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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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

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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

 $10 - 20%$ the speed of light*

*Speed depends on the ion used.

OVERVIEW OF ORIGINAL ATLAS AI-ML PROJECT

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

 \Box At ATLAS, we switch ion beam species every 3-4 days $\ldots \rightarrow$ Using AI could streamline beam tuning & help improve machine performance

❑ Project objectives and approach:

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

ACCOMPLISHMENTS VS. ORIGINAL OBJECTIVES

- o **Data collection, organization and classification, towards a fully automated and electronic data collection for both machine and beam data**… established
- o **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
- o **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.
- \Box 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
	- o Adwaith Ravichandran, started in December'23
	- o 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:

- o 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.
- o 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

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

NEW ATLAS DASHBOARD INTERFACE (2)

Development of a User Interface for the Operators

GUI ONLINE TEST #1: PII TO BOOSTER LINE

GUI ONLINE TEST #2: PII TO BOOSTER LINE

NEW ATLAS BADGER INTERFACE

Development of a Developer Interface for the Experts

Select Algorithm & Parameters

Setup the problem's variables and objectives

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

BO Model Hyperparameters: • Beta : 0.1 • No of candidates: 1 • No of restarts: 20 • Max Iterations: 2000 • No of Monte Carlo Samples: 128

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

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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 Varying 6 quads + 4 steerers

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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 \sim 85% in \sim 50 iterations x 8 sec \sim 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

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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 ²⁵²Cf fission fragments $(10^2 – 10^4$ pps, few keV/u)
- **nuCARIBU** a major upgrade in progress to increase beam intensities via neutron induced $\mathbb N$ fission
- Essential for ATLAS multi-user upgrade (post-accel. beams, 3-10 MeV/u)
- 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 \hat{m} , γ) $\hat{k}40B$ a 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 CONTROLS – SIMPLIFIED VIEW Splitting in sections, each with 10 or less control parameters 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)

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❑ 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)
- Generation of simulation data
- Different conditions and inputs
- Integration with AI/ML modeling

BAYESIAN OPTIMIZATION – A BRIEF DESCRIPTION

✓ **Surrogate Model: A probabilistic model approximating the objective function**

[Gaussian Process with Radial Basis Function (RBF) Kernel and Gaussian likelihood]

- ✓ **Acquisition Function 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)**
- o **Optimization of beam transmission**
- o **Case of ¹⁴N3+ : 29 historical + 33 random tunes**

o **Case of ⁴⁰Ar9+ : 29 historical tunes**

MULTI-OBJECTIVE BAYESIAN OPTIMIZATION

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

Beam Symmetry vs Transmission - MOBO ^{16}O **MOBO** liffe **Results**: Pareto Front

REINFORCEMENT LEARNING – A BRIEF DESCRIPTION

Basic Concept 14 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

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

 \checkmark 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 \sim 1%, a surrogate model will be developed based on the simulations

MORE SLIDES

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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 ¹⁶O TO ²²NE - BO

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

Training model on ¹⁶O Applying same model to ²²Ne

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

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**.

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

Aperture

Actual Experiment

Doublet-1 Doublet-2 **2xSteerers**

- 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

