2024 DOE/NP ARTIFICIAL INTELLIGENCE/MACHINE LEARNING PRINCIPAL INVESTIGATOR EXCHANGE MEETING GAITHERSBURG, MD, DECEMBER 4-5, 2024

#### USE OF AI-ML TO OPTIMIZE ACCELERATOR OPERATIONS & IMPROVE MACHINE PERFORMANCE



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#### **OTHER CONTRIBUTORS**

Calem Hoffman, Physicist Adwaith Ravichandran, Postdoc Sergio Lopez-Caceres, Postdoc





# OUTLINE

### Completion of the Original ATLAS AI-ML Project

### □Accomplishments & Main Conclusions

### □The New AI-ML Project – Overview & Objectives

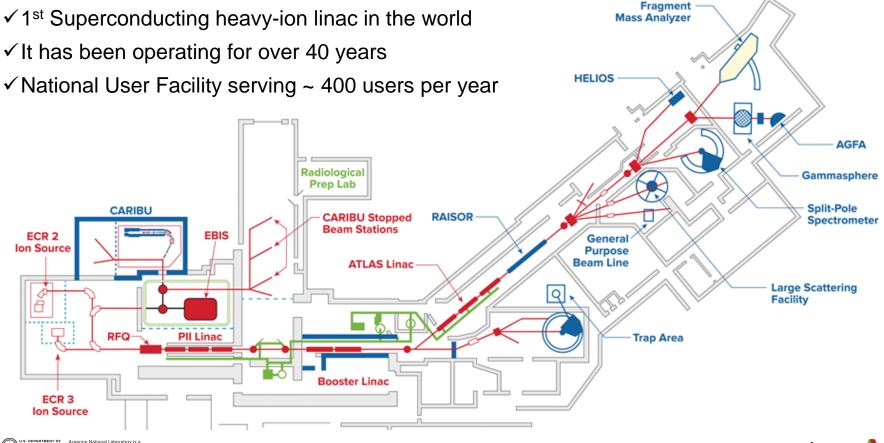
### Development and Testing of AI-ML User Interface(s)

### Recent Progress & Highlights – ATLAS & CARIBU

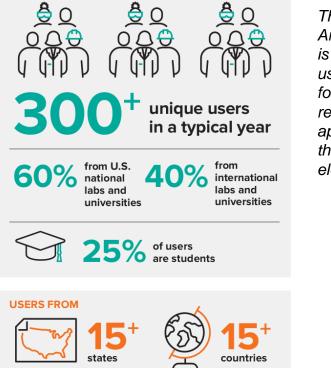




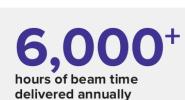
### ATLAS: ARGONNE TANDEM LINEAR ACCELERATOR SYSTEM



### ATLAS BY THE NUMBERS In FY24, served 400+ unique users

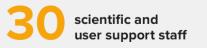


The ATLAS accelerator at Argonne National Laboratory is a DOE/SC/NP national user facility that supports forefront nuclear physics research, national security applications, and studies of the origin of chemical elements.

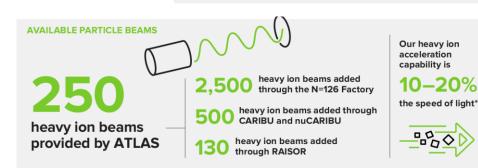


40% of requested beamtime approved as high priority

1–2 calls for proposals per year



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https://www.anl.gov/atlas

# **OVERVIEW OF ORIGINAL ATLAS AI-ML PROJECT**

# Use of artificial intelligence to optimize accelerator operations and improve machine performance

□ At ATLAS, we switch ion beam species every 3-4 days ... → Using AI could streamline beam tuning & help improve machine performance

□ Project objectives and approach:

- Data collection, organization and classification, towards a fully automated and electronic data collection for both machine and beam data
- Online tuning model to optimize operations and shorten beam tuning time in order to make more beam time available for the experimental program
- Virtual model to enhance understanding of machine behavior to improve performance and optimize particular/new operating modes



### **ACCOMPLISHMENTS VS. ORIGINAL OBJECTIVES**

- Data collection, organization and classification, towards a fully automated and electronic data collection for both machine and beam data... established
- Online tuning model to optimize operations and shorten beam tuning time in order to make more beam time available for the experimental program... achieved for short beam lines, commissioning of a new beamline
- Virtual model to enhance understanding of machine behavior to improve performance and optimize particular/new operating modes ... good progress, a long-term goal...





# MAIN CONCLUSIONS FROM ORIGINAL PROJECT

- Developed and used Bayesian Optimization (BO) for multiple beamlines. BO is very effective for beam tuning even with no prior data.
- □ BO typically converges in 50 iterations or less for a few parameter problem (< 10). With every iteration taking ~15 s, that's 10-15 min, this is comparable to operators' time.
- Used BO to support the commissioning of a new beamline (AMIS), it was more competitive and helpful in this task (new to operators). Also, for multi-objective optimization MOBO, it's not an easy task for the operators.
- Demonstrated transfer learning: We were able to save a BO model from one beam and used it as starting point (prior knowledge) to tune another beam leading to faster accelerated convergence.
- □ Transfer from a simulation model was not as successful due to discrepancy between the model and the actual machine. We need a more realistic simulation or surrogate model.
- Developed and used Reinforcement Learning (RL) for the AMIS line with different parameter combinations. RL requires a lot of prior data and training, which is very expensive to perform online.
- □ We were able to train RL models with 3, 5 & 7 parameters in ~1000 iterations which took ~ 4 hours each. Once trained, an RL model converges in 2-3 iterations, less than 1 min!
- □ We made good progress on the virtual machine model based on TRACK simulations. Once ready, it will be very helpful to train BO & RL models offline, then apply them directly to the machine with no or minimal further online training...





### THE NEW ATLAS AI-ML PROJECT (2023 FOA)



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# THE NEW CONSOLIDATED PROJECT (2023 FOA) – THREE SUBPROJECTS

- □ Stable beams in ATLAS Brahim Mustapha
- □ Inflight radioactive beams from RAISOR Calem Hoffman
- □ Radioactive beams from CARIBU Daniel Santiago
- Consolidation: close collaboration, exchange of ideas, codes and effort...
- Two new postdocs joined the ATLAS and CARIBU projects
  - Adwaith Ravichandran, started in December'23
  - Sergio Lopez-Caceres, started in June'24





### ATLAS NEW PROJECT: DEPLOYMENT...

Same project title: Use of artificial intelligence to optimize accelerator operations and improve machine performance

□ The main objectives of the phase II project are:

- Deploy the autonomous beam tuning tools developed during our previous project, evaluate their impact on both automating the tuning process and saving on tuning time.
- Develop tools for new operating modes such as multi-user operation of the ATLAS linac and high-intensity beams, as well as developing virtual diagnostics to supplement existing ones.





### **PROGRESS - MOST RECENT DEVELOPMENTS...**

Development of an AI-ML Graphics User Interface – ATLAS Dashboard

- Offline tests using simulation model successful
- Online tests at ATLAS not yet successful, but promising
- Adapted the existing AI-ML GUI, Badger from SLAC, for use at ATLAS
  - Well supported and offers more options / optimization algorithms
  - Not as friendly or customized as the ATLAS Dashboard GUI
- □ Tuning the beam to an end target station
  - Issues with tuning intermediate sections using only beam transmission
- □ Re-tuning the beamline after an energy change
  - $\circ~$  A time-consuming process when done manually



### **DEVELOPMENT & TESTING OF** AI-ML USER INTERFACE(S)



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### **NEW ATLAS DASHBOARD INTERFACE**

#### **Development of a User Interface for the Operators**

ATLAS - Dash	board				ATLAS - Dashboard						
Get/Read Settings	Set/Vary Settings	Get/Read BPMs	Get/Read FCP	Ps ▲	<ul> <li>Get/Read</li> <li>Settings</li> </ul>	Set/Vary Settings	Get/Read BPMs	Get/Read FCPs			
Instructions	Task Setup	Beamlines	Execution		Instructions	Task Setup	Beamlines	Execution			
Please, follow th	e instructions bel	ow:		0	pen the beam	n lines you are inte	rested in and sele	ect the elements			
	devices will be accessible.				PII Two Beamline						
2. In Beamlines, select v	which elements will be read	d and the data will be sa	ived.		PII Exit Beamline						
<ol> <li>In Beamlines, select v</li> <li>In Execution, click to</li> </ol>		d and the data will be sa	ived.		PII Exit Beamline						
,	execute or run.	d and the data will be sa	ived.		PII Exit Beamline	shboard					
3. In Execution, click to	execute or run.	d and the data will be sa	● Get/Read FCPs			shboard Set/Vary Settings	C Get/Read BPMs	Get/Read FCPs			
3. In Execution, click to ATLAS - Dar	execute or run. shboard				ATLAS - Das		Get/Read BPMs Beamlines	Get/Read FCPs Execution			
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### **NEW ATLAS DASHBOARD INTERFACE (2)**

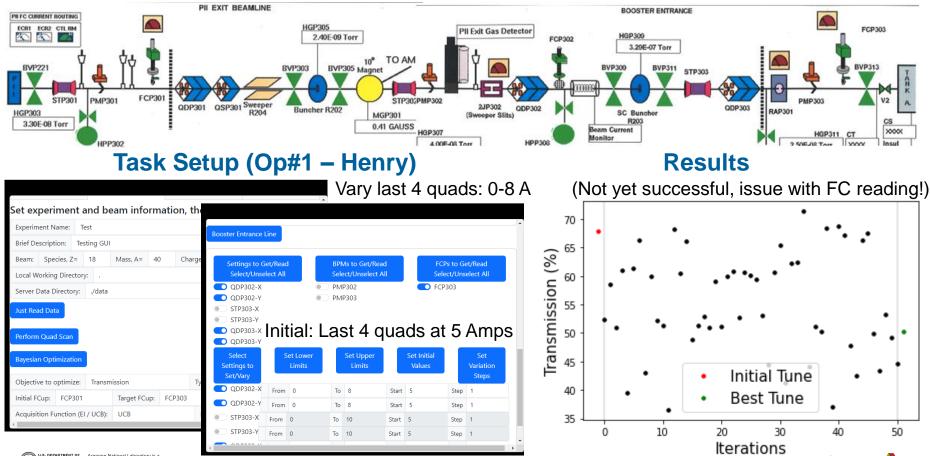
#### **Development of a User Interface for the Operators**

ATLAS - Dashboard					ATLAS - Dashboard								
Get/Read Settings	Set/Vary Settings G Get/Read BPMs Get/Read ECPs			Settings to Get/Read Select/Unselect All								FCPs to Get/Read Select/Unselect All	
Instructions	Task Setup	Beamlines	Execution	STP301-X     PMP301     STP301-Y     OPDP001					0	FCP301			
Open the beam l PII Two Beamline PII Exit Beamline	ines you are inter	rested in and sele	ct the elements		QDP301-X QDP301-Y QSP301-X STP302-X STP302-Y								
	ad BPMs to 0		FCPs to Get/Read	2	Select Settings Set/Vary	to		ngs Lower Limits		Settings Upper Limits		Settings Initial Values	
Settings to Get/Rea Select/Unselect A STP301-X		select All S	elect/Unselect All		STP301-X	From From			To To		Start Start		
<ul> <li>STP301-Y</li> <li>QDP301-X</li> <li>QDP301-Y</li> </ul>					QDP301-X	From From				10 10	Start Start		
<ul> <li>QSP301-X</li> <li>STP302-X</li> </ul>					QSP301-X	From From			To To	10 10	Start Start		
• STP302-Y			· · · ·		STP302-Y	From	0	-	То	10	Start	5	+





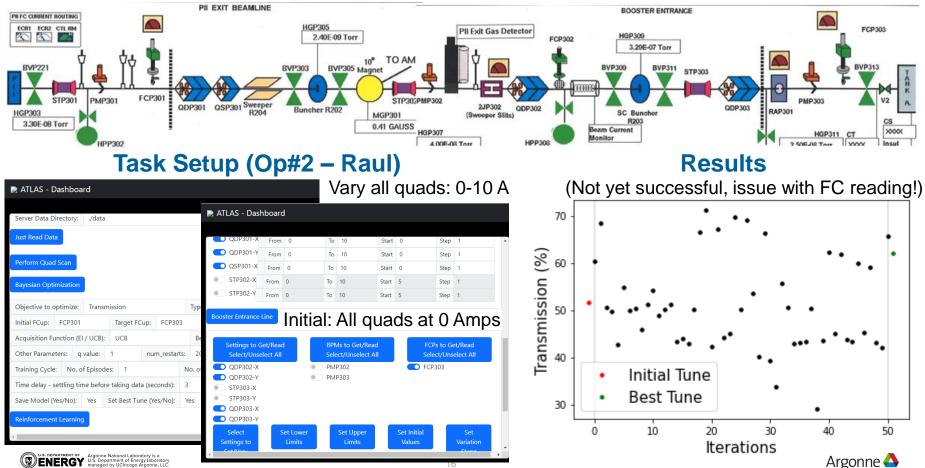
### **GUI ONLINE TEST #1: PII TO BOOSTER LINE**



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Argonne

### **GUI ONLINE TEST #2: PII TO BOOSTER LINE**



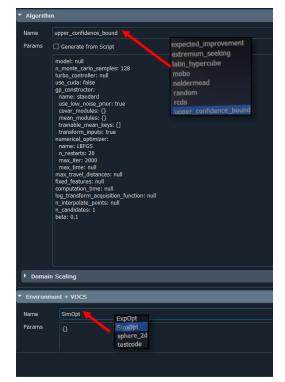
### **NEW ATLAS BADGER INTERFACE**

#### **Development of a Developer Interface for the Experts**

#### Setup the problem's variables and objectives

Variables	Filter	variables	Add Limit Variable Ra	ange			0	Show Check	ed Only				
	☑	QDP301X				4	.0000	12.0000	H				
	•	QDP301Y				4	.0000	12.0000					
	☑	QSP301X				4	.0000	12.0000	9				
	V	QDP403X				1	0.0000	20.0000					
	•	QDP403Y				1	0.0000	20.0000	ПЧ				
	▼ In	itial Points											
		Add Row							łł				
					QDP403X		QDP403						
		5.4	10.19	7.12	11.254	16.339							
Objectives			8	Show Check	ed Only								
			Name										
									MINIMIZE				

#### Select Algorithm & Parameters



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### **NEW ATLAS BADGER INTERFACE (2)**

#### **Developer Interface testing using simulations with different setups**



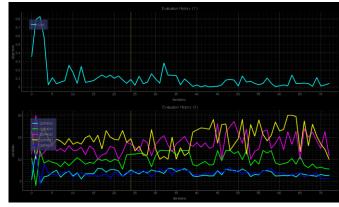
#### **BO Model Hyperparameters:**

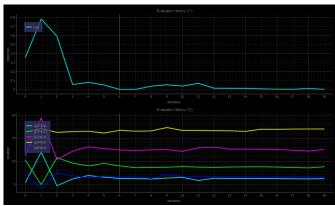
- Beta : 2.0
- No of candidates: 1
- No of restarts: 20
- Max Iterations: 2000
  - No of Monte Carlo Samples: 128



- Beta : 0.1
- No of candidates: 1
- No of restarts: 20
- Max Iterations: 2000
  - No of Monte Carlo Samples: 128

18







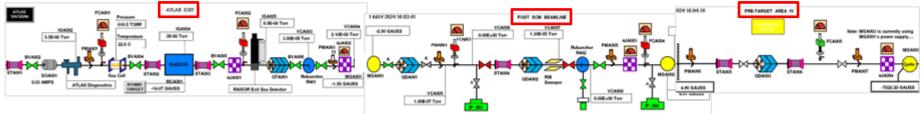
### **RECENT PROGRESS & HIGHLIGHTS - ATLAS**



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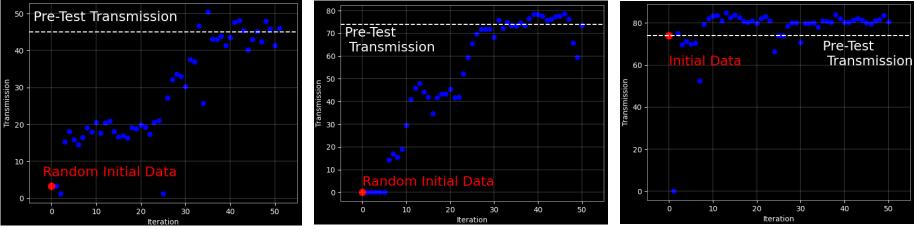


### **TUNING THE BEAM - ATLAS EXIT TO FMA TARGET**



**Problem**: Maximize transmission, use BO **Tuning parameters**: up to 9 quads & 6 steerers (v&h) **Method**: Don't vary all parameters at once, find the most sensitive set of parameters...

Iterations & Time: Typically, 50 iterations x 15 sec (reading two FCs), x 8 sec (reading one FC)



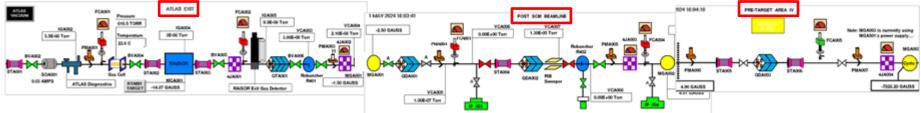
Varying 6 quads + 2 steerers  $\rightarrow$  Change initial data point



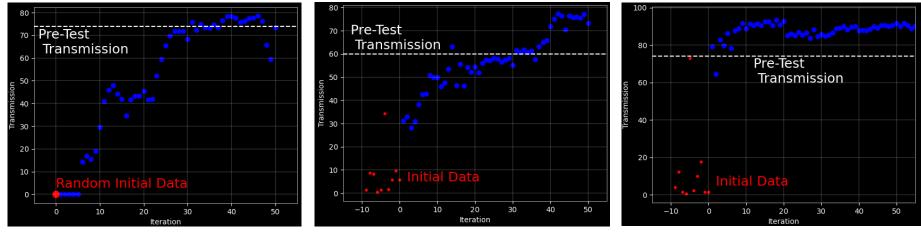
Varying 6 guads only

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### **TUNING THE BEAM - ATLAS EXIT TO FMA TARGET (2)**



**Problem**: Maximize transmission, use BO **Tuning parameters**: up to 9 quads & 6 steerers (v&h) **Method**: Change number of initial data points for BO model, also explore more  $\beta = 0.1 \rightarrow 1.5$ **Iterations & Time**: Best transmission 95% in less than 50 iterations x 8 sec ~ 7 min



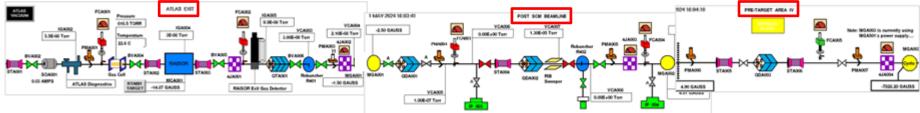
Varying 6 quads + 2 steerers  $\rightarrow$  Using 10 initial data points

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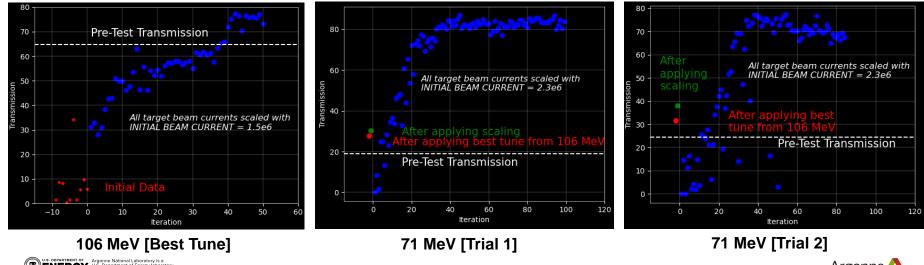


Varying 6 guads + 4 steerers

### **RE-TUNING THE BEAMLINE AFTER ENERGY CHANGE**



**Problem**: Switch to a lower energy tune, 106 MeV  $\rightarrow$  71 MeV, retune for max. transmission **Method**: Load 106 MeV tune after energy change, scale to 71 MeV and re-optimize... **Iterations & Time**: Best transmission ~ 85% in ~ 50 iterations x 8 sec ~ 7 min





### **RECENT PROGRESS & HIGHLIGHTS - CARIBU**



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**DECEMBER 4TH, 2024** 

#### THE CARIBU-MATIC PROJECT AUTOMATION FOR THE TRANSPORT OF RADIOACTIVE BEAMS FROM THE CARIBU/NUCARIBU SOURCE



#### DANIEL SANTIAGO-GONZALEZ

Physicist Physics Division Argonne National Laboratory



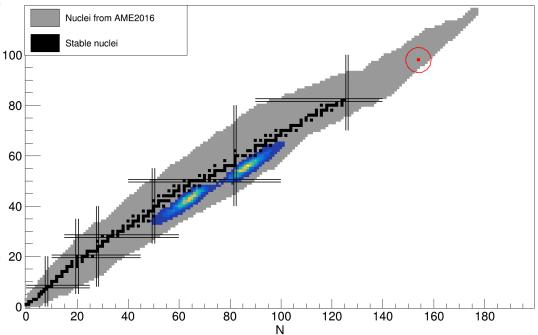
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# WHAT IS CARIBU?

#### A radioactive ion source part of the ATLAS national user facility

- CARIBU provides beams of heavy ions made from <sup>252</sup>Cf fission fragments (10<sup>2</sup> – 10<sup>4</sup> pps, few keV/u)
- nuCARIBU a major upgrade in progress to increase beam intensities via neutron induced <sup>N</sup> fission
- Essential for ATLAS multi-user upgrade (post-accel. beams, 3-10 MeV/u) 20
- User statistics: in FY24, ATLAS enabled research directly impacting over 430 unique users (many come more than once per year, about 25 are students)



https://www.anl.gov/atlas/caribu-beams



### SCIENCE ENABLED BY THE CARIBU SOURCE Selected highlights

- CARIBU beams enable a diverse user program that produces cutting-edge scientific publications with impact in the fields of:
  - nuclear structure
  - nuclear astrophysics
  - national nuclear security, and others
- Selected publications include:
  - Mass measurements that help us better understand how the chemical elements were produced in stellar environments – Van Schelt et al. PRL 111, 061102 (2013)
  - First direct experimental evidence of a "pear-shaped" nucleus Bucher et al. PRL 116, 112503 (2016)
  - First study of the 139Ba(m,γ) #40Ba reaction to constrain the conditions for the astrophysical *i* process Spyrou et al. PRL 132, 202701 182502 (2024)

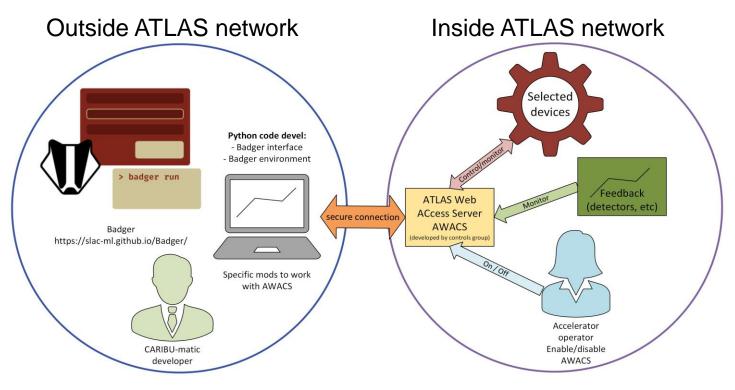
These state-of-the-art investigations are possible in part because the CARIBU staff scientists deliver close to 2500 hours (or about 100 days) of beam time per year to our users





### **CARIBU-MATIC PROJECT**

Our approach for secure radioactive beams tuning automation







### RECENT MILESTONES - JUL/2024 FOUNDATIONAL WORK COMPLETED - AUG/2024 CARIBU-MATIC LIVE OPTIMIZATION

**TASK:** IN A SINGLE SESSION, TRANSPORT A RADIOACTIVE BEAM USING BAYESIAN OPTIMIZATION (60+ CONTROL PARAMS)

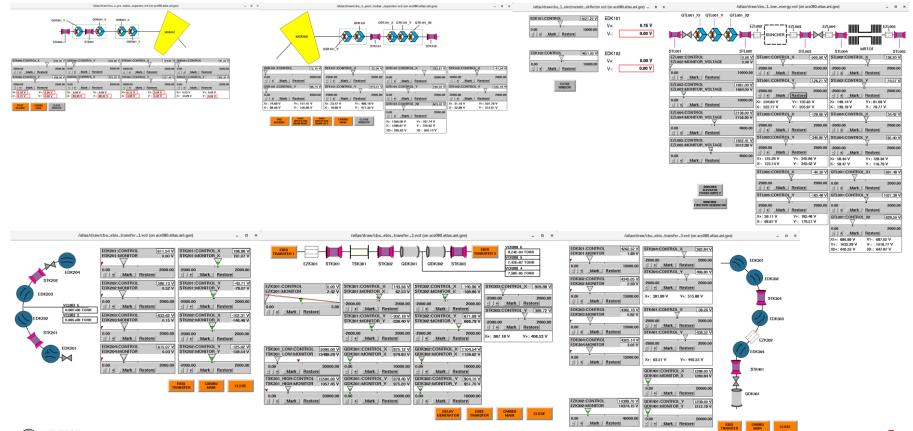


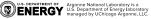
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### **CARIBU CONTROLS FOR THIS TEST**

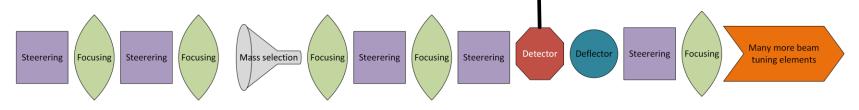
#### 60+ control parameters to transport beam from start to finish





# CARIBU CONTROLS – SIMPLIFIED VIEW

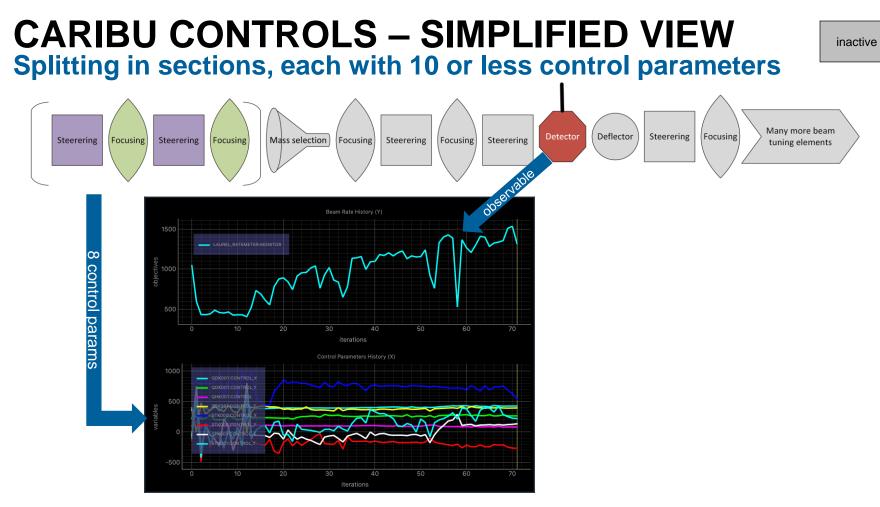
60+ control parameters to transport beam from start to finish

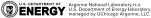




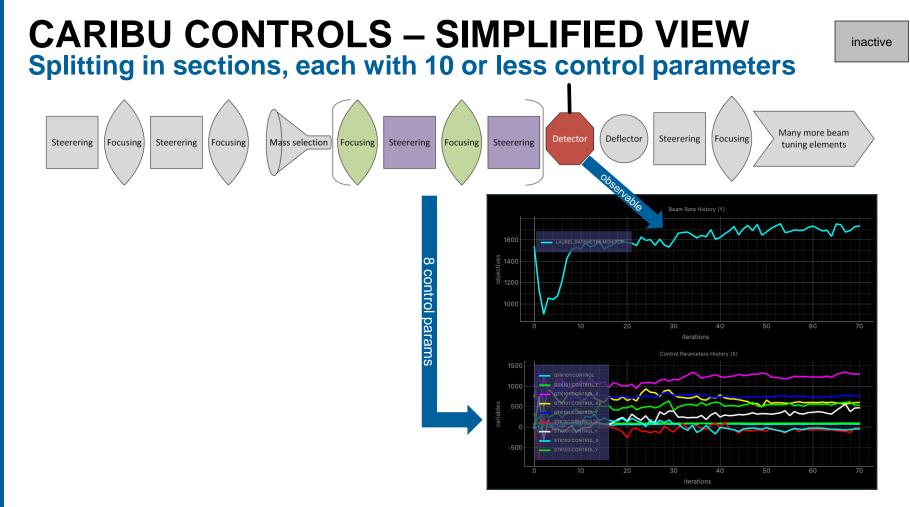


inactive













# CARIBU-MATIC TEST RESULTS (NOT A SIMULATION)

#### Serial optimization of 60+ elements to transport radioactive beam

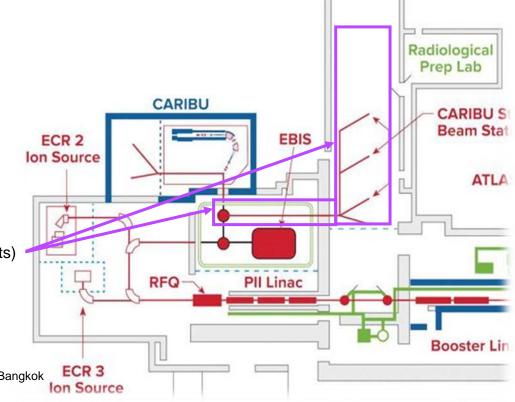
- Transport efficiency
  - 40% from first detector to last detector
  - On par with typical hand tune
- Optimization time
  - About 10-15 minutes per section
  - Comparable to hand tune approach

#### **Next steps**

- Refine code
- Extend to **target stations** (100+ different elements)
- Automate multi-section optimization

#### Badger web sites and reference

https://slac-ml.github.io/Badger/ https://github.com/SLAC-ML/Badger Zhang, Z., et al. "Badger: The missing optimizer in ACR", Proc. IPAC'22, Bangkok







### THANK YOU



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## MANY THANKS TO

□ Students & Postdocs:

Jose Martinez, Adwaith Ravichandran and Sergio Lopez – Postdocs Anthony Tran (MSU) and Onur Gilanliogullari (IIT) – Students

□ ATLAS Controls Group:

Daniel Stanton, Kenneth Bunnell and David Novak

□ ATLAS Operations Group:

Ben Blomberg, Eric Letcher, Gavin Dunn, Henry Brito and Raul Patino





### **BACK-UP SLIDES**



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## **ORIGINAL PROJECT -PROGRESS & HIGHLIGHTS**



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## **SUMMARY OF PROGRESS & HIGHLIGHTS**

Automated data collection and two-way communication established

- Bayesian Optimization (BO) successfully used for online beam tuning
- □ Multi-Objective BO (MOBO) to optimize transmission and beam size
- □ AI-ML supporting the commissioning of a new beamline (AMIS)
- □ Transfer learning from one ion beam to another (BO)
- □ Transfer learning from simulation to online model (BO with DKL)

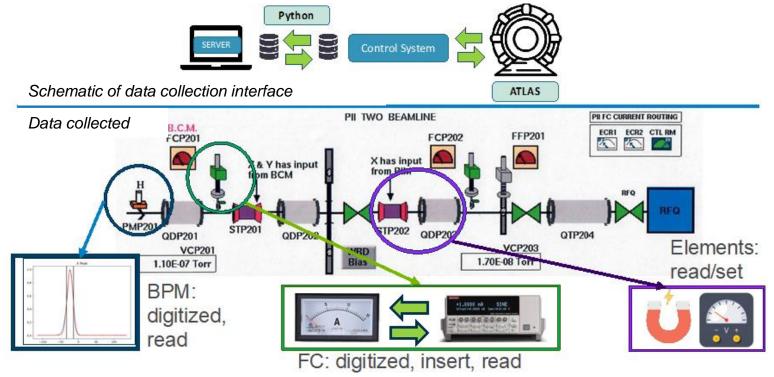
Reinforcement Learning (RL) for online beam tuning – Exp. Success

Good progress on the virtual machine model / physics model



# **AUTOMATED DATA COLLECTION - ESTABLISHED**

- ✓ Beam currents and beam profiles digitized
- $\checkmark$  A python interface developed to collect the data automatically

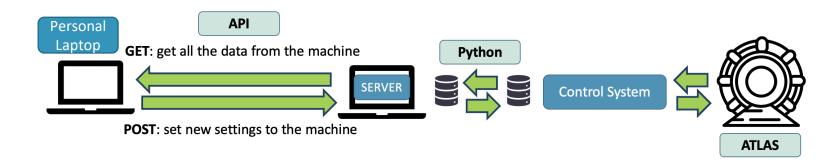




Now working on reducing acquisition time ...



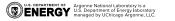
# **ONLINE – INTERFACE WITH CONTROL SYSTEM**



## **OFFLINE – INTERFACE WITH BEAM SIMULATION**

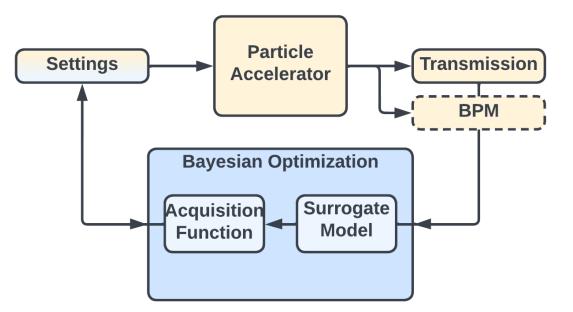
- ✓ Python wrapper for TRACK (Simulation Code)
- $\checkmark$  Generation of simulation data
- ✓ Different conditions and inputs
- ✓ Integration with AI/ML modeling







### **BAYESIAN OPTIMIZATION – A BRIEF DESCRIPTION**



- <u>Surrogate Model</u>: A probabilistic model approximating the objective function [Gaussian Process with Radial Basis Function (RBF) Kernel and Gaussian likelihood]
- ✓ <u>Acquisition Function</u> tells the model where to query the system next for more likely improvement
- Bayesian Optimization with Gaussian Processes guides the model and gives a reliable estimate of uncertainty



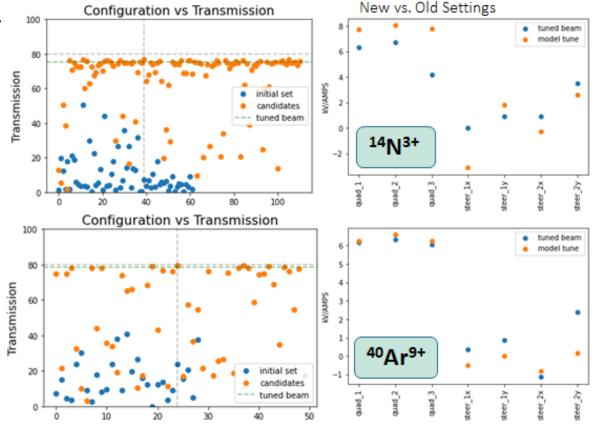
## **BAYESIAN OPTIMIZATION USED IN ONLINE TUNING**

### Beamline under study



- o 7 variable parameters
   (3 quadrupoles + 2x2 steerers)
- Optimization of beam transmission
- Case of <sup>14</sup>N<sup>3+</sup>: 29 historical +
   33 random tunes

Case of <sup>40</sup>Ar<sup>9+</sup> : 29 historical tunes

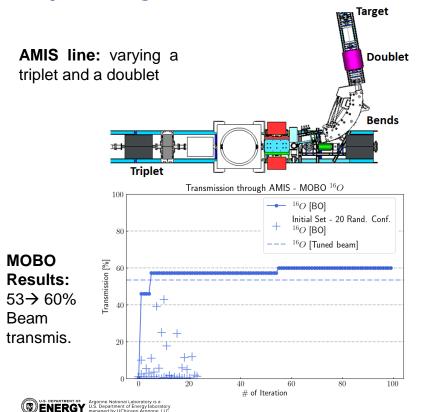


# **MULTI-OBJECTIVE BAYESIAN OPTIMIZATION**

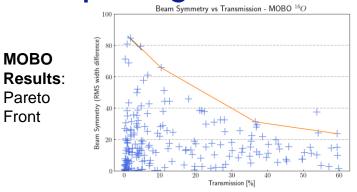
Multi-Objective Problem: Optimize transmission and beam profiles on target - Not easy for an operator!

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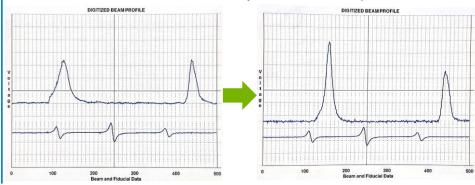
Improving Beam Transmission



### **Improving Beam Profiles**



MOBO Results: More symmetric beam profiles

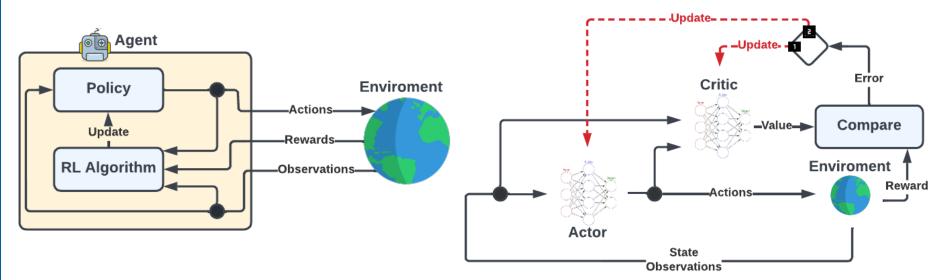




# **REINFORCEMENT LEARNING – A BRIEF DESCRIPTION**

### **Basic Concept**

### Implementation Example

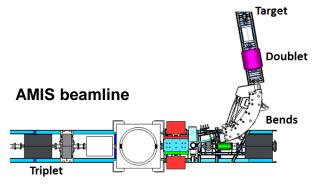


- ✓ **Essence:** Learning from experience based on interaction with the environment
- ✓ Action: Varies the parameters/variables of the problem
- ✓ Reward: Measures the goal function to maximize/optimize
- ✓ Policy: How the process evolves/learns
- ✓ Algorithm used: Deep Deterministic Policy Gradient (DDPG); Actor-Critic Approach



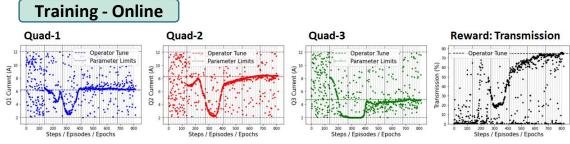
# **REINFORCEMENT LEARNING: FIRST EXP. SUCCESS**

### Beamline under study



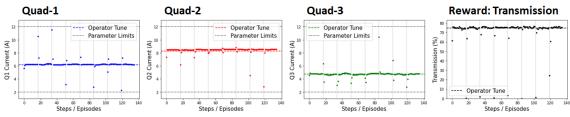
**Objective**: Maximize beam transmission

- Varying 3 magnetic quads
- Current limits: 2 12 Amps
- Max. Action: Full range



Training done in 816 total steps/evaluations (48 episodes)

### **Testing - Online**



- Testing done for 8 episodes (16 steps/episode)
- Model converges in 2-3 steps, starting from random config.

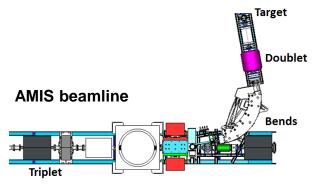
➢ RL is much slower than BO, requiring significantly more data → more iterations to train, but once trained, it takes fewer steps to converge to the best solution …



# **REINFORCEMENT LEARNING: MORE PARAMETERS**

Ouad-2

### Beamline under study



#### **Training: Quad-1** Operator Tune Operator Tune ---- Operator Tune Parameter Limits Steps / Episodes / Epochs Steps / Episodes / Epochs

Ouad-3

**Training - Online** 

Ouad-4

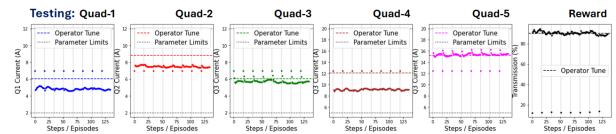
Ouad-5

Reward

### Training done in 816 total steps/evaluations (48 episodes)

### **Objective**: Maximize beam transmission

- Varying 5 magnetic quads
- Triplet 2–12 A, Doublet 5-15 A
- Max. Action: Full range

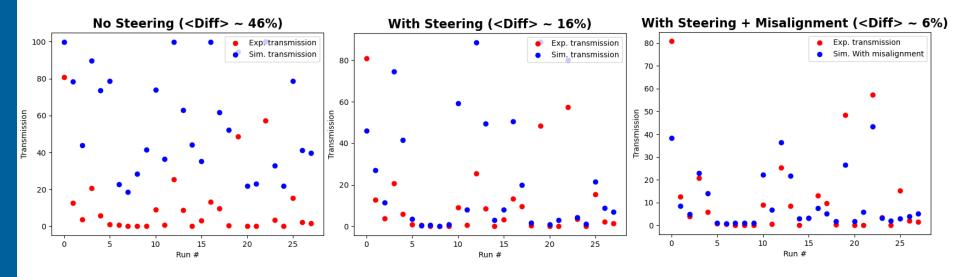


**Testing - Online** 

- Testing done for 8 episodes (16 steps/episode)
- Model converges in 2-3 steps, starting from same config.



# **PROGRESS ON THE VIRTUAL MACHINE MODEL**



- In order to develop a realistic virtual machine model, we need first to improve the predictability of the physics model based on beam dynamics simulations (using TRACK code)
- ✓ Significant improvement was realized by adding steering effects, using steerers settings
- ✓ Further improvement achieved by adding misalignment effects, obtained using BO inference
- ✓ Adding information about the initial beam distribution should close the gap even further
- ✓ Once the agreement is ~ 1%, a surrogate model will be developed based on the simulations



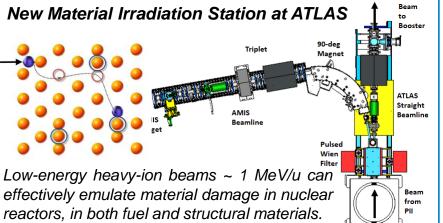
# **MORE SLIDES**



**ENERGY** Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

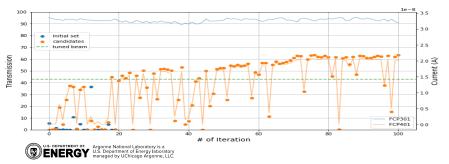


# **AI/ML SUPPORTING AMIS LINE COMMISSIONING**



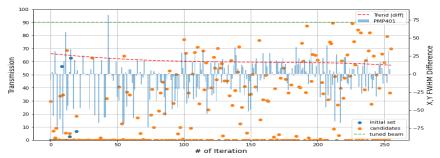
### **Improving Beam Transmission**

**Problem**: Maximize beam transmission by varying a triplet, two dipoles and two steerers [BO]; **Results**:  $40 \rightarrow 70\%$ 

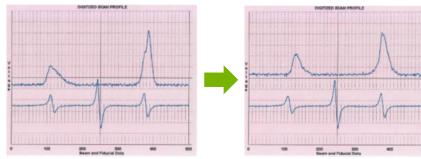


### **Improving Beam Profiles**

**Problem**: Produce symmetric beam profiles by varying a triplet and a steerer [BO]



Training online, slow convergence but steady progress. Competition between nice profiles and beam transmission!

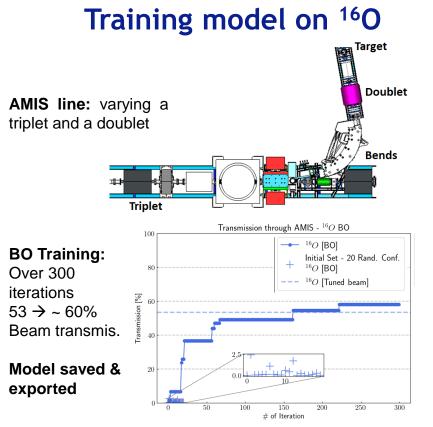


### Very encouraging first results!

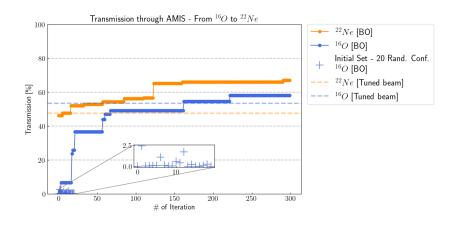


# TRANSFER LEARNING FROM <sup>16</sup>O TO <sup>22</sup>NE - BO

**Goal**: Train a model using one beam then transfer it to tune another beam  $\rightarrow$  Faster switching and tuning



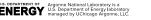
### Applying same model to <sup>22</sup>Ne



**160 Model loaded for 22Ne**: Initial transmission improved in 7 iterations:  $48 \rightarrow 55 \%$ 

With more training for 22Ne:  $48 \rightarrow 67\%$ 

Scaling was applied from 16O to 22Ne, re-tuning is often needed because of different initial beam distributions

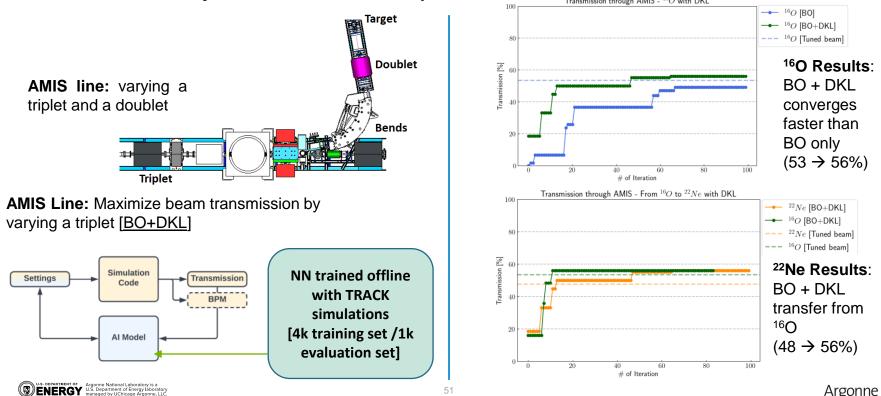




# TRANSFER LEARNING FROM SIMULATION TO ONLINE

**Goal**: Train a model using simulations then use it for online tuning  $\rightarrow$  Less training & faster convergence online

Method: Deep kernel learning (DKL) to combine the representational power of neural networks with the reliable uncertainty estimates of Gaussian processes. Transmission through AMIS - <sup>16</sup>O with DKL



# **REINFORCEMENT LEARNING: FIRST ATTEMPT...**

### Simulation Case

- Focusing the beam through an aperture using an electrostatic triplet (3 Quadrupoles)
- ✓ Voltage limites: E- Triplet
   2 10 kV
  - Max. action:



+/- 0.25 kV

### Actual Experiment

Doublet-1 Doublet-2

- Maximizing beam transmission using 2 doublets (4 quads) and 2x2 steerers
- ✓ Electrostatic Quadrupoles :
  - 2 kV to 10 kV
  - Max action +/- 0.25 kV
- ✓ Steering Magnets:
  - -1 A to 1 A
  - Max action +/- 0.25 A

