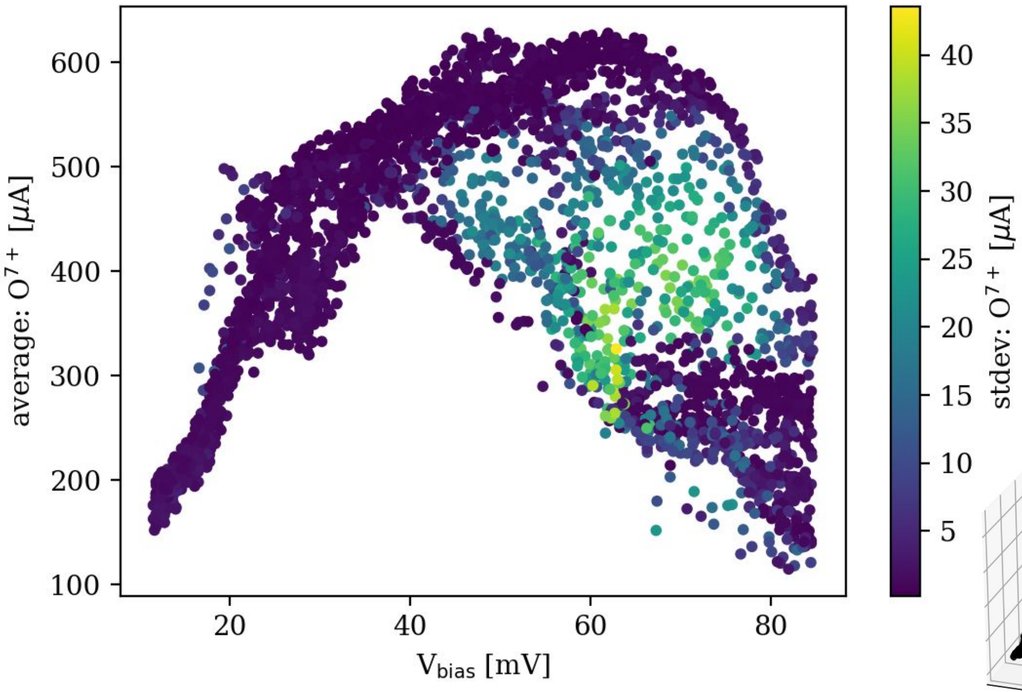
Data Sets

- VENUS is continuously recording; data points are ***averages*** of stable periods
- 1st half: Weeks 1-4 → coil currents were modified
- 2nd half: Weeks 5-8 → bias voltage and gas input valve were modified

Week ID	Actual date (2022)	#Data
1	Feb. 18 – Feb. 21	1057
2	Mar. 18 – Mar. 20	931
3	Apr. 29 – May 2	939
4	Jul. 15 – Jul. 18	Invalid
1st Half		2927
5	Sep. 2 – Sep. 6	3288
6	Sep. 16 – Sep. 18	2126
7	Sep. 30 – Oct. 1	626
7.5	Oct. 2 – Oct. 3	689
8	Oct. 7 – Oct. 10	1135
2nd Half		7864
Total		**10791**

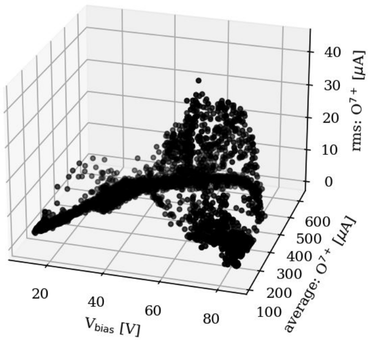
2 Data Analytics and Insight for VENUS

More Data = More Insight



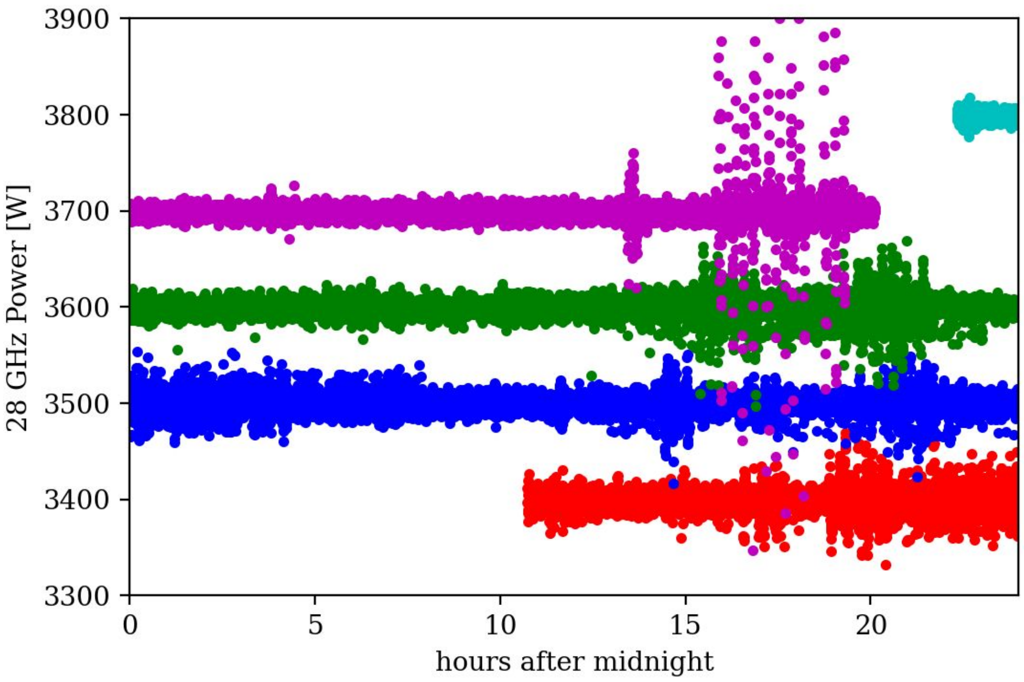
Example run:

- 1 weekend of data varying two parameters to maximize O^{7+} current
- 221,760 data points — at least two orders of magnitude more data that humans could take in the same period of time
- Each data point is a snapshot of 63 different plasma/beam diagnostic



2 Data Analytics and Insight for VENUS

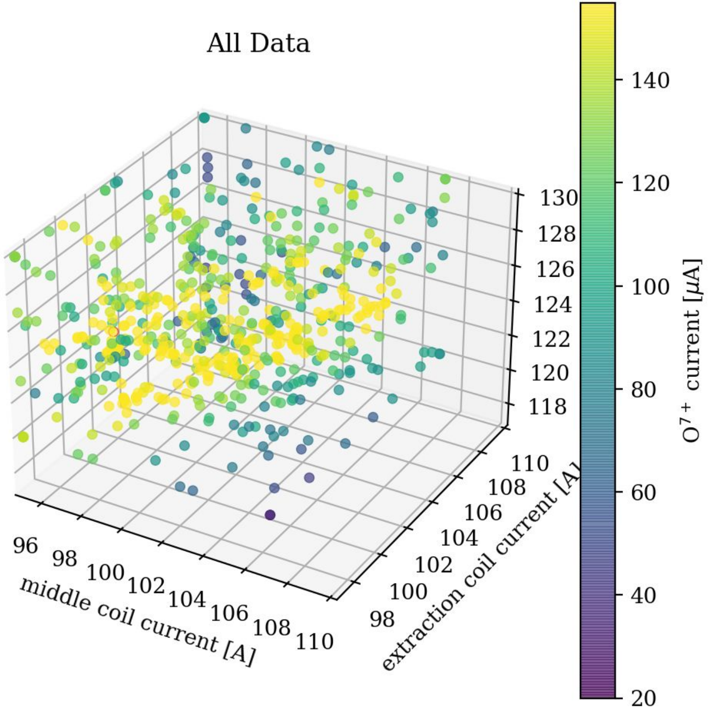
Monitoring has led to identification of previously-unknown system instabilities



3 Bayesian Optimization for Parameters of VENUS

Investigation of the Parameter Space

- Automated tuning was used as a method to explore a portion of the parameter space for VENUS - 3 magnet currents specifically
- Concept: Use Bayesian optimization to find the configuration with the best beam properties - defined for now as the highest Faraday cup current
- Use Gaussian Process regressor for parameter space modeling



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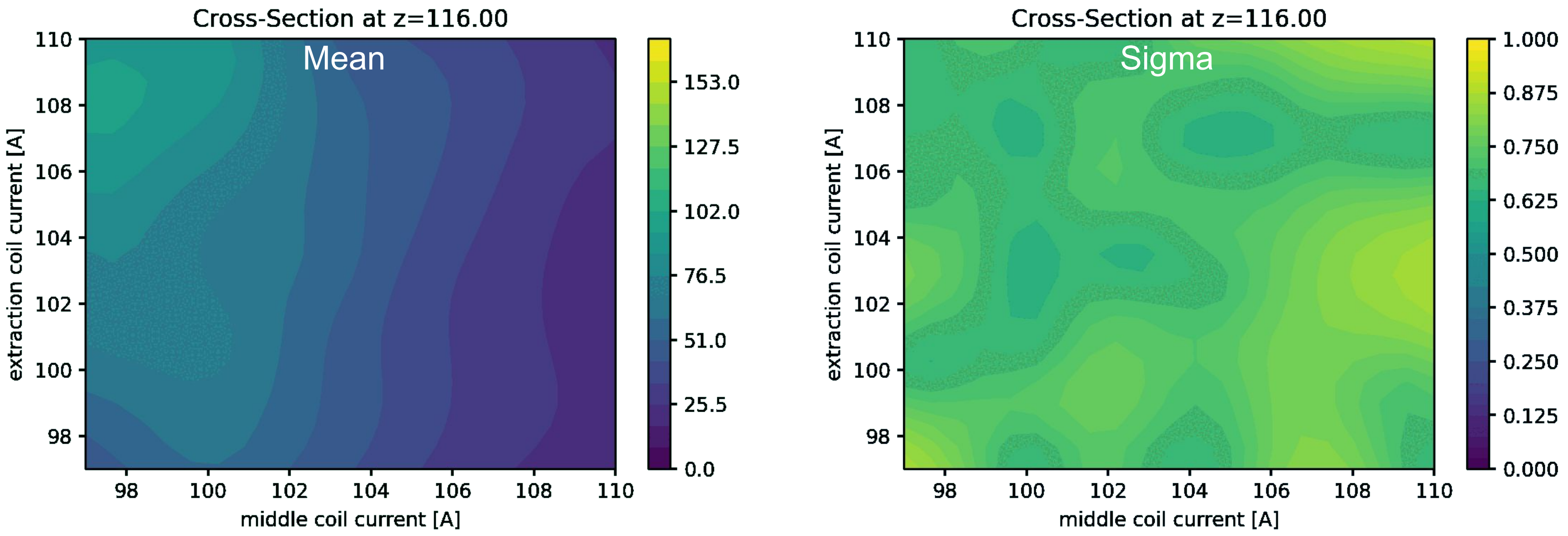


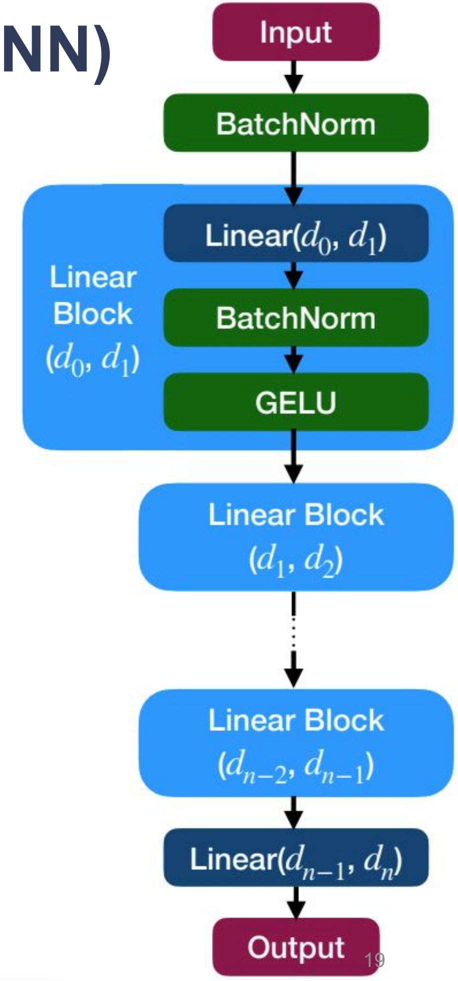
Next steps? Apply Bayesian optimization on the model to tune hyper-parameters.

4 Modeling VENUS with a Neural Network (NN)

Given a specific set of parameters what is the output beam current?

Neural Network Structure

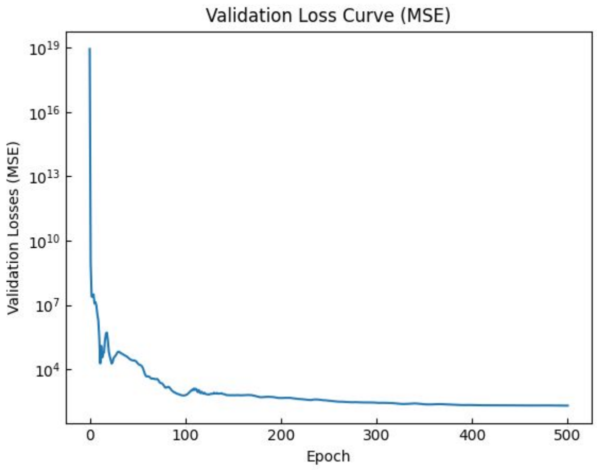
- Fully connected NN (n = 4)
- $\{d_i \mid i \in \mathbb{N}(n+1)\}$: Layer sizes
  - d_0 = 63: Input dimension
  - d_n = 1: Output dimension
- Actual dimensions: 63, 256, 64, 8, 1

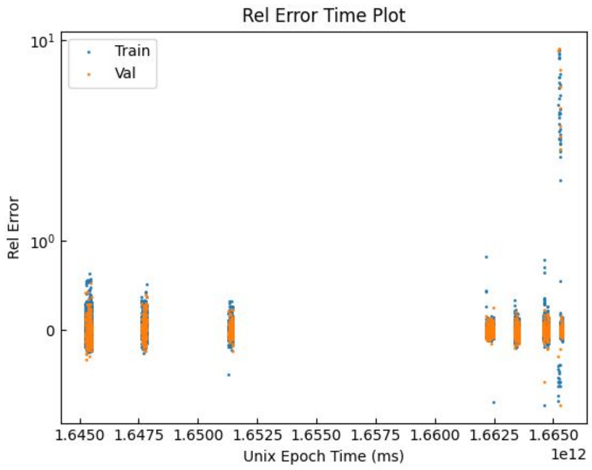


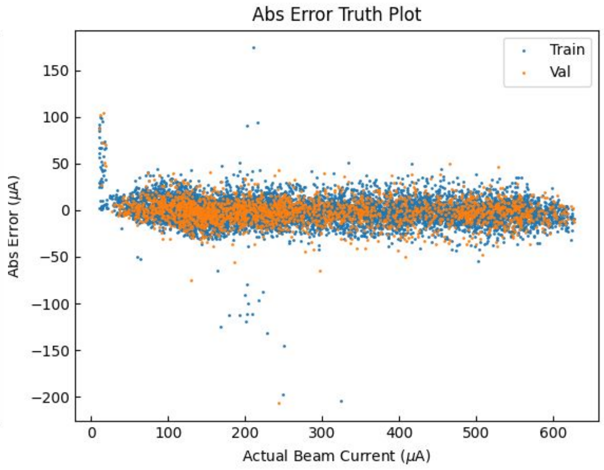
4 Modeling VENUS with a Neural Network (NN)

Results - Training with All Weeks

- Random training-validation split (4:1 ratio)
- Trained 500 epochs, using mean-squared error (MSE) as loss



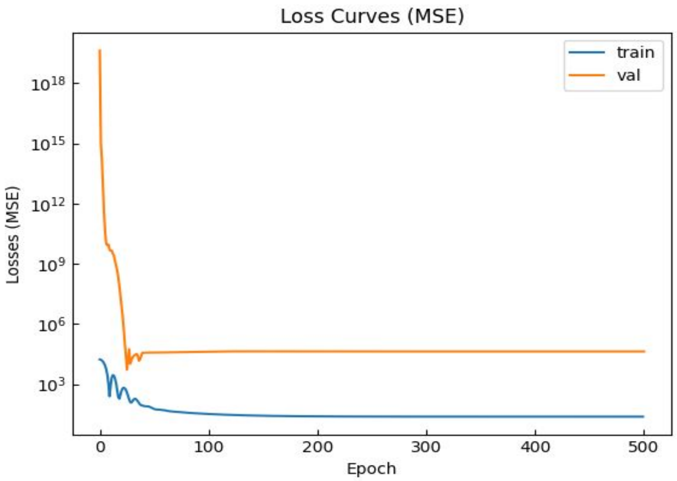


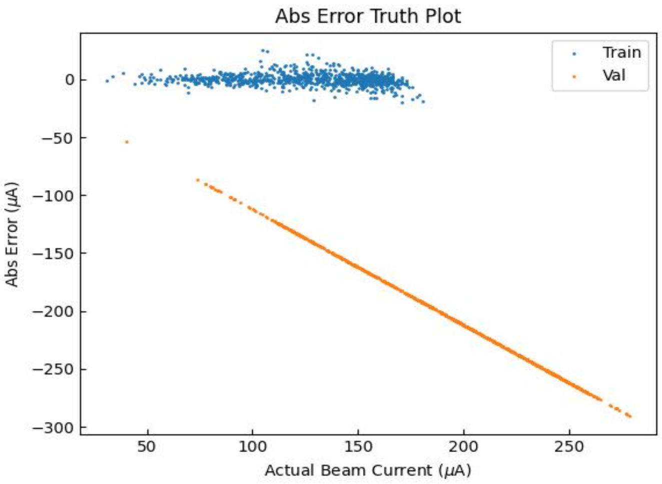


4 Modeling VENUS with a Neural Network (NN)

Results - Generalizability

- Model trained by one week **cannot** be used to predict the data in another week
- Train on week 2; validate on week 3:





4 Modeling VENUS with a Neural Network (NN)

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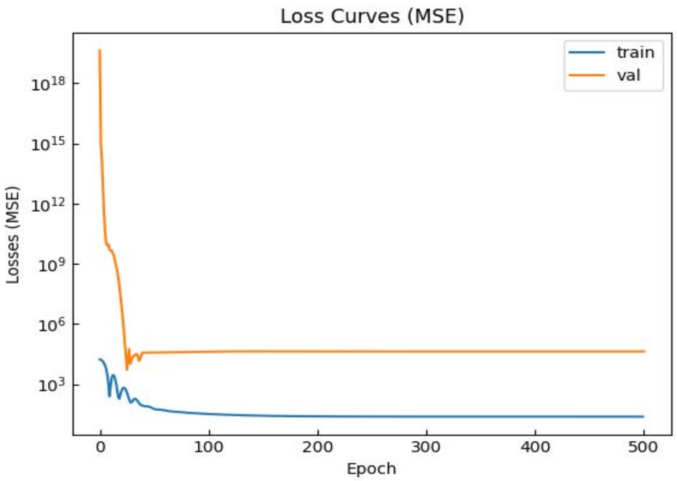
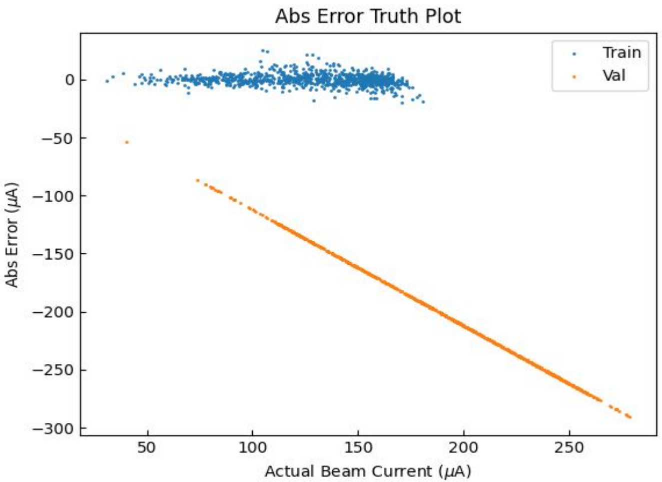




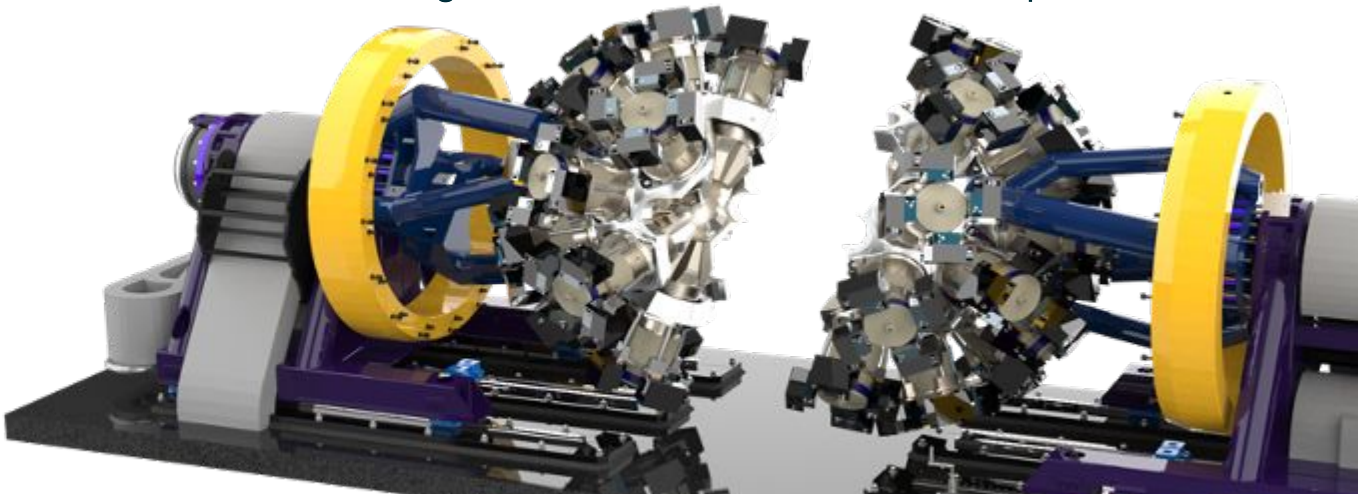
Next steps?

Transfer learning, based on naive or recurrent NN, and expansion of the parameter space

5 Data Source for GRETA

An even broader set of data sources than VENUS

- GRETA data will come from a broad range of sources - e.g. PLC controls system, EPICS slow controls, Prometheus database (used in GRETA computing), on-line data analysis software
- As GRETA systems are still in production, assembly of all data sources together for fault detection efforts has not yet started
- Planned approach is a modular system of libraries for each data source and an interface to a database similar to that used for VENUS → general framework for ML/AI setup in diverse systems

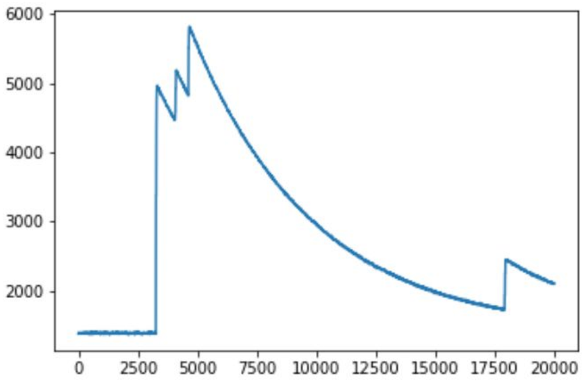


6 Energy Filter Optimization

The first task for GRETA, using offline optimization

- Recorded streamed data sets for a single channel of a GRETA detector is available to be used to optimize energy filter (trapezoidal filter) algorithm
- Just started – currently exploring least-square and gradient descent algorithms for optimization of a single parameter in the energy filter

- Ultimate implementation will be changing parameters online for the entire array to optimize



Project Details

Budget, Schedule and Milestones

Budget and Expenditures

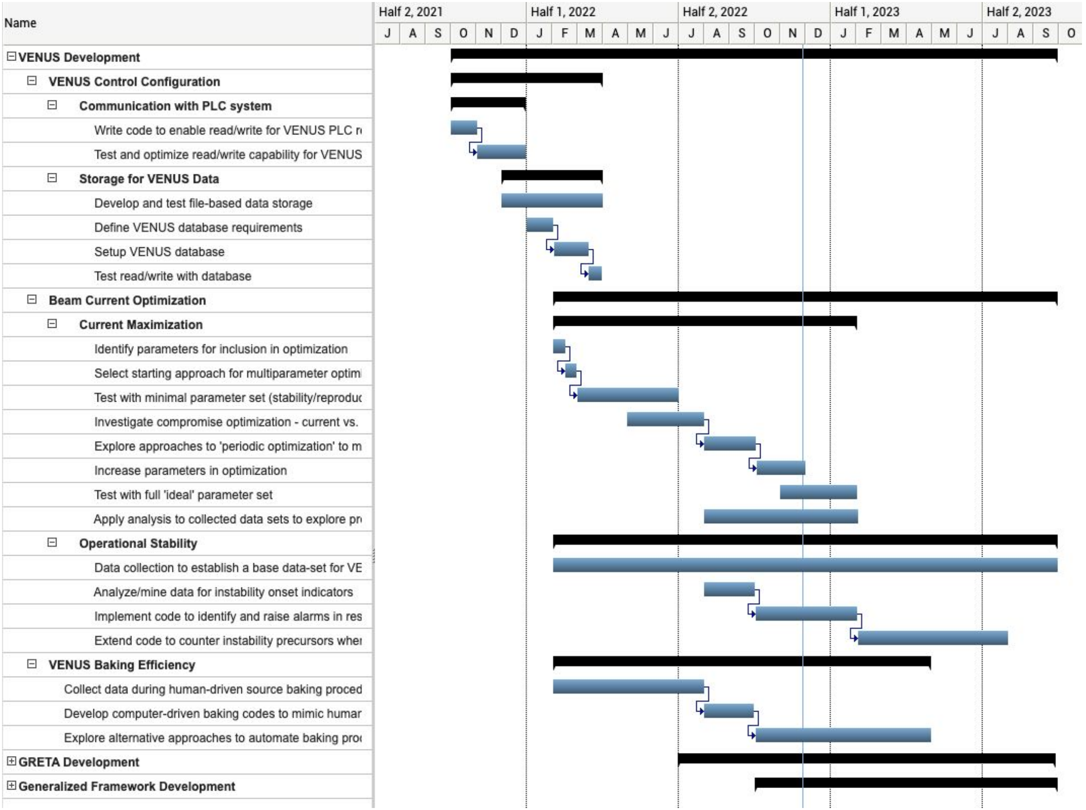
	FY22 ($k)	FY23 ($k)	Total ($k)
Funds Allocated	500	500	1000
Actual Costs to Date	187*	53	240*

* our postdoc (V. Watson) did not start until 08/2022; he is now 100% on this project

Schedule

Early effort has been focused on VENUS

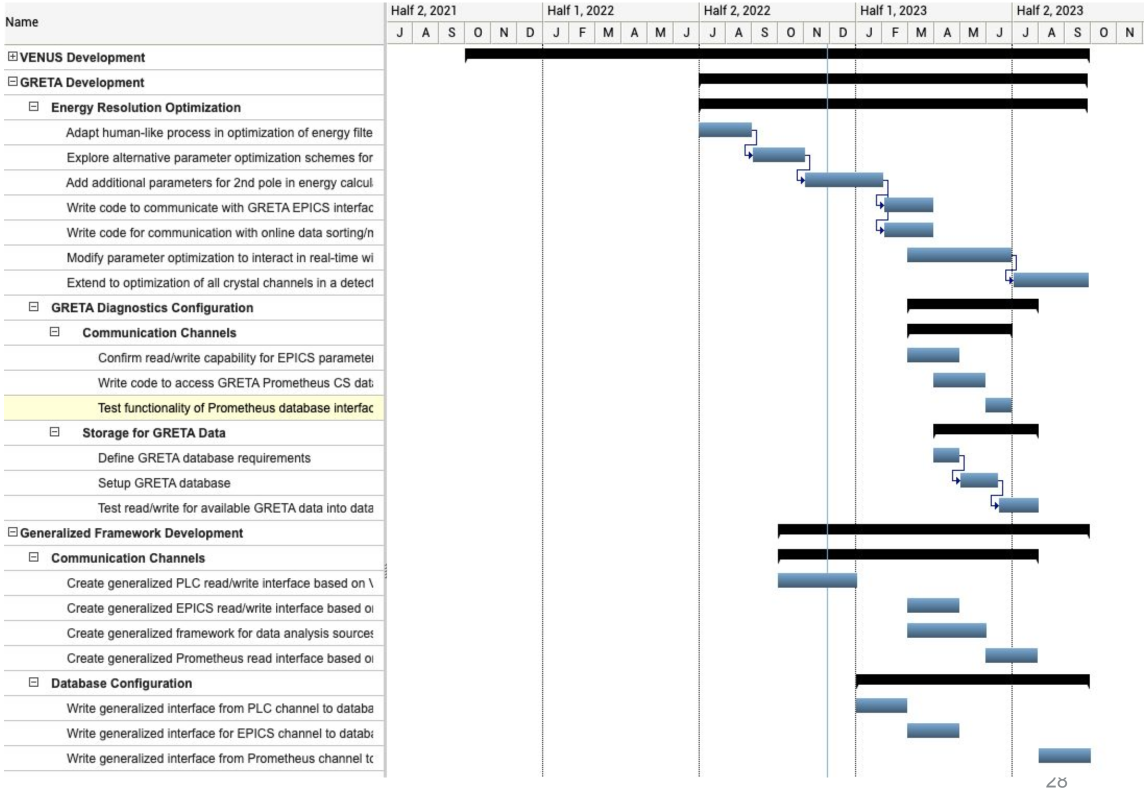
- As VENUS is an operating device, it was ready to go and efforts began here
- We are currently expanding the parameter space under exploration and beginning implementation of key “baking” process for VENUS



Schedule

GRETA and “general framework” efforts are now ramping up

- GRETA work has started using offline analysis, and will transition next to using the EPICS interface for online energy filter optimization
- Creation of general interfaces will be a focus in the next several months



Project Milestones

WBS	Milestone	Description	Projected Milestone Date	Status
1.1.1	**VENUS** PLC Interface Complete	Develop and test code to read/write from the VENUS PLC control system.	Dec-2021	✓
1.1.2	**VENUS** Database Implemented	Database for logging of VENUS parameters is defined, established and configured for use.	Mar-2022	✓
1.2.1	**VENUS** Current Optimization Started	Optimization of VENUS beam current through automated search of a limited parameter space has started.	May-2022	✓
2.1	**GRETA** Off-line Energy Resolution Optimization Implemented	Human-like process for optimization of energy filters in off-line data analysis for GRETA streamed data is complete.	Sept-2022	✓
1.3	**VENUS** Baking Control First Attempt Complete	Computer-driven codes to implement baking procedure for VENUS guided by human approach complete.	Dec-2022	In progress
1.2.1	Full Parameter Space **VENUS** Optimization Implemented	Optimization of VENUS beam current implemented exploring the full parameter space of the controls system.	Feb-2023	
2.1	**GRETA** SFB Optimization Enabled	Optimization of the energy filter parameters is implemented for the signal filter board hardware via the EPICS interface in GRETA.	Jun-2023	
2.2.2	**GRETA** ML/AI Database Established	Database for logging of GRETA parameters is defined, established and configured for use.	Jun-2023	
3.1	Generalized Framework Communication Channels Complete	Complete generally configurable versions for all communication types used in VENUS and GRETA.	Aug-2023	

Summary

- Recruitment challenges and personnel shortages have meant a slower start than initially hoped
- An impressive team of undergraduates have made substantial headway
  - VENUS data collection is now routine and dedicated data sets are in hand for training and assessment purposes
  - NN and Bayesian optimization approaches are both showing promise
  - GRETA work is now ramping up as the GRETA systems near construction completion
- We are excited to keep moving forward and having much more to report on soon!

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Thank you!