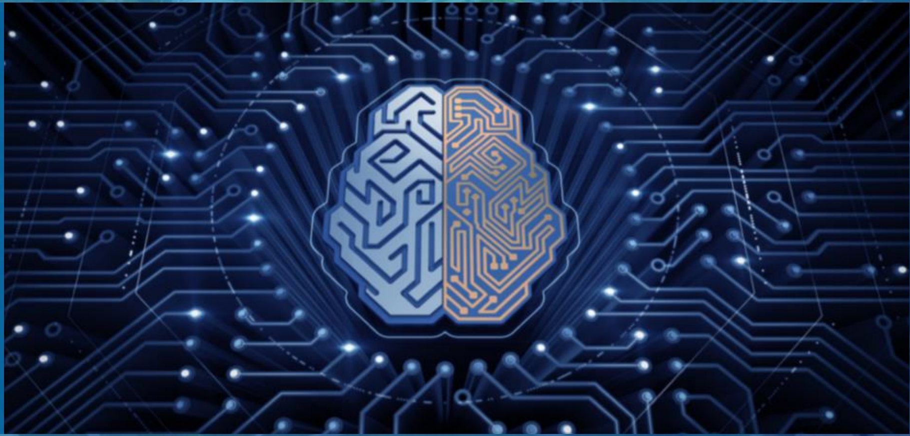
ACCELERATOR PHYSICS & ENGINEERING SEMINAR
OCTOBER 7, 2024, FRIB, MSU

AI - ML TOOLS FOR HEAVY-ION LINAC OPERATIONS



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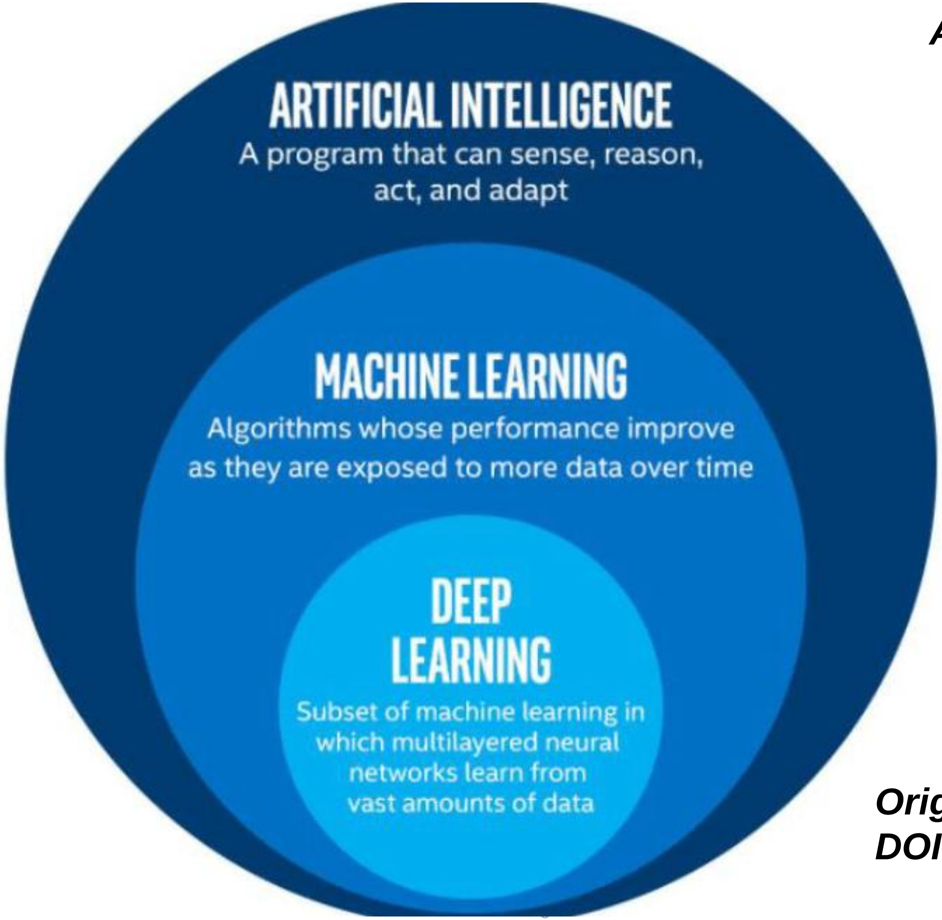
A BRIEF INTRODUCTION TO AI – ML

- Evolving concept of computing …
  - Passive computing: everyday use, relies on the user's input
    (in some cases: garbage in garbage out!)
  - Active & interactive computing: machine learns, starts making predictions and suggestions, capable of surpassing the user's "expectation" / "imagination"!

- Machine Learning vs. Artificial Intelligence?
  - Artificial Intelligence: The machine mimicking human intelligence, with the goal of replacing it wherever possible.
  - Machine Learning: The machine learns how to perform a specific task(s) and provide accurate results/predictions (a part/subset of artificial intelligence).

MACHINE LEARNING VS. ARTIFICIAL INTELLIGENCE

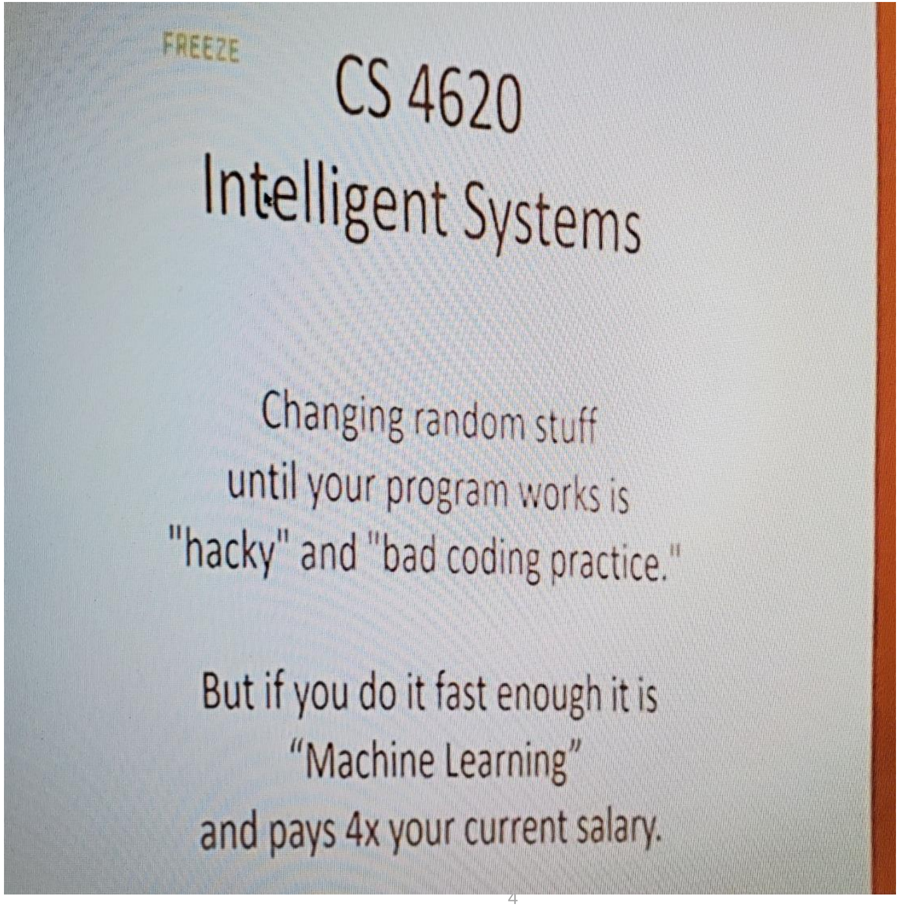


Artificial Intelligence includes

- ***Automation: Robotics***
- ***Natural language processing***
- ***Chatbots***
- ***Computer Vision***
- ***Machine Learning, DL, NN***
- ***…***

Origin: R. Khalkar et al.
DOI:10.17148/IARJSET.2021.86148

ANOTHER DEFINITION OF MACHINE LEARNING!



Origin: Cornell U. lecture in computer science

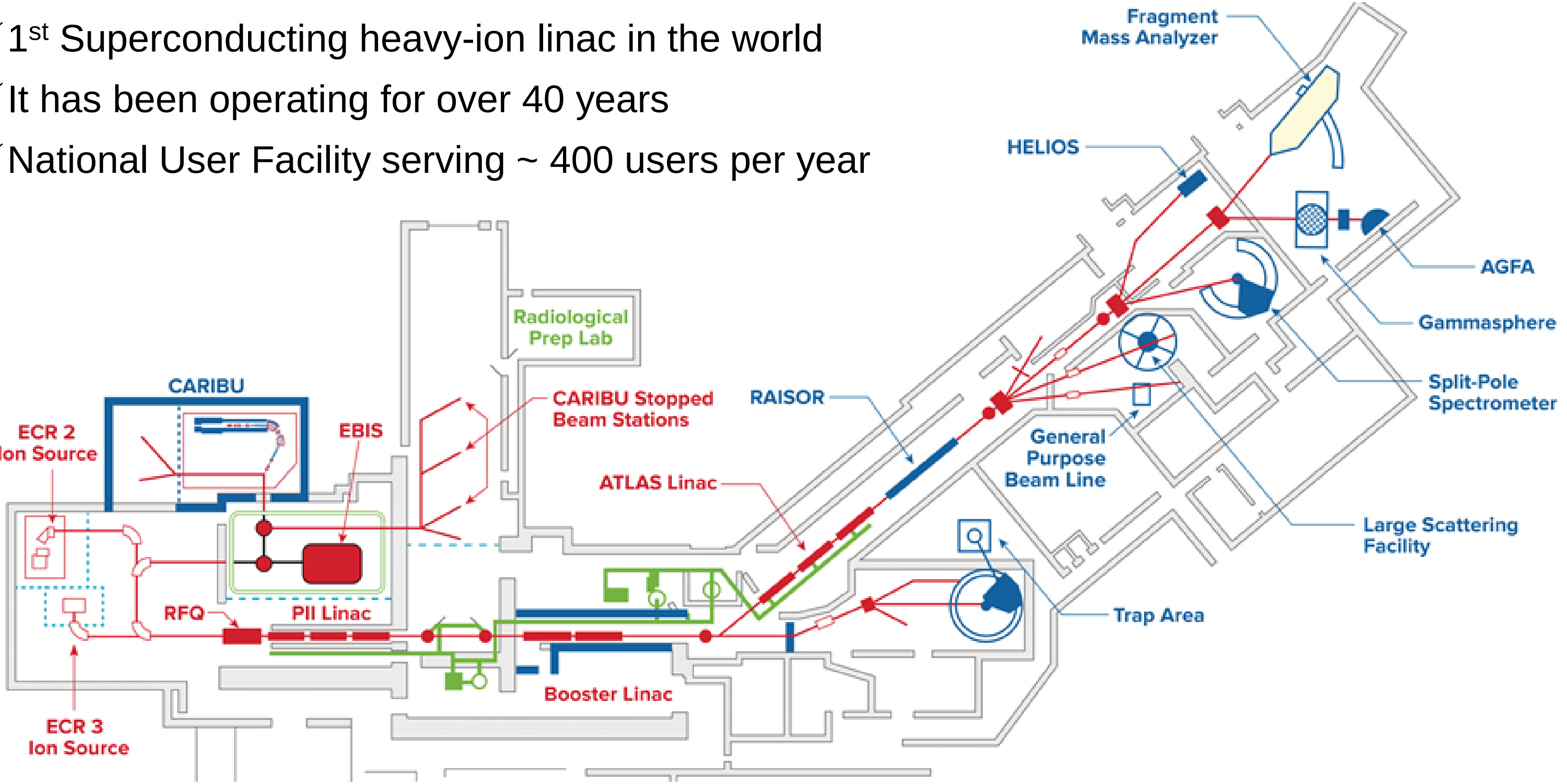
THE ATLAS AI-ML PROJECT – OVERVIEW & HIGHLIGHTS

OUTLINE

- ❑Brief Introduction to the ATLAS Facility at Argonne
- ❑Overview of the ATLAS AI-ML Project
- ❑Summary of Progress & Highlights
- ❑Main Conclusions
- ❑Future Plans

ATLAS: ARGONNE TANDEM LINEAR ACCELERATOR SYSTEM

- ✓1st Superconducting heavy-ion linac in the world
- ✓It has been operating for over 40 years
- ✓National User Facility serving ~ 400 users per year



BRIEF OVERVIEW OF THE 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
- The 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**

SUMMARY OF PROGRESS & HIGHLIGHTS

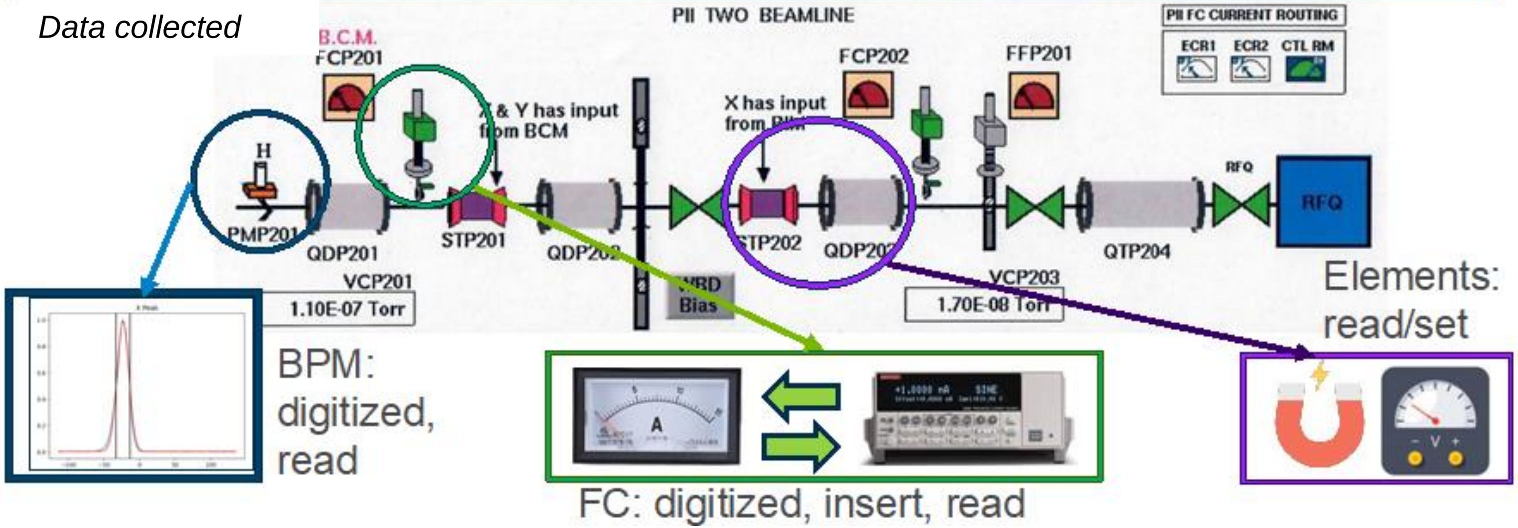
- ❑ Automated data collection and two-way communication established
- ❑ Bayesian Optimization (BO) successfully used for online beam tuning
- ❑ Multi-Objective BO (MOBO) to optimize transmission and beam size
- ❑ AI-ML supporting the commissioning of a new beamline (AMIS)
- ❑ Transfer learning from one 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
- ✓ A python interface developed to collect the data automatically

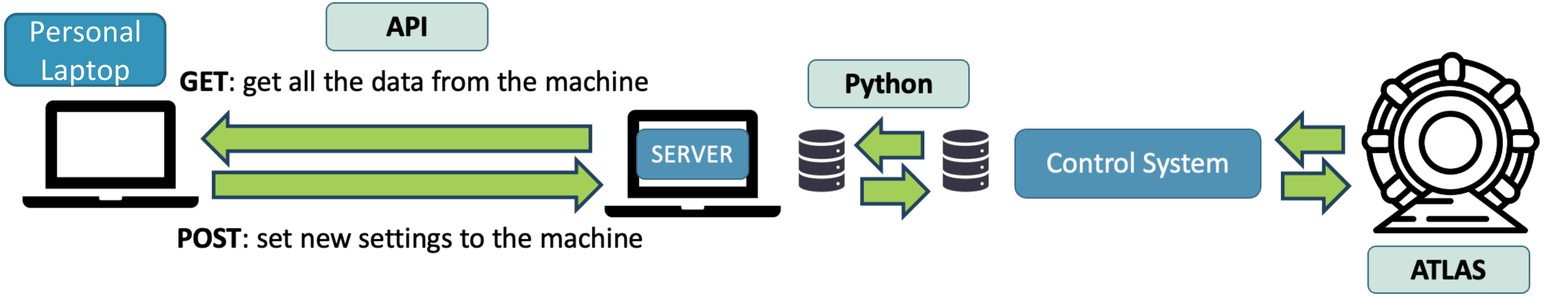
Schematic of data collection interface

Data collected



Now working on reducing acquisition time …

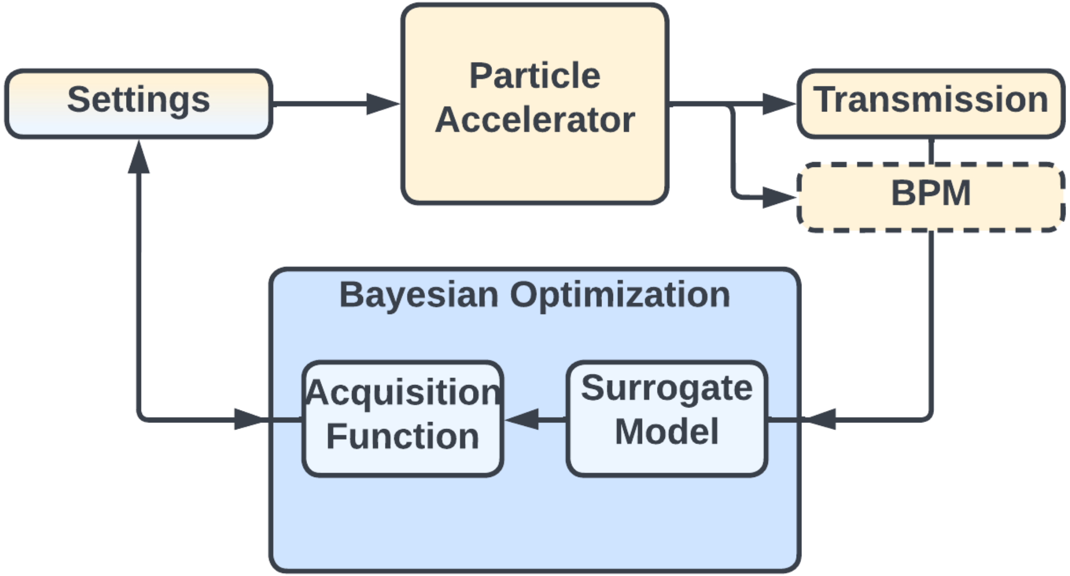
ONLINE – INTERFACE WITH CONTROL SYSTEM



OFFLINE – INTERFACE WITH BEAM SIMULATION

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

BAYESIAN OPTIMIZATION – A BRIEF DESCRIPTION

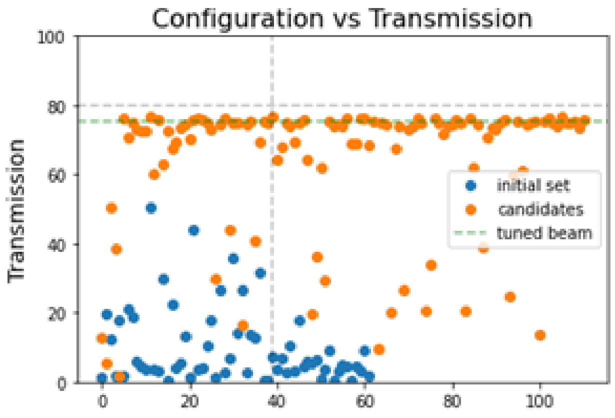


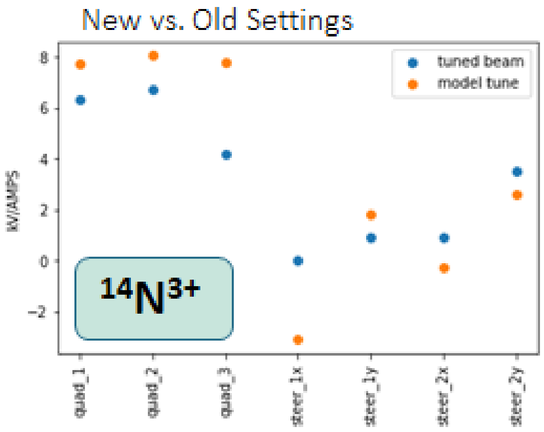
- ✓ **<u>Surrogate Model</u>: A probabilistic model approximating the objective function**
  [Gaussian Process with Radial Basis Function (RBF) Kernel and Gaussian likelihood]
- ✓ **<u>Acquisition Function</u> tells the model where to query the system next for more likely improvement**
- ➢ **Bayesian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

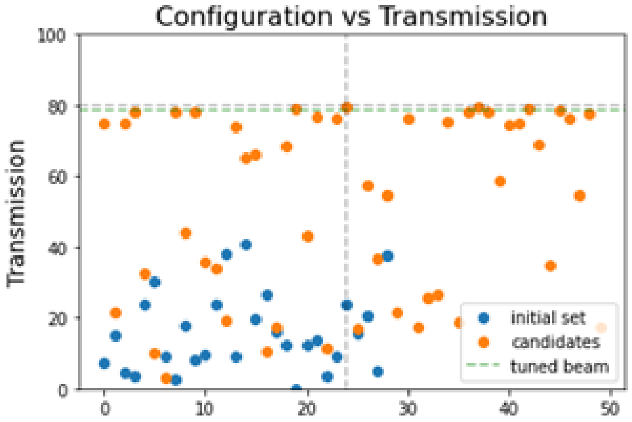
BAYESIAN OPTIMIZATION USED IN ONLINE TUNING

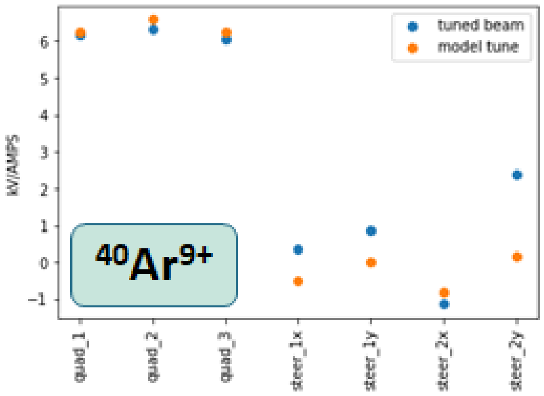
Beamline under study

- 7 variable parameters (3 quadrupoles + 2x2 steerers)
- Optimization of beam transmission
- Case of $^{14}N^{3+}$: 29 historical + 33 random tunes
- Case of $^{40}Ar^{9+}$: 29 historical tunes



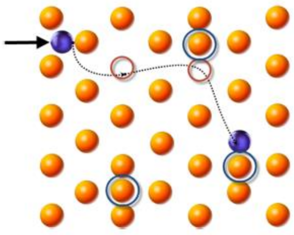


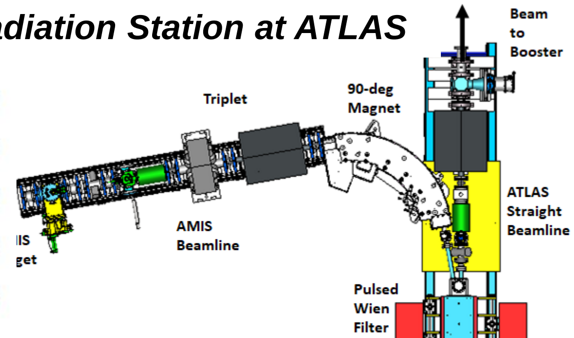




AI/ML SUPPORTING AMIS LINE COMMISSIONING

New Material Irradiation Station at ATLAS

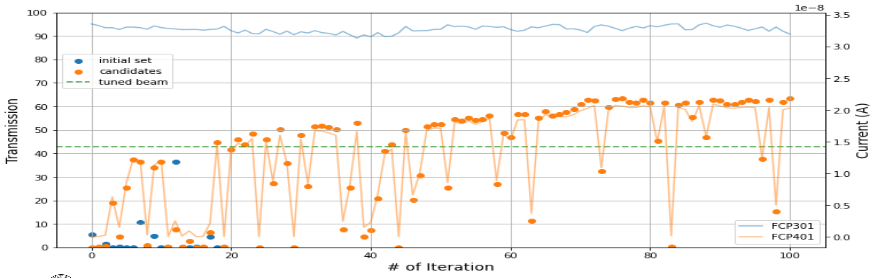




Low-energy heavy-ion beams ~ 1 MeV/u can effectively emulate material damage in nuclear reactors, in both fuel and structural materials.

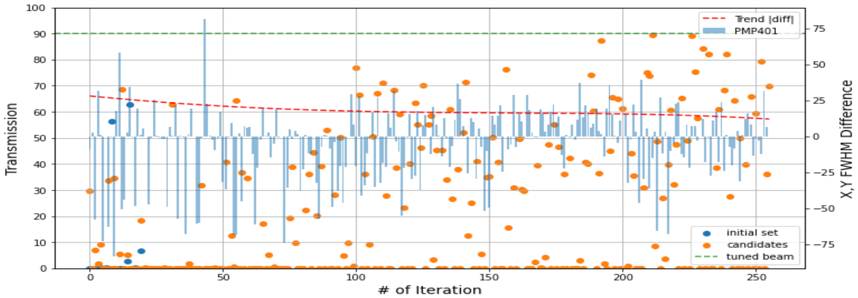
Improving Beam Transmission

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

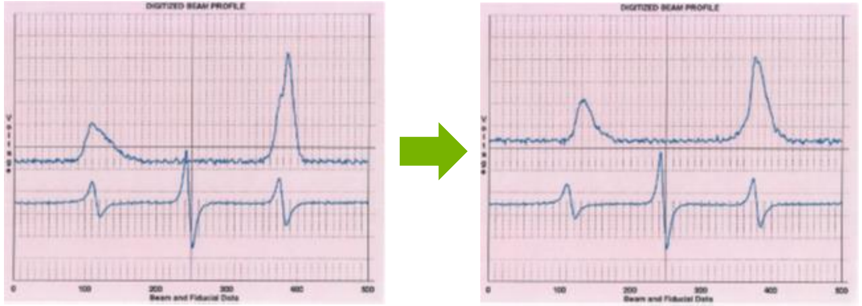


Improving Beam Profiles

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!



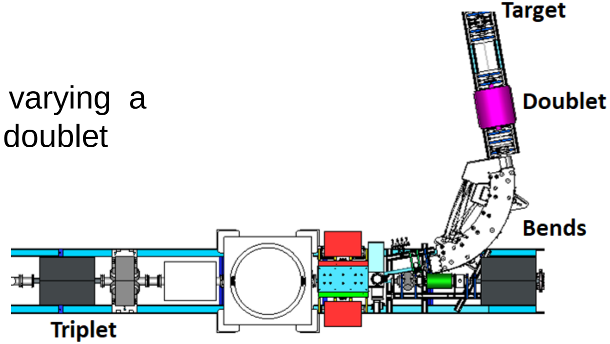
Very encouraging first results!

MULTI-OBJECTIVE BAYESIAN OPTIMIZATION

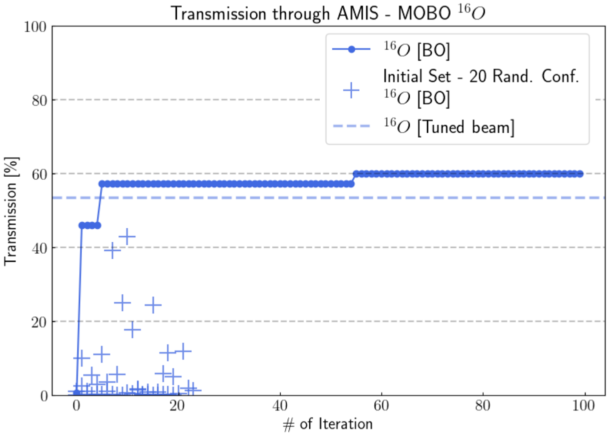
Multi-Objective Problem: Optimize transmission and beam profiles on target - Not easy for an operator!

Improving Beam Transmission & Improving Beam Profiles

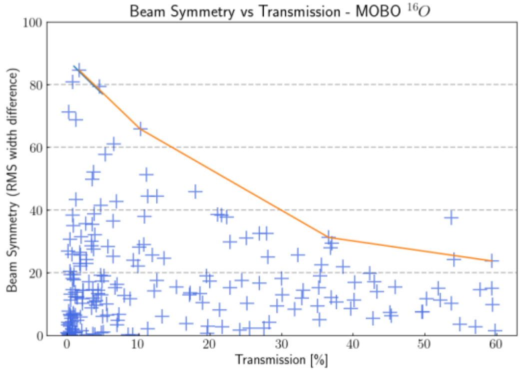
AMIS line: varying a triplet and a doublet



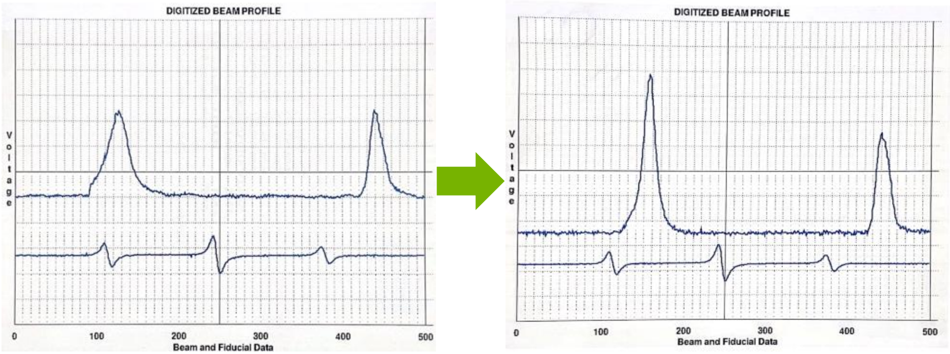
MOBO Results: 53→ 60% Beam transmis.



MOBO Results: Pareto Front



MOBO Results: More symmetric beam profiles

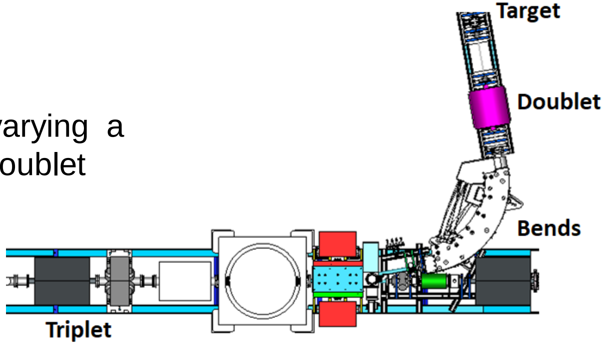


TRANSFER LEARNING FROM ^{16}O TO ^{22}NE - BO

Goal: Train a model using one beam then transfer it to tune another beam → Faster switching and tuning

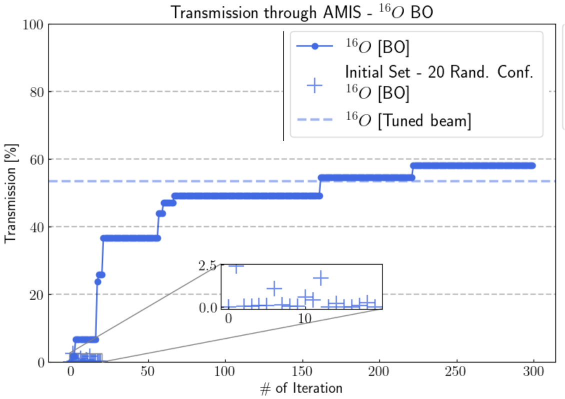
Training model on ^{16}O → Applying same model to ^{22}Ne

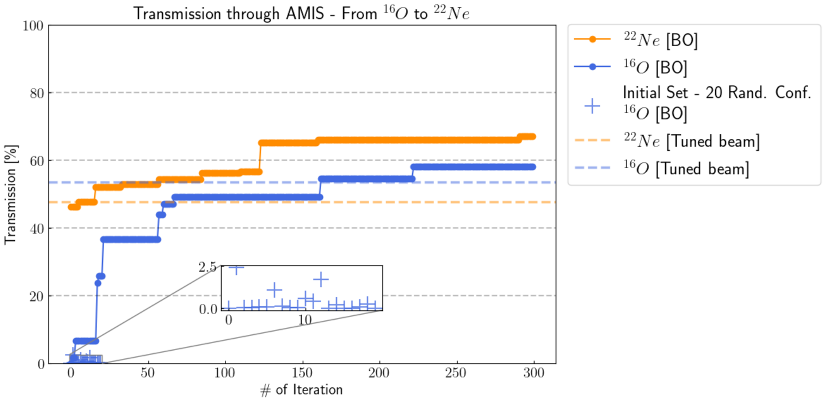
AMIS line: varying a triplet and a doublet



BO Training:
Over 300 iterations
53 → ~ 60% Beam transmis.

Model saved & exported





16O Model loaded for 22Ne: Initial transmission improved in 7 iterations: 48 → 55 %

With more training for 22Ne: 48 → 67%

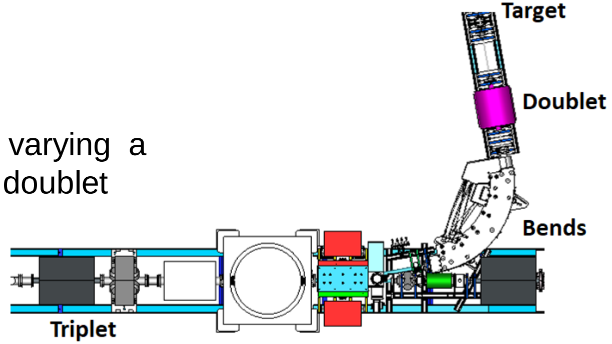
Scaling was applied from 16O to 22Ne, re-tuning is often needed because of different initial beam distributions

TRANSFER LEARNING FROM SIMULATION TO ONLINE

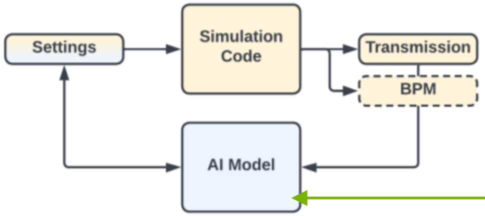
Goal: Train a model using simulations then use it for online tuning → Less training & faster convergence online

Method: Deep kernel learning (DKL) to **combine the representational power of neural networks with the reliable uncertainty estimates of Gaussian processes**.

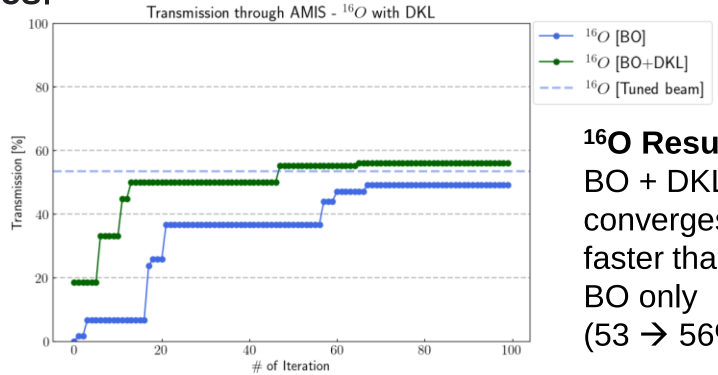
AMIS line: varying a triplet and a doublet



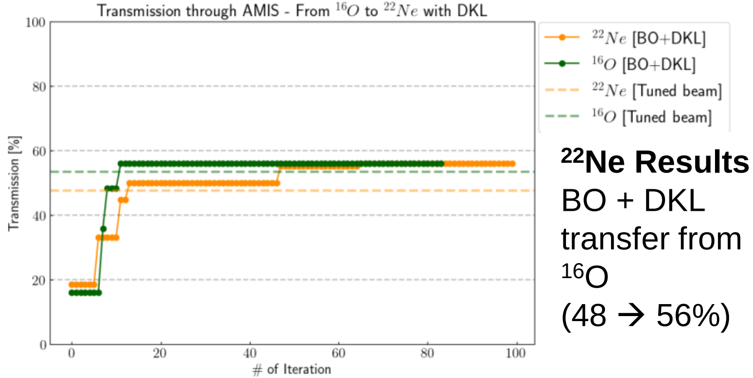
AMIS Line: Maximize beam transmission by varying a triplet [BO+DKL]



NN trained offline with TRACK simulations [4k training set /1k evaluation set]



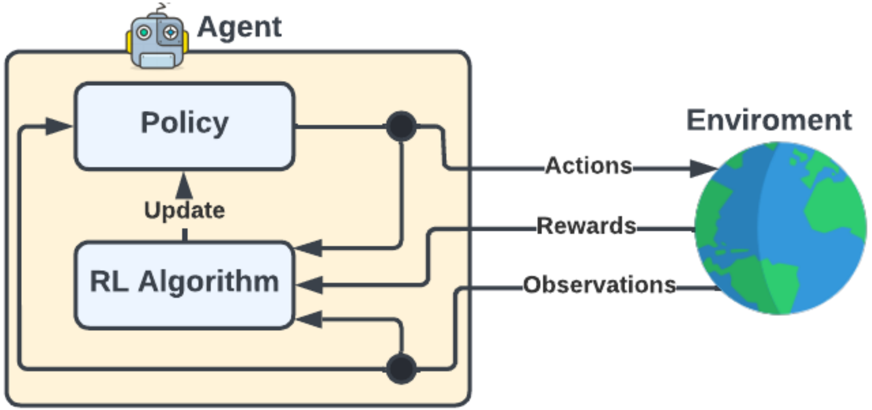
^{16}O Results: BO + DKL converges faster than BO only (53 → 56%)



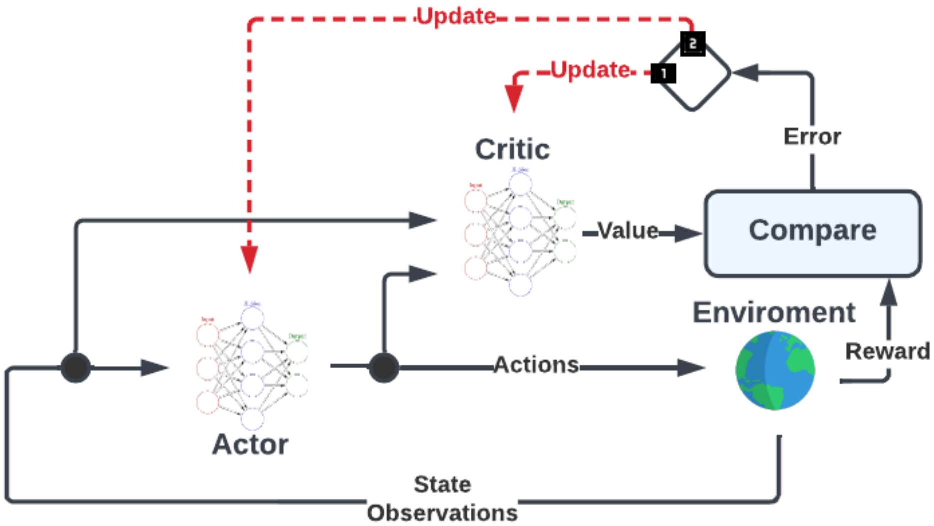
^{22}Ne Results: BO + DKL transfer from ^{16}O (48 → 56%)

REINFORCEMENT LEARNING – A BRIEF DESCRIPTION

Basic Concept



Implementation Example

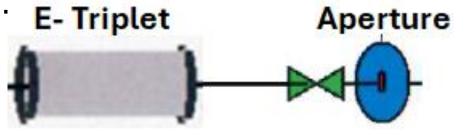


- ✓ **Essence:** Learning from experience based on interaction with the environment
- ✓ **Action:** Varies the parameters/variables of the problem
- ✓ **Reward:** Measures the goal function to maximize/optimize
- ✓ **Policy:** How the process evolves/learns
- ✓ **Algorithm used:** Deep Deterministic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

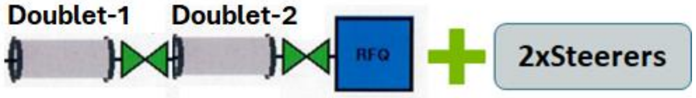
REINFORCEMENT LEARNING: FIRST ATTEMPT…

Simulation Case

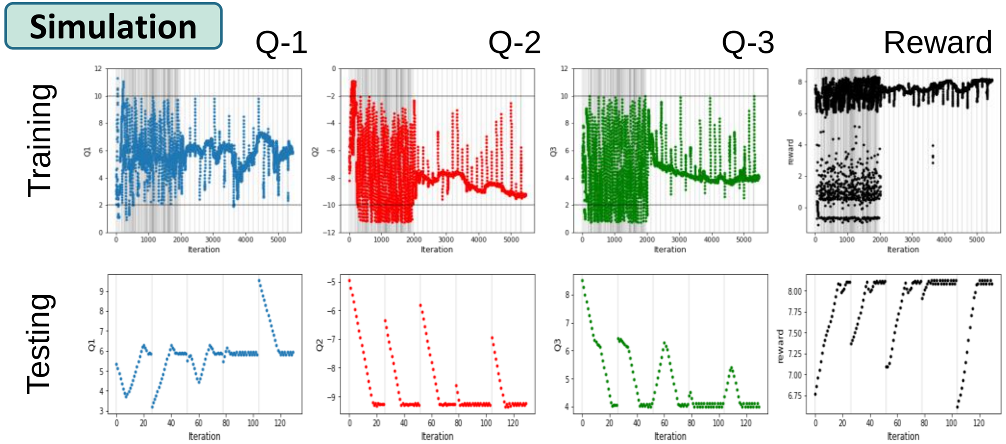
- ✓ Focusing the beam through an aperture using an electrostatic triplet (3 Quadrupoles)
- ✓ Voltage limites: 2 – 10 kV
- ✓ Max. action: +/- 0.25 kV

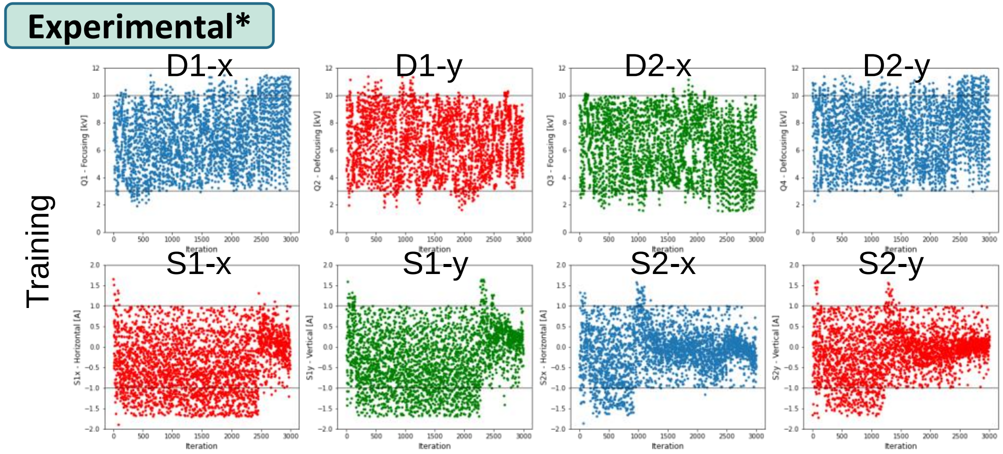


Actual Experiment



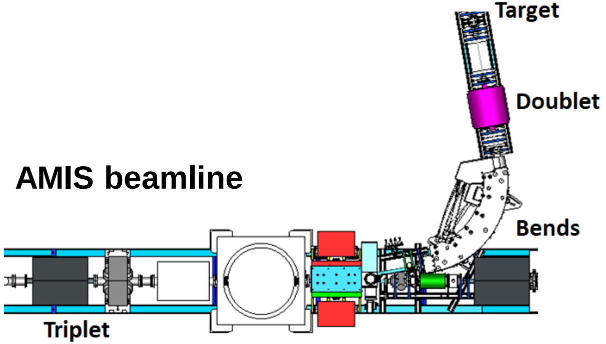
- ✓ Maximizing beam transmission using 2 doublets (4 quads) and 2x2 steerers
- ✓ Electrostatic Quadrupoles :
  - 2 kV to 10 kV
  - Max action +/- 0.25 kV
- ✓ Steering Magnets:
  - -1 A to 1 A
  - Max action +/- 0.25 A





REINFORCEMENT LEARNING: FIRST EXP. SUCCESS

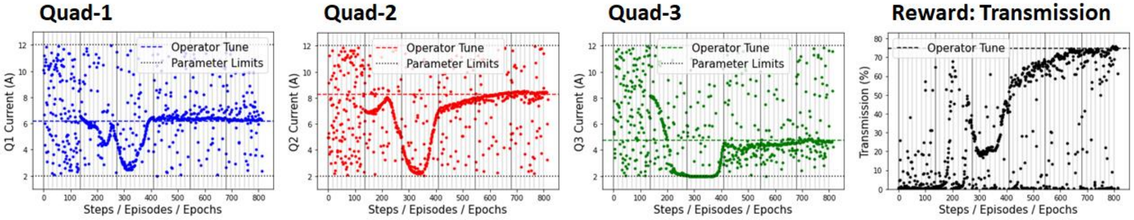
Beamline under study



Objective: Maximize beam transmission

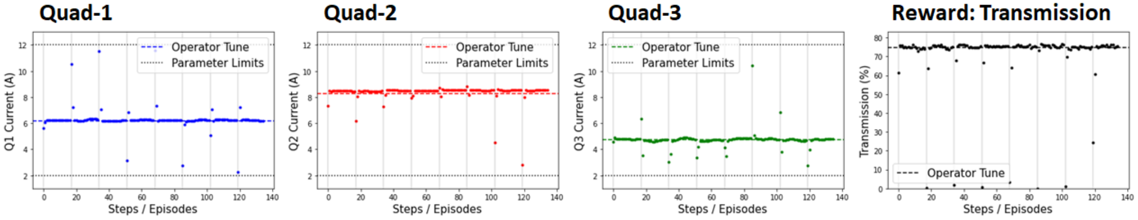
- Varying 3 magnetic quads
- Current limits: 2 – 12 Amps
- Max. Action: Full range

Training - Online



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

Testing - Online

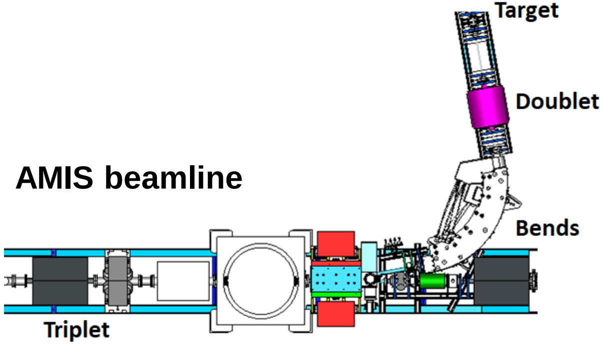


➢ Testing done for 8 episodes (16 steps/episode)
➢ Model converges in 2-3 steps, starting from random config.

➢ **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

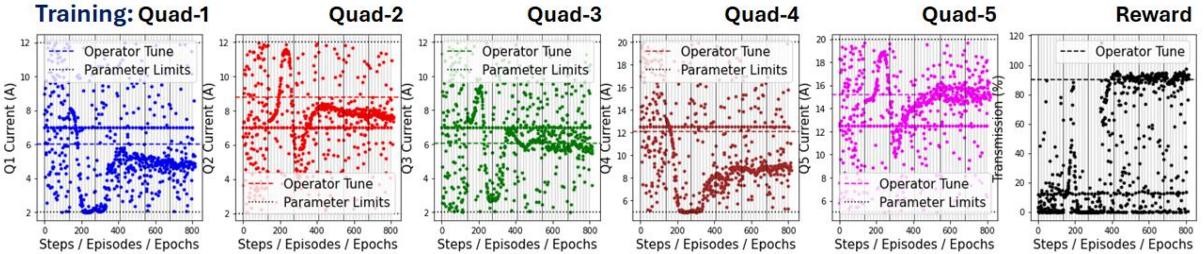
Beamline under study



Objective: Maximize beam transmission

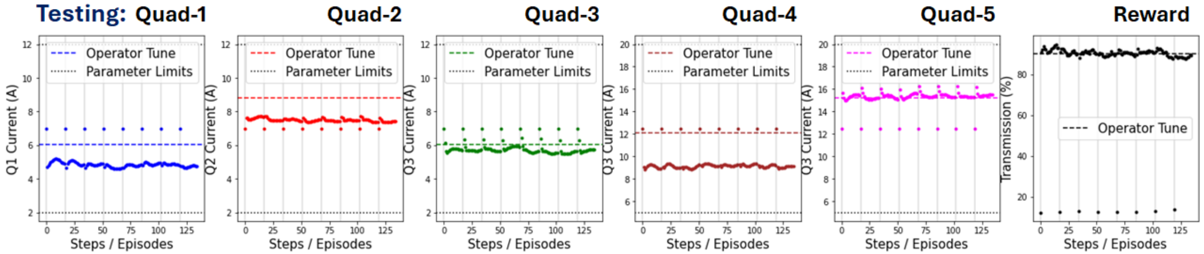
- Varying 5 magnetic quads
- Triplet 2–12 A, Doublet 5-15 A
- Max. Action: Full range

Training - Online



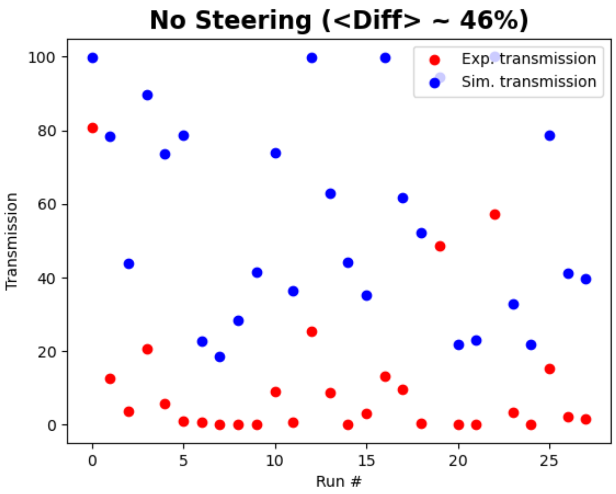
- ➢ Training done in 816 total steps/evaluations (48 episodes)

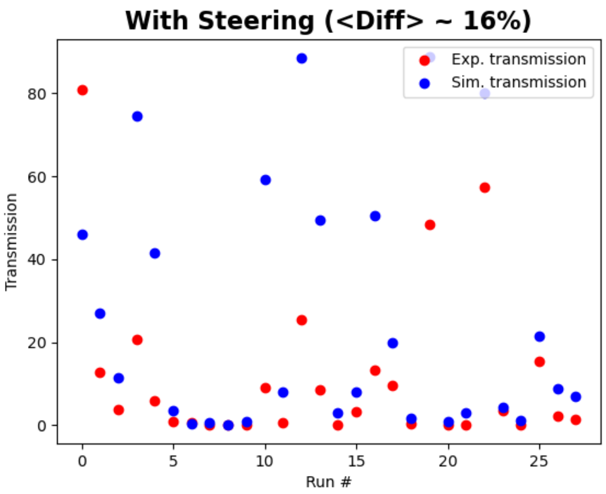
Testing - Online

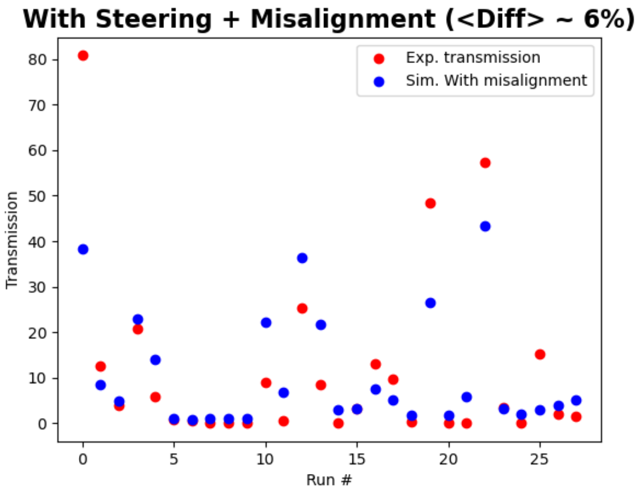


- ➢ Testing done for 8 episodes (16 steps/episode)
- ➢ Model converges in 2-3 steps, starting from same config.

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

MAIN CONCLUSIONS

- ❑ Bayesian Optimization is very effective for beam tuning with no prior knowledge, and typically converges in 50 iterations or less for few parameter problems (< 10). With every iteration taking ~15 s, that's 10-15 min, which's comparable to operators.
- ❑ BO was more competitive and helpful for beam commissioning (new to operators), and for multi-objective optimization, which is not an easy task for the operators.
- ❑ We were able to save a BO model from one beam and use it as starting point (prior knowledge) to tune another beam which accelerated convergence. Transfer from a simulation model was not as successful due to discrepancy with the actual machine.
- ❑ Reinforcement Learning requires prior training which is very expensive to perform online. We were able to train a model with ~ 5 parameters in ~1000 iterations which took ~ 4 hours, but once trained it converged in 2-3 iterations, less than 1 min!
- ❑ We made good progress on the virtual machine model or digital twin, which once ready, it will be very helpful to train the models offline then apply them directly to the machine, hopefully without requiring further online training…

PROJECT ACCOMPLISHMENTS VS. OBJECTIVES

- Original Project 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…

WHAT'S NEXT – A NEW PROJECT PHASE…

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

- The main objectives of the new 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.

MANY THANKS TO

- Jose Martinez: project postdoc, did most of the work …

- ATLAS Controls Team:

  Daniel Stanton and Kenneth Bunnell

- ATLAS Operations Team:

  Ben Blomberg, Eric Letcher and Gavin Dunn

- ATLAS Users Liaison:

  Daniel Santiago

THANK YOU

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