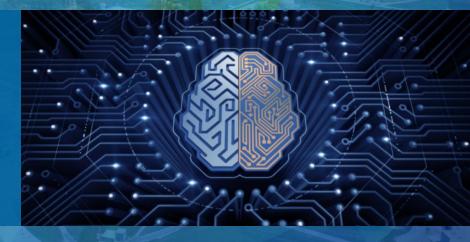
2025 DOE/NP ARTIFICIAL INTELLIGENCE/MACHINE LEARNING PRINCIPAL INVESTIGATOR EXCHANGE MEETING VIRTUAL, VIA ZOOM, NOVEMBER 19-20, 2025

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



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OTHER CONTRIBUTORS

Adwaith Ravichandran, Postdoc Sergio Lopez-Caceres, Postdoc Anthony Tran, Student





OUTLINE

☐ The ATLAS AI-ML Project (Phase II) – Overview & Status

☐ Progress on the ATLAS Sub-project

☐ Progress on the RAISOR Sub-project

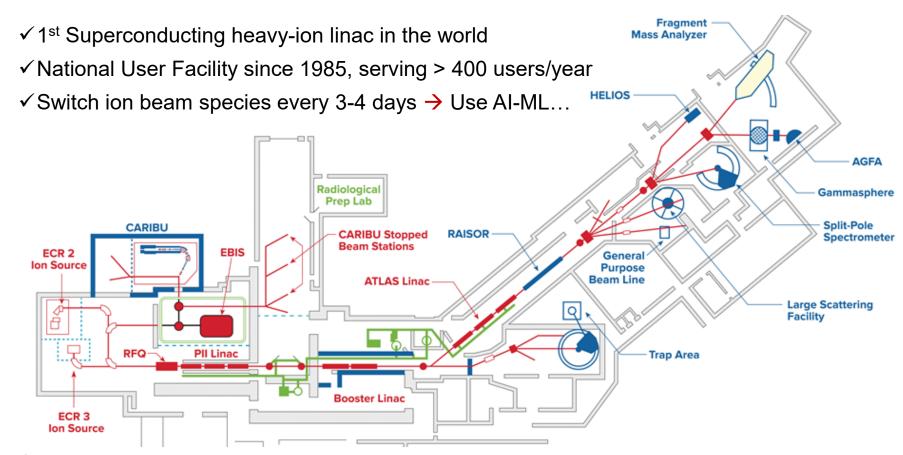
☐ Progress on the CARIBU Sub-project

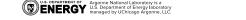
☐ Summary & Future Work





ATLAS: ARGONNE TANDEM LINEAR ACCELERATOR SYSTEM





ATLAS AI-ML PROJECT – PHASE II (2023 FOA)

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

- Consolidated Three subprojects
 - ATLAS Sub-project: Stable beams in main Linac Brahim Mustapha
 - RAISOR Sub-project: Inflight radioactive beams Calem Hoffman
 - CARIBU Sub-project: Reaccelerated radioactive beams 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 SUB-PROJECT: ONLINE DEPLOYMENT...

- ☐ 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...

- □ New AI-ML Tools Development / Longitudinal Tuning
 - Bunching optimization
 - Automated energy change
- ☐ The ATLAS AI-ML Interface / Dashboard
 - Example Online Applications
 - Operators Experience
- ☐ The Virtual Accelerator (VA) Model
 - Development & Fine-Tuning of VA Model
 - Example VA Applications using same AI-ML Interface
- ☐ Summary & Future work



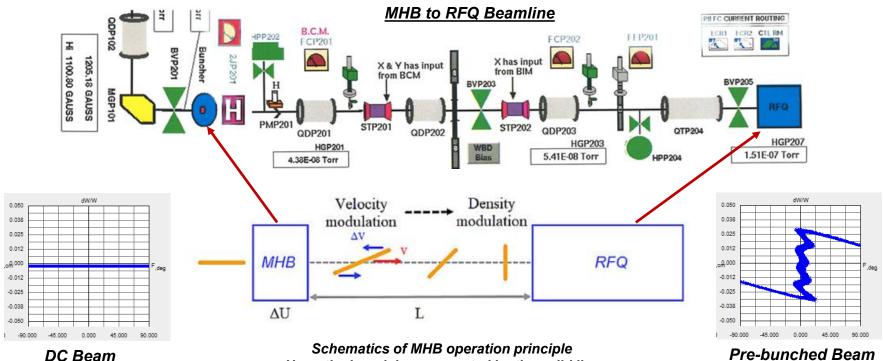








BEAM PRE/BUNCHING – MULTI-HARMONIC BUNCHER

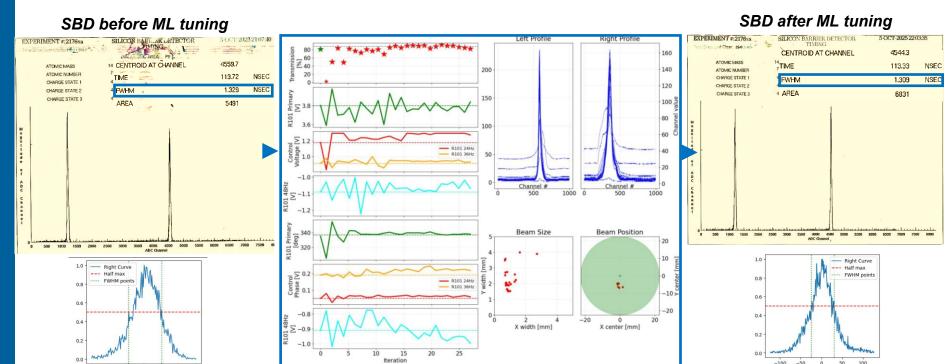


Schematics of MHB operation principle Here, the bunch is represented by the solid line, v: beam velocity, Δv : velocity change of end particles due to applied voltage ΔU , L: distance between MHB and RFQ [1]

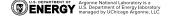


DC Beam

BUNCH WIDTH OPTIMIZATION - FROM OPERATOR TUNE

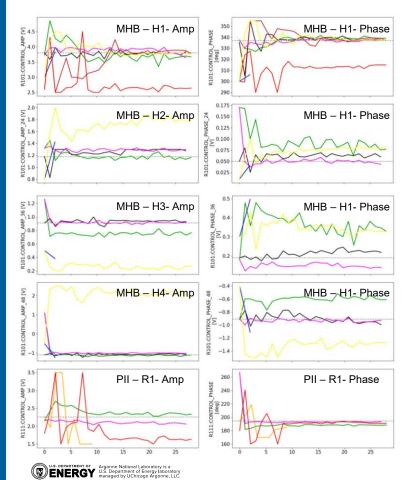


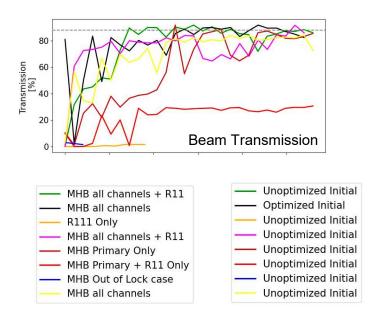
- ☐ Operator tuned values of MHB channels used as starting point to see if bunch width can be improved
- ☐ Control channel window limit made narrow relative to initial values
- ☐ After ML tuning, bunch width [FWHM] slightly reduced, but more importantly tuning from scratch...





BUNCH WIDTH OPTIMIZATION – MORE CASES

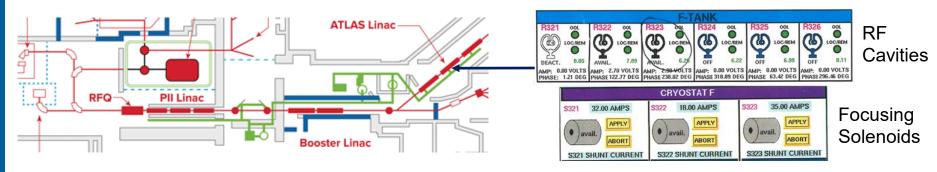




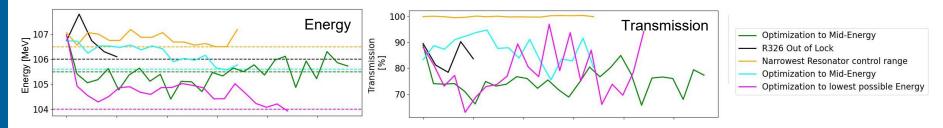
- ☐ Plots shows ML model changing the MHB settings (4 harmonics) to optimize for transmission, used as indirect observable
- ☐ Most cases converge in ~ 15 iterations; different paths show possibility of multiple optima in solution space
- ☐ Dotted lines indicate operator tuned values



RAPID ENERGY CHANGE & BEAMLINE RETUNING



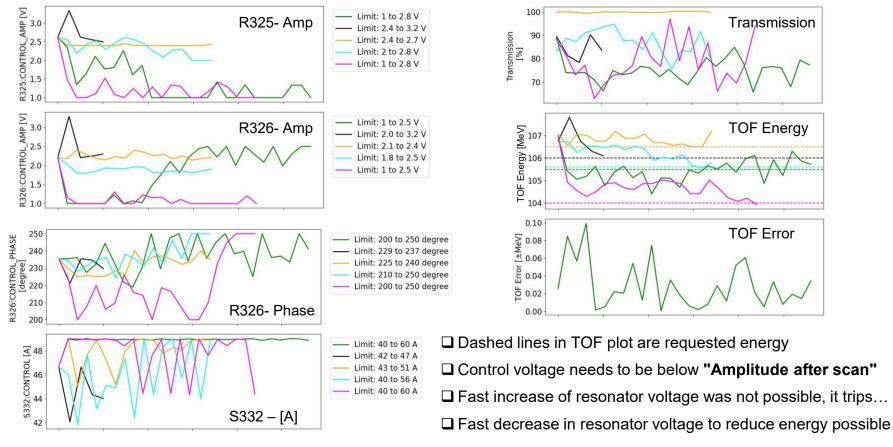
- ☐ Some experiment requires different beam energies; energy change & retuning can time consuming
- ☐ Energy change requires adjusting RF resonators voltages and phases, and retuning of transport line
- ☐ Example shows the F Cryostat of the last section of ATLAS housing 6 RF cavities and 3 solenoids
- ☐ Here, only the last two cavities were adjusted, along with the last solenoid for focusing & transmission
- ☐ Initial energy tuned for **106.74 MeV**, Resonators R325+R326 energy window: **2 MeV/resonator**







ENERGY CHANGE & RETUNING OPTIMIZATION





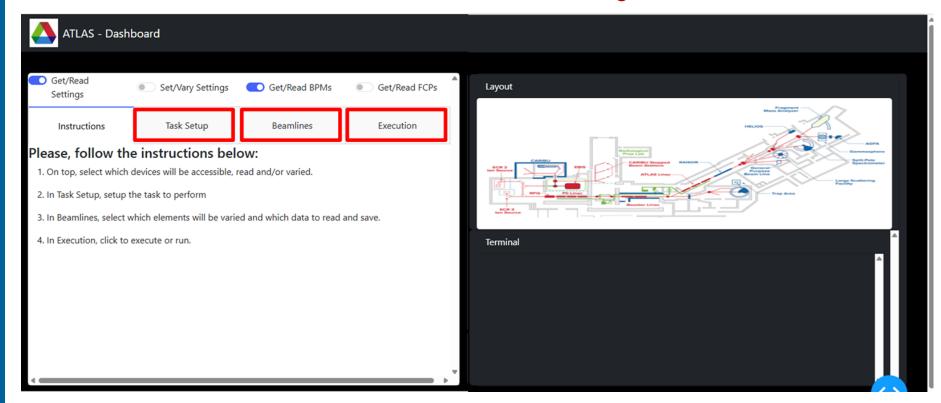






ONLINE AI-ML INTERFACE – LANDING PAGE

A browser-based interface that uses API through an URL address...

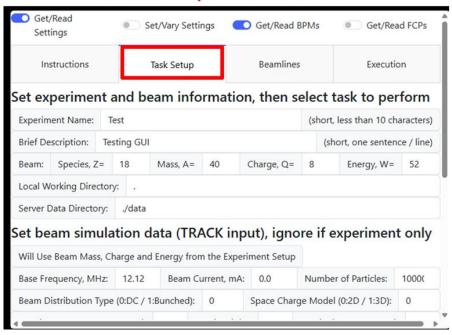




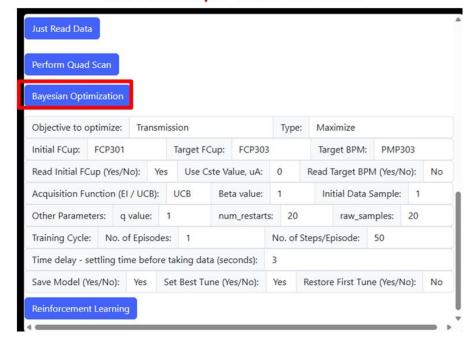


ONLINE AI-ML INTERFACE - TASK SETUP

Task Setup: Beam Infos



Task Setup: Task Choice

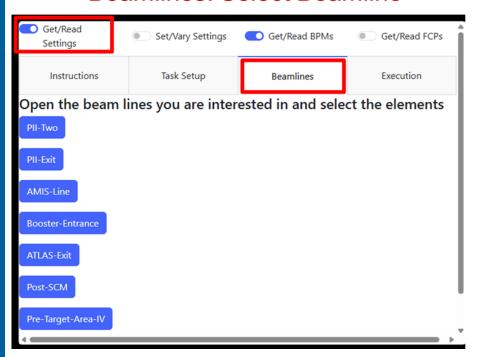




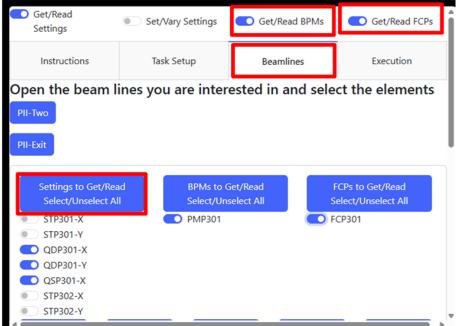


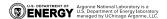
ONLINE AI-ML INTERFACE – BEAMLINE SETUP

Beamlines: Select Beamline



Beamlines: Data to Get/Collect

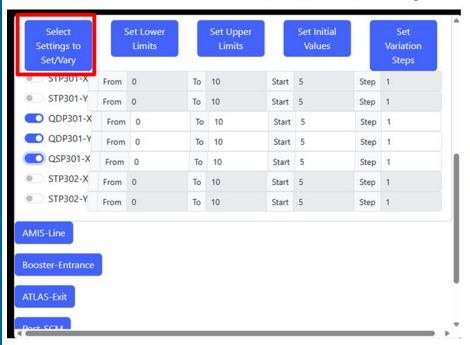




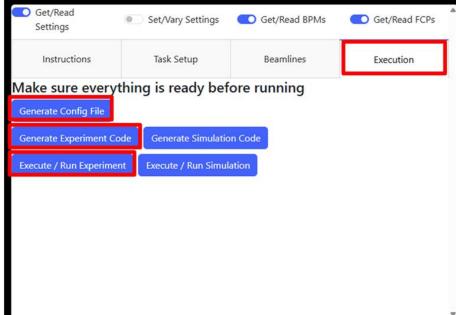


ONLINE AI-ML INTERFACE - PARAMETERS / RUN

Beamlines: Parameters to Set/Vary



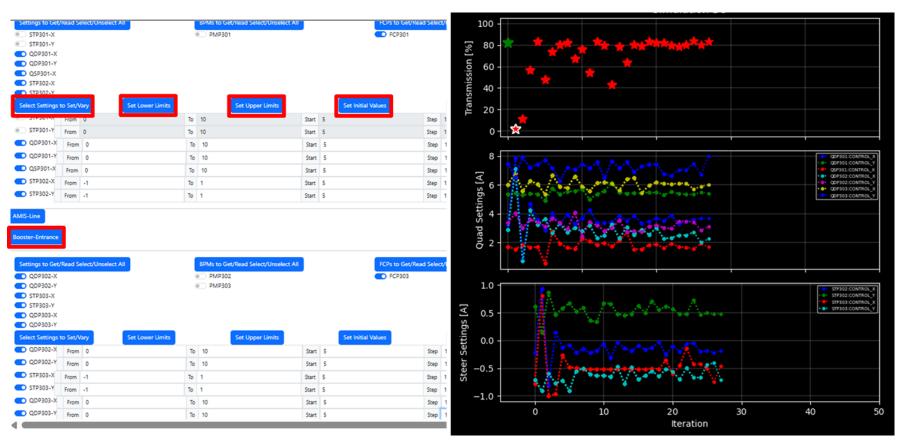
Execution: Experiment or Simulation

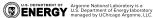






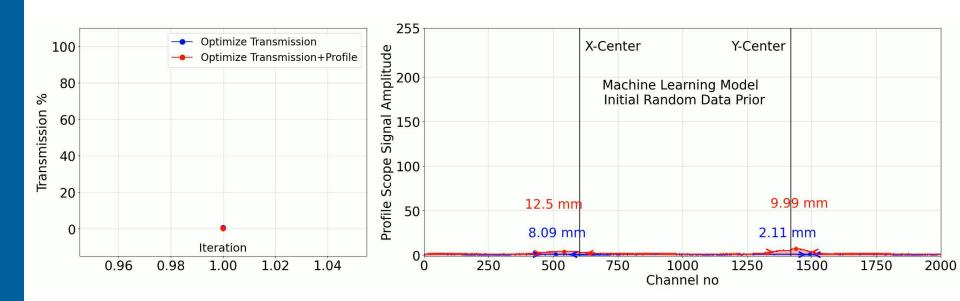
ONLINE TEST – OPTIMIZING BEAM TRANSMISSION







OPTIMIZING BOTH BEAM TRANSMISSION & PROFILE



Issue: Optimization based on beam transmission only is not sufficient. An optimum may be found for one section, but the beam is not well matched / not optimum for the next section...

Solution: Adding more observables to the objective function, in our case, beam profiles





OPERATORS EXPERIENCE - TIMING & PERFORMANCE

Beamline	Objective	Prior Data	Elements / Parameters	Model Transmission Change	Operator Transmission Reference	Model tune time	Operator tune time
PII – Booster	Beam Transmission	Random	7 Quads + 2 steerers / 11	0 to ~85%	~90%	9 min	~5 min
PII – Booster	Beam Transmission	Experimental	7 Quads + 2 steerers / 11	0 to ~85%	~90%	1.5 min	<mark>∼5 min</mark>
AMIS	Beam Transmission	Random	3 Quads + 1 steerer / 5	0 to ~80%	~90%	4 min	∼15 min
ATLAS Exit – PT	Beam Transmission	Random	6 Quads + 2 steerers / 10	0 to ~70%	~80%	6.5 min	~5 min
ATLAS Exit – PT	Beam Transmission	Random	6 Quads + 4 steerers / 14	0 to ~90%	~85%	15.5 min	~15 min
ATLAS Exit – PT	Beam Transmission	Optimized Initial	6 Quads + 2 steerer / 10	75 to ~90%	~85%	<mark>2 min</mark>	N/A
ATLAS Exit – GS	Beam Transmission	Random	6 Quads + 5 steerer / 16	0 to ~85%	~85%	22 min	~20 min
ATLAS Exit – GS	Transmission + Profile	Random	6 Quads + 5 steerer / 16	0 to ~80%	~85%	19 min	<mark>∼20 min</mark>
ATLAS Exit – GS	Transmission + Profile	Optimized Initial	6 Quads + 5 steerer / 16	56 to ~90%	~85%	16 min	N/A

- ☐ **Timing:** Table shows tuning time using ML model (BO) compared to approximate manual operator tuning
- ☐ **Performance**: Table shows higher beam transmission achievable compared to manual tuning values
- ☐ Using prior experiment data significantly reduces tuning time by ~75% relative to manual tune [PII-Booster line]
- □ Optimizing profile width along with beam transmission reduces total tune time by ~25% [ATLAS EXIT-GAMMA SPHERE line]





AI-ML TOOLS SUMMARY - EVALUATION & BENEFITS

- ☐ 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 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.









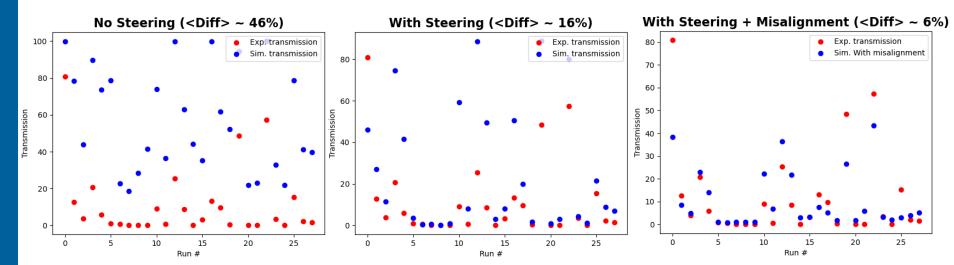
VIRTUAL ACCELERATOR - DESIRED CAPABILITIES

- ☐ Mimics the machine as much as possible, with the same online experience in terms of control, beam diagnostics and optimizable observables...
- ☐ Allows both Offline and Online Use:
 - Prepare tunes for future experiments or new operating modes
 - Train ML models offline, such as RL-based models that can be very time consuming to be trained online
 - Train operators on AI-ML tools offline before using them online
 - Run optimizations on the virtual accelerator, then set the optimum operating point to the machine online
- ☐ However, the most important feature is that the virtual accelerator reproduces and predicts the machine behavior very well, to a few % level, 1% if possible ...





VIRTUAL MODEL - IMPROVING PREDICTIVE POWER

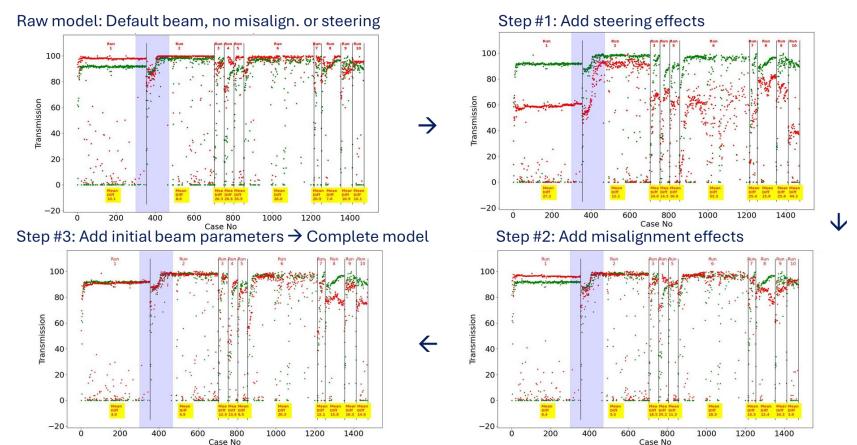


To develop a realistic virtual accelerator model with high predictive power, we need:

- Start with an existing physics model, full beam dynamics simulations if possible
- Use realistic models for all beamline elements, 3D models if possible
- Use the right calibrations and conversion factors (B vs. I for example)
- Include misalignment and steering effects, use recent surveys or infer from the data
- Use realistic initial beam distribution / parameters, measure if possible or infer from the data
- Once the agreement is ~ 1%, a surrogate model may be developed based on the simulations



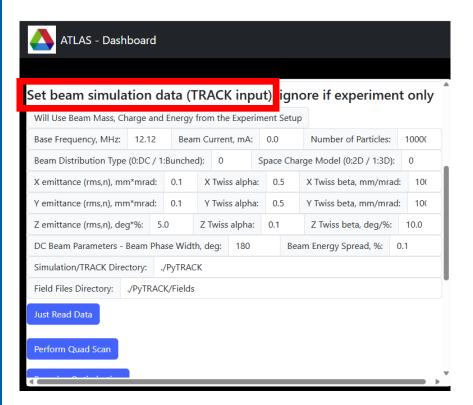
VIRTUAL MODEL TUNING – IMPROVED RESULTS

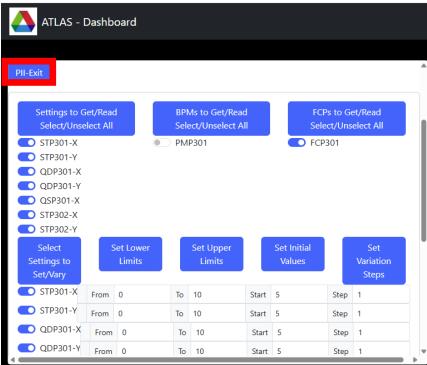






VIRTUAL ACCELERATOR – OFFLINE TEST EXAMPLE...

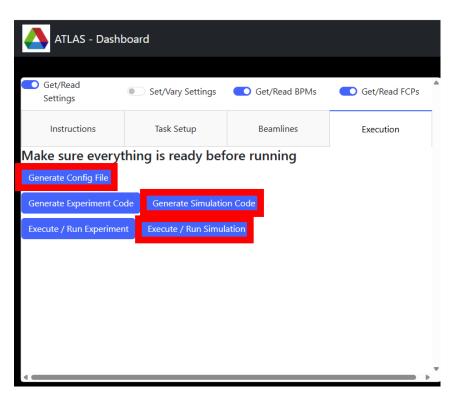


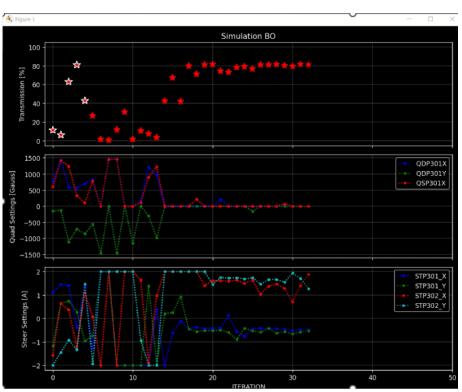


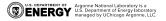




VIRTUAL ACCELERATOR – OFFLINE TEST EXAMPLE

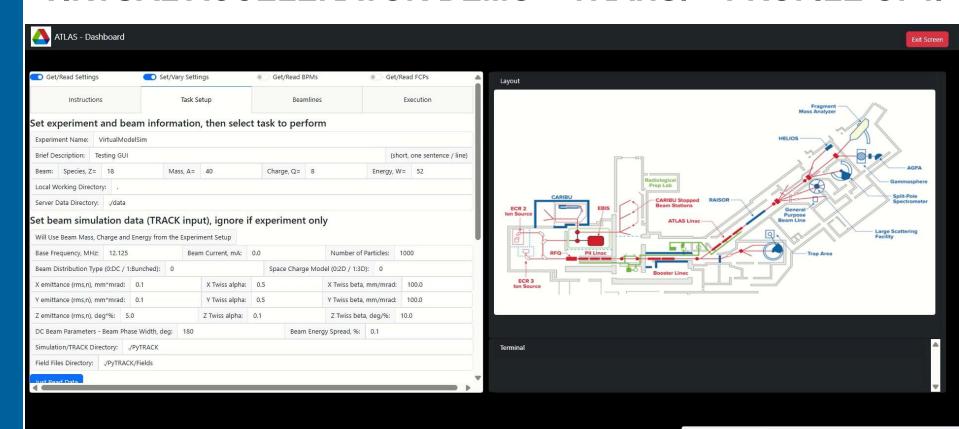








VIRTUAL ACCELERATOR DEMO – TRANS. + PROFILE OPT.







△ Errors ¾ Callbacks v3.0.4 Dash update available - v3.2.0 Server ② (>>)

VIRTUAL ACCELERATOR – SUMMARY

- ☐ Developed a virtual accelerator model based on beam simulations using the TRACK code
- ☐ The model predictability was significantly improved through fine-tuning by adding misalignment and steering effects as well as initial beam parameters inferred from data
- ☐ For example, difference in beam transmission between experiment and simulation reduced
 - from ~46% down to ~16% after adding steering effects,
 - o down to ~6% after including misalignments, and
 - down to ~2% after including initial beam parameters
- ☐ Using the described model tuning procedure, a highly accurate virtual accelerator is now at the core the ATLAS AI-ML Dashboard interface
- ☐ Ongoing & Future work
 - Developing a surrogate to the full simulation model for speed
 - Deploying the virtual model online to support operations & offline for testing / training
 - Developing models for other sections of the linac





SUMMARY & FUTURE WORK

- ☐ Recently developed tools and capabilities tested for longitudinal beam tuning, will enable future end-to-end tuning of complete beamlines both transverse and longitudinal
- ☐ The ATLAS AI-ML Dashboard Interface is fully developed and currently being used for online beam tuning and optimization by expert operators, working on full deployment...
- □ Developed a virtual accelerator model based on beam simulations using the TRACK code.

 Using fine-tuning procedure, a highly accurate virtual model (Error < 2%) is now at the core of the same Al-ML Interface, model already being used for offline experimental preparations
- □ Added features like combined objective optimization improves performance while using prior experimental data significantly reduces tuning time relative to manual tuning, by ~70%
- ➤ Working on "successive sectional tuning" from the ion source through the low-energy beam transport (LEBT), MHB, RFQ to the first accelerating section (PII) [first in virtual model, online]
- > Develop a neural network surrogate model to the TRACK simulation model for speed
- ➤ Deploy the virtual accelerator online with bidirectional data flow Virtual ↔ Physical







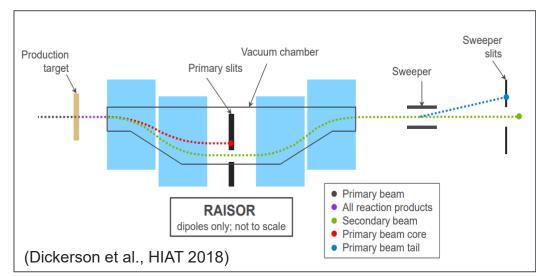


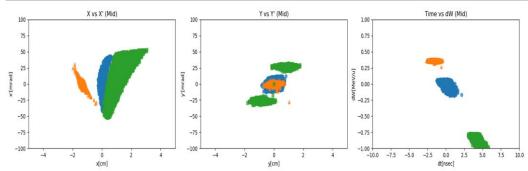


THE RAISOR INFLIGHT SEPARATOR AT ATLAS

32S Primary Core

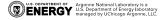
- Primary Goal: Separate secondary radioactive beams produced from the interaction of a primary beam with a target.
- Separation Technique: Magnetic separation (momentum and charge, Bρ), followed by time-offlight separation (RF Sweeper)
- Configuration: Magnetic Chicane made of 4 Dipole Magnets (separation based on rigidity) and 4 Quadrupole Magnets (focus the beam and provide momentum separation resolution)





33Cl Secondary beam

32S Primary Tail



MOTIVATION FOR RAISOR VIRTUAL MODEL

A RAISOR Virtual Model would allow:

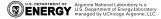
Preparation for Experiments – *Predictive tuning for beam purity and separation efficiency, Virtual testing before online experiments*

Reduction of Trial-Error, Risk and Time – Better define the operating parameter space to minimize risk and reduce online tuning time

Foundation for Automation – Develop and test AI-ML techniques offline using the same online experience via the same interface

Reproducing experimental data, different from stable beam:

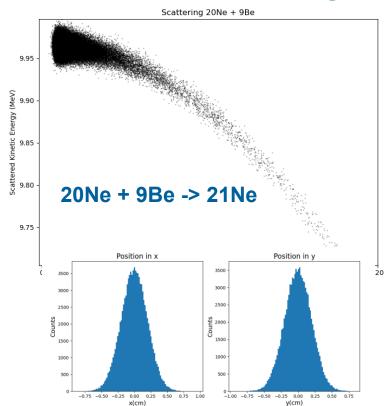
- Simulate the nuclear reaction and secondary beam production
- Multiple beams are produced, simulate and track multiple beams, including different charge states for each specie
- Identify and separate the beam of interest



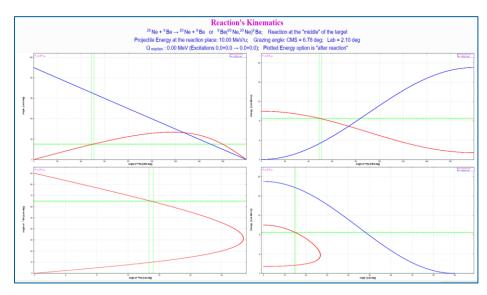


GENERATING PHASE SPACE FOR MULTIPLE BEAMS

Rutherford Scattering



Nuclear Reaction Models / MC

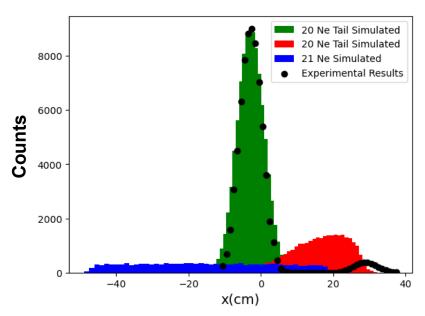


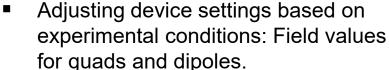
- Nuclear reaction models or user cross-sections based on previous data
- Primary beam parameters (position, size, angular & energy spread)
- Monte Carlo simulations, i.e. LISE++



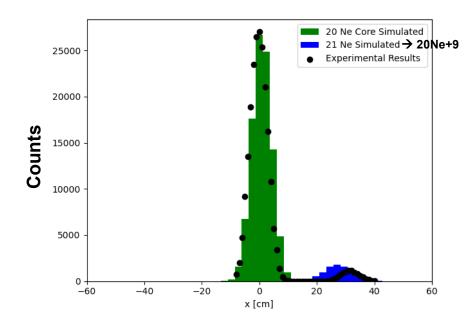


MATCHING MODEL TO EXPERIMENTAL RESULTS





Extra peak, a different contaminant?



- Identifying the contaminant: 20Ne+9
- Other charge states are relevant
- Good overall match between simulation and experimental results.
- Complete virtual model, offline RAISOR testing followed by online experimental tuning







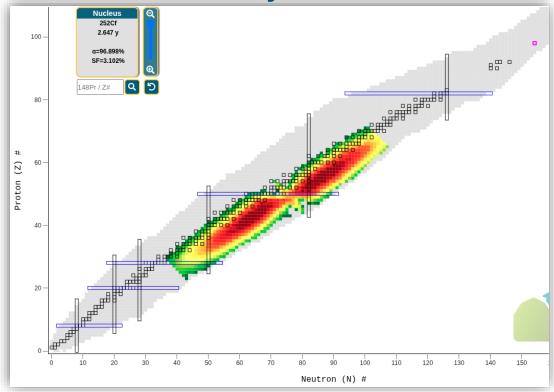




WHAT IS CARIBU/nuCARIBU?

A radioactive ion source part of the ATLAS facility

- CARIBU = CAlifornium Rare Isotope Breeder Upgrade
- CARIBU ended Aug/2024
- CARIBU provided beams of heavy ions made from fission fragments of ²⁵²Cf (10² – 10⁴ pps)



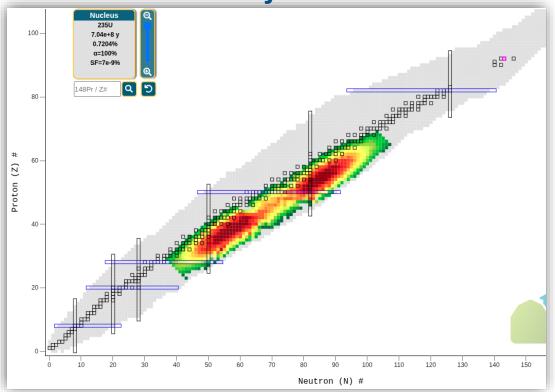




WHAT IS CARIBU/nuCARIBU?

A radioactive ion source part of the ATLAS facility

 nuCARIBU - a major upgrade in progress to increase the source intensities by using neutron-induced fission on ²³⁵U (and possibly other fissionable targets)



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

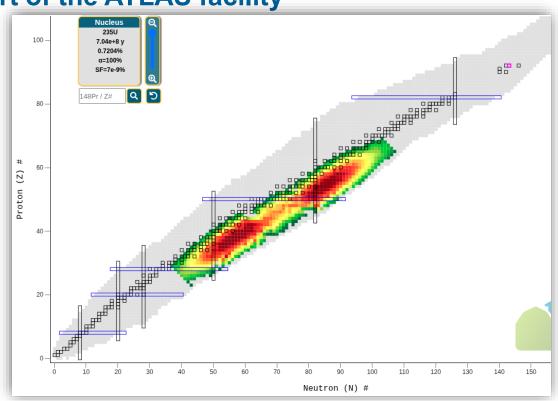




WHAT IS CARIBU/nuCARIBU?

A radioactive ion source part of the ATLAS facility

- **nuCARIBU** a major upgrade in progress to increase the source intensities by using neutron-induced fission on ²³⁵U (and possibly other fissionable targets)
- nuCARIBU
 - The nu (v) is for neutron
 - But there is no CAlifornium
 - An upgrade of an upgrade
- Essential for ATLAS multi-user upgrade (post-accel. beams, 3-10 MeV/u)



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





OUR HIGH-LEVEL GOALS

To increase nuCARIBU operational efficiency via automation



Automate radioactive beam extraction and transport from source to target station (user or charge breeder for reacceleration)



Publish results



Create documentation for ATLAS operations



nuCARIBU-MATIC ML TOOL DEPLOYED

Used online during nuCARIBU commissioning operations Jul/2025

Task

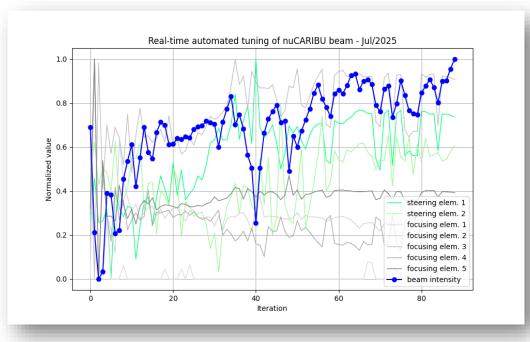
- Extract and transport radioactive beam (¹⁰⁰Zr) from source to charge breeder
- Perform online optimization of 100+ beam line elements divided in sections of 5-10 elements

Transport efficiency

- ~35% from source to charge breeder
- In some sections demonstrated significant improvements in transport efficiency compared to initial tune performed by human experts

Optimization time

- 5-10 minutes per section (21 sections)
- ~3 hours from source to charge breeder







PUBLICATION AND PRESENTATIONS

On nuCARIBU-matic sub-project

Conferences

2024 Fall Meeting of the APS Division of Nuclear Physics

October 6-10, 2024; Boston

Contributed - The CARIBU-matic project: automation for the transport of radioactive beams from the CARIBU source

https://meetings.aps.org/Meeting/DNP24/Session/F11.3

ICALEPCS 2025 - The 20th International Conference on Accelerator and Large Experimental Physics Control Systems

September 20-26, 2025; Chicago

Contributed - *Al-driven autonomous tuning of radioactive ion beams* https://indico.jacow.org/event/86/contributions/10115/

2025 Fall Meeting of the APS Division of Nuclear Physics

October 17-20, 2025; Chicago

Invited - Enhancing Radioactive Beam Transport at CARIBU through Aldriven Automation

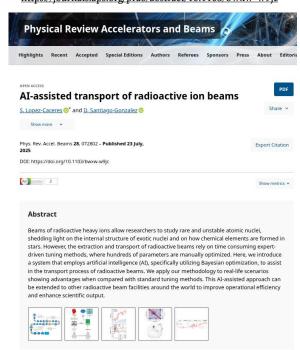
https://schedule.aps.org/dnp/2025/events/L05/1

Peer-reviewed article

AI-assisted transport of radioactive ion beams

Published Jul/2025

Physical Review Accelerators and Beams https://journals.aps.org/prab/abstract/10.1103/bwxw-w9ic



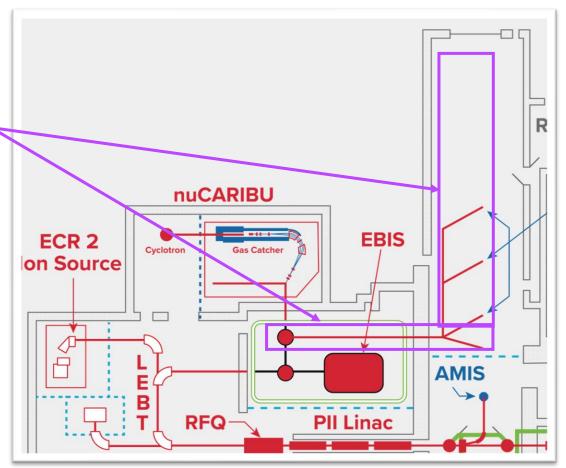




NEXT STEPS

On going efforts

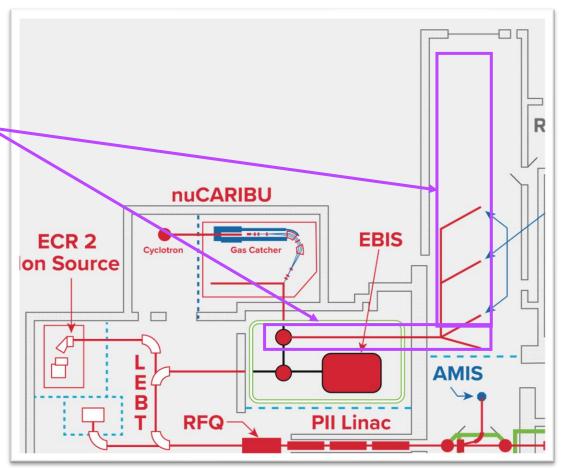
- Refine codes (possibly speed up opt)
- Extend to target stations (100+ different elements, about 200 in total)
- Create ML application documentation



NEXT STEPS

On going efforts

- Refine codes (possibly speed up opt)
- Extend to target stations (100+ different elements, about 200 in total)
- Create ML application documentation
- Automate multi-section optimization via LLM Agent (Sergio Lopez-Caceres)



nuCARIBU-MATIC PROJECT

Deliverables

Deploy ML application for online optimization of nuCARIBU beams

Publish results
3 conference presentations
1 journal paper

Pending deliverables

Expand ML application

Automate optimization of multiple beamline sections (Al agent)

Documentation for accelerator operations











THANKS TO

☐ Students & Postdocs:

Adwaith Ravichandran and Sergio Lopez – Postdocs

Anthony Tran (MSU) and Onur Gilanliogullari (IIT) – PhD Students

Dilan Arik (Minerva U.) – Undergrad. Student

☐ ATLAS Controls Group:

David Novak, Kenneth Bunnell and Daniel Stanton

☐ ATLAS Operations Group:

Ben Blomberg, Gavin Dunn, Henry Brito, Raul Patino and Brendon Zavala











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





ORIGINAL PROJECT - SUMMARY OF PROGRESS

- ☐ 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





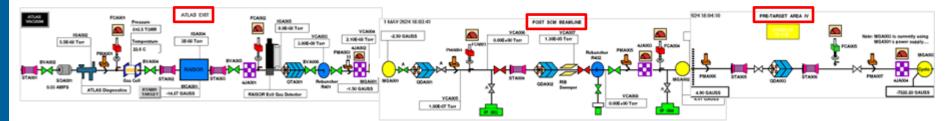
2024 PROGRESS & DEVELOPMENTS...

- ☐ 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
 - o Issues with tuning intermediate sections using only beam transmission
- ☐ Re-tuning the beamline after an energy change
 - A time-consuming process when done manually



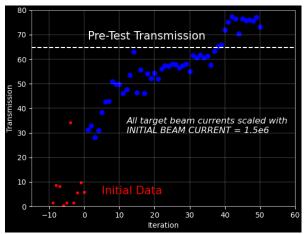


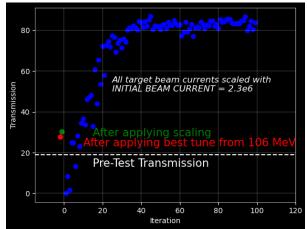
FAST BEAMLINE RETUNING AFTER ENERGY CHANGE

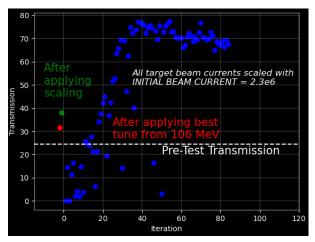


Problem: Switch to a lower energy, ¹⁶O 106 MeV → 71 MeV, retune for max. transmission **Method**: Load 106 MeV tune after energy change, scale to 71 MeV and re-optimize...

Iterations & Time: Best transmission ~ 85% in ~ 50 iterations x 8 sec ~ 7 min



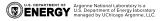




106 MeV [Initial Tune]

71 MeV [Retune 1]

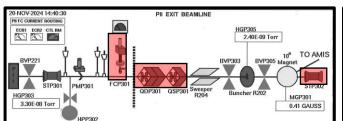
71 MeV [Retune 2]

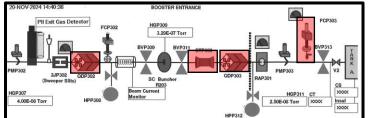


VIRTUAL MODEL TUNING – COLLECTING DATA

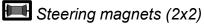
Data Collection: Could be existing data or specifically collected for this purpose

PII-BOOSTER BEAMLINE



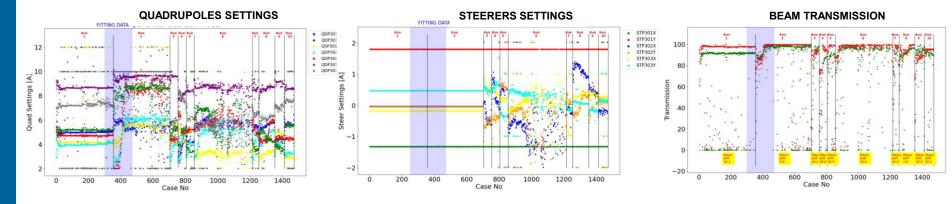


Quadrupoles (7 total)





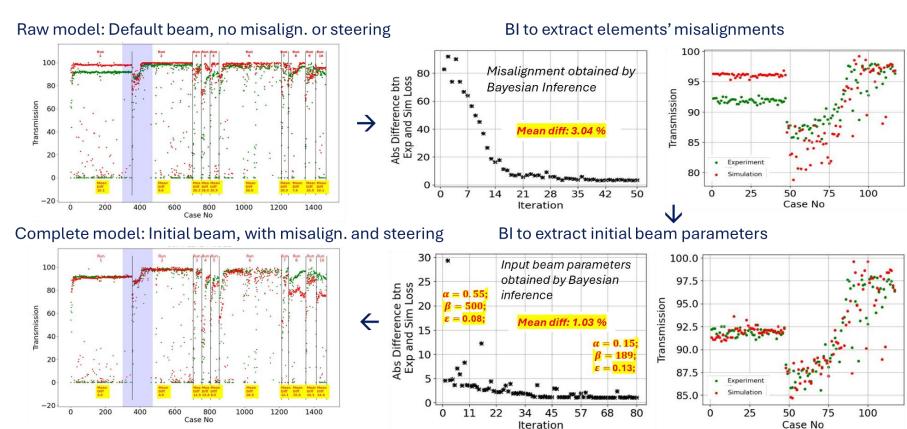
Faraday cups (3)







VIRTUAL MODEL TUNING – INFERRING MISSING INFO

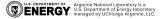






Automating parts of the nuCARIBU beam tuning process could:

- increase efficiency of facility operations (in this case rad. beams)
- set the stage for optimum delivery of nuCARIBU beams in the era of ATLAS multi-user operations
- increment the number of experiments and facility users per FY
- accelerate the pace of discovery





References

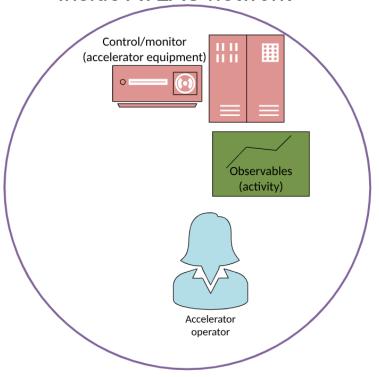
- [1] https://xopt-org.github.io/Badger/
- [2] Zhang, Z., et al. "Badger: The missing optimizer in ACR", Proc. IPAC'22, Bangkok

THE nuCARIBU-MATIC PROJECT

Our approach for secure radioactive beams tuning automation

Outside ATLAS network Python code devel: - Badger interface - Badger environment - AWACS get/post badger run Badger https://xopt-org.github.io/Badger/ nuCARIBU-matic developer

Inside ATLAS network





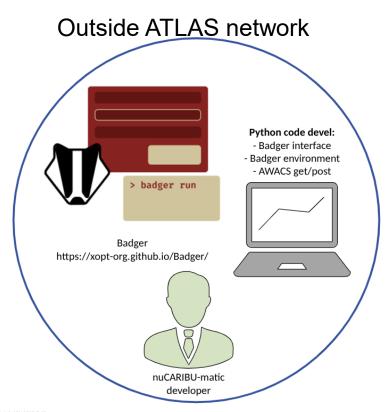


References

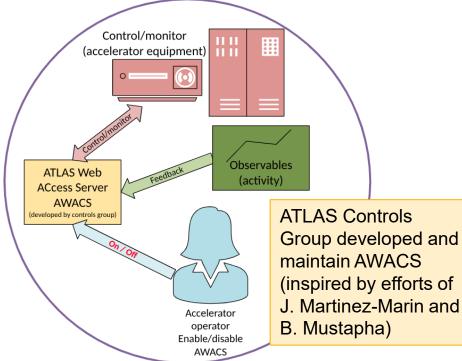
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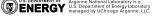
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Inside ATLAS network







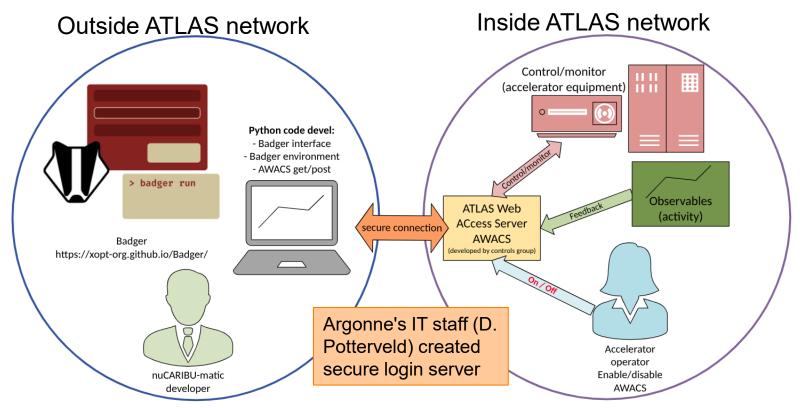
References

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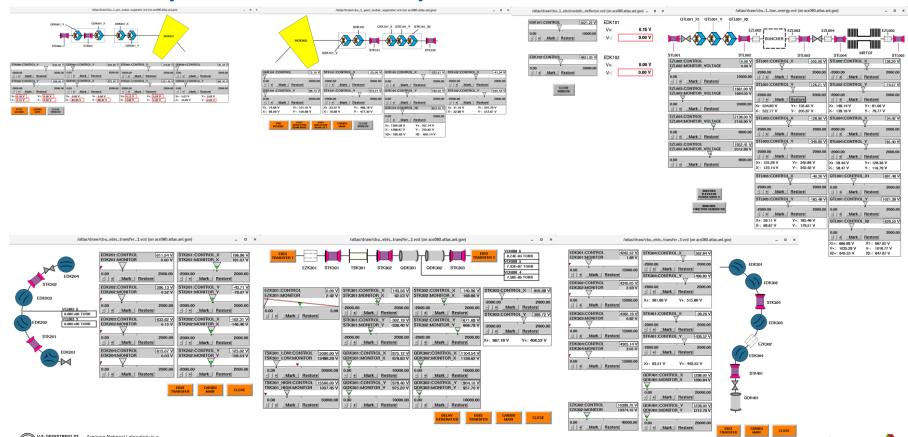


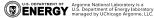




NUCARIBU CONTROLS

60+ control parameters to transport beam from start to finish

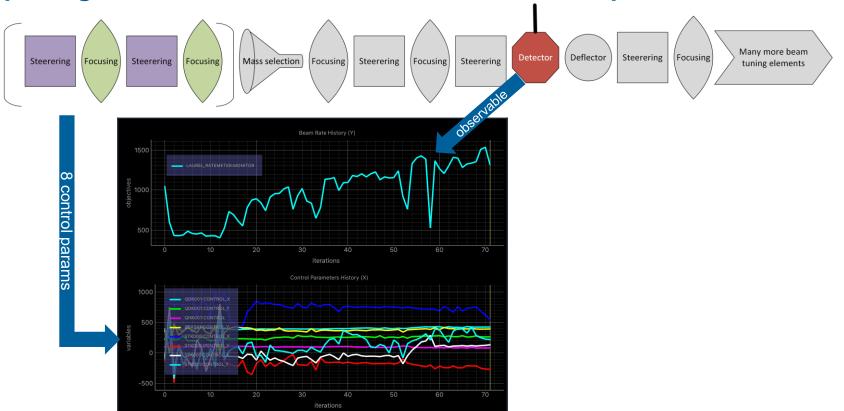


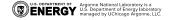


NUCARIBU CONTROLS – SIMPLIFIED VIEW

inactive

Splitting in sections, each with 10 or less control parameters



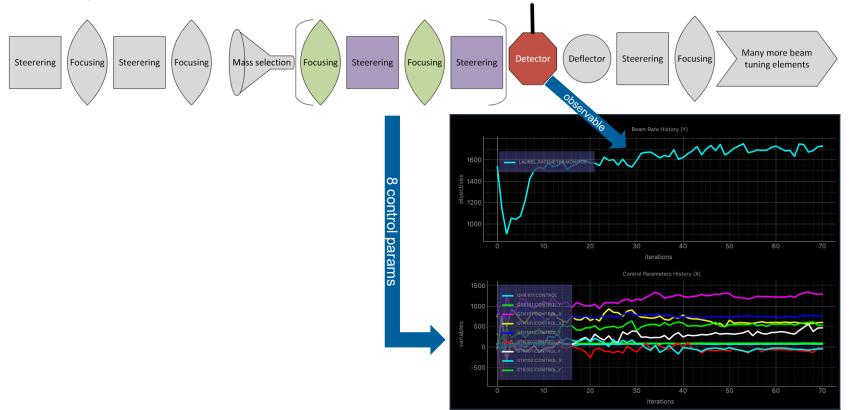




NUCARIBU CONTROLS – SIMPLIFIED VIEW

inactive

Splitting in sections, each with 10 or less control parameters





NO BEAM CASE

Impact of parameter "beta" (exploration v. exploitation)

