Swiss Institute of Particle Physics





ACTIVE DEEP LEARNING FOR SINGLE-PARTICLE BEAM DYNAMICS STUDIES D. DI CROCE<sup>2</sup>, M. GIOVANNOZZI<sup>1</sup>, G. IADAROLA<sup>1</sup>, E. KRYMOVA<sup>4</sup>, T. PIELONI<sup>2</sup>, S. RADAELLI<sup>1</sup>, M. SEIDEL<sup>2,4</sup>, F. F. VAN DER VEKEN<sup>1</sup> <sup>1</sup>CERN, <sup>2</sup>EPFL, <sup>3</sup>PSI, <sup>4</sup>SDSC

> 9<sup>TH</sup> LOW EMITTANCE RINGS WORKSHOP – 19<sup>TH</sup> JUNE 2024, UNIGE - GENEVA CHIPP 2024 ANNUAL MEETING

This work was carried out under the auspices and with the support of the Swiss Accelerator Research and Technology programme (CHART) and the Swiss Data Science Centre (SDSC)

# **MACHINE LEARNING 4 FUTURE CIRCULAR COLLIDER**

- The ML4FCC project is a collaboration between EPFL, CERN, and The Swiss Data Center (SDSC): <u>https://www.epfl.ch/labs/lpap/machine-learning-applied-to-accelerators/</u>
- Our focus is on applying Machine Learning techniques to improve the understanding of Beam Dynamics in various accelerator setups.
- Currently, developing tools and benchmarking models on an existing accelerator (LHC) to demonstrate the ML effectiveness before moving to the design of a future, large accelerator (FCC).
- For the case of lepton accelerators, additional effects (e.g. synchrotron radiation) should be included.



## **MACHINE LEARNING 4 FUTURE CIRCULAR COLLIDER**

- Extracting Physics-Relevant Features with ML: Identify key features for predicting beam loss from accelerator variables: betatron tunes, chromaticities, octupole strength, realization of magnet errors, phase advance, crossing angles and separation, beam energy, emittance, bunch intensity, anharmonicities and more.
- Ultra-Fast Simulations: ML enables rapid and efficient simulations, significantly accelerating the exploration of machine configurations for the optimization of current machines and the design of future accelerators as FCC.
- Knowledge Preservation: models capture and store physics knowledge, reducing the need for numerical simulations to acquire the same physics insights.

#### **DEEP LEARNING FOR DYNAMIC APERTURE**

- The Dynamic Aperture (DA) is defined as the extent of the connected phase-space region within which the dynamics of a single particle remains bounded in circular accelerators
- DA is important to assess linear and non-linear optics, lattice imperfections, beam-beam, e-cloud, and incoherent effects!
- The dataset is based on simulation (MADX) and tracking (Xsuite) on LHC.
- Tracked the particles distributed in polar coordinates (44 angles and 0.06  $\sigma$  radial steps) for every machine configuration.
- Goal is to regress the evolution of the stable region (angular DA) in 12 different number of turns (up to 10<sup>5</sup> turns) [Red points].



- 20k sets of accelerator parameters generated by variating chromaticity, octupole current, betatron tunes, and magnet realizations (also called seeds) of the magnetic field errors for the 2 beams.
- Other machine variables included: anharmonicities, maximum  $\alpha$  and  $\beta$  and phase-advance at IPs.

#### **DEEP LEARNING FOR DYNAMIC APERTURE**

- Multilayer Perceptron with 4 hidden layers with ReLU and 5% dropout.
- Trained with Reduce on Plateau for learning rate scheduler, NADAM optimizer and Mean Absolute Error (MAE) as Loss Function.
- Test MAE = 0.34 beam  $\sigma$  and MAPE = 11.91 %.
- Inference of a single machine in 0.5 ms (~1  $\mu$ s/angular DA prediction)





# **ESTIMATING THE PREDICTION ERROR**

- By leveraging dropout at inference time, we introduce diversity among the predictions (different angular DAs every time). This technique is known as Monte Carlo (MC) dropout.
- The variation in these predictions are utilized to estimate uncertainty: dropout at 1% between the first hidden layers and 1 std of 128 variations as error.





- DA and error prediction (129 inferences) in
  0.75 s/machine configuration.
- Tracking on Xsuite takes 147s/machine configurations (using HT-Condor). Our model, once trained, is approximately 200 times faster!

Simulation	10k configs	15k configs
MADX + Xsuite *	425 h	612 h
DA Regressor **	126h (3.4x faster)	136h (4.5x faster)

\*MADX and Xsuite simulations with HT-Condor (1000 simultaneous jobs) \*\*Including the simulation time of an initial dataset of 5k and training time

## **ADAPTABILITY TO DIFFERENT OPTICS CONFIGURATIONS**

- We want to ensure that the model can adapt to different optics configurations, which is a key advantage, especially in scenarios where the optics are unknown to the model like in designing a new accelerator.
- We included merely 1k configurations from 2016 optics (which can be simulated in 5 days) in conjunction with the 20k from 2023, enabling the model to become predictive for 2016 as well.
- Learning solely from physics variables reduces the need for extensive retraining and provides adaptability to new optics.



# **PREDICTION OF REAL OBSERVABLES**

- Another crucial aspect is the capability to link simulations with real observables, such as loss rates, to enhance the practicality and reliability of our models.
- We combined theoretical calculations of beam intensity into our ML models. The theoretical Intensity loss for a gaussian distribution considering their angles:

$$\mathcal{L} = N_P \left( 1 - 4 \int_0^{\frac{\pi}{2}} \int_0^{DA_{\theta}} r^3 e^{-r^2} \sin \theta \cos \theta \, dr \, d\theta \right)$$

- Loss rates estimated by computing the derivate of the intensity loss.
- This month we performed an 8h MD to measure LHC intensity loss for several machine configurations to compare with the predicted ones.



# **ACTIVE LEARNING FRAMEWORK**

- We integrated the DNN model alongside its error estimator into an innovative Active Learning (AL) framework.
- AL framework also enables smart sampling of simulations: by prioritising predictions with higher errors, it efficiently determines the sequence in which to simulate new machine configurations.



PUBLISHED BY IOP PUBLISHING FOR SISSA MEDIAI	inst
RECEIVED: December 29, 2	J
ACCEPTED: February 6, 2	
PUBLISHED: April 4, 2	

68th ICFA Advanced Beam Dynamics Workshop on High-Intensity AND HIGH-BRIGHTNESS HADRON BEAMS - HB2023

#### Optimizing dynamic aperture studies with active learning

Di Croce <sup>©</sup> , <sup><math>a</math>,*</sup> M. Giovannozzi, <sup><math>b</math></sup> E. Krymova, <sup><math>c</math></sup> T. Pieloni, <sup><math>a</math></sup> S. Redaelli, <sup><math>b</math></sup> M. Seidel, <sup><math>a</math>,<math>d</math></sup> Tomás <sup><math>b</math></sup> and F.F. Van der Veken <sup><math>b</math></sup>
LPAP, École Polytechnique Fédérale de Lausanne,
BSP — Rte de la Sorge, Lausanne, Switzerland
ABP, CERN,
Espl. des Particules 1, Meyrin, Switzerland
SDSC, The Swiss Data Science Center,
Wasserwerkstrasse 10, Zurich, Switzerland
GFA, Paul Scherrer Institut,
Forschungsstrasse 111, Villigen, Switzerland
E-mail: davide.dicroce@epfl.ch
BSTRACT: Dynamic aperture is an important concept for the study of non-linear beam dynamics

INST in circular accelerators. It describes the extent of the phase-space region where a particle's motion \_\_\_\_ 9 Þ 

remains bounded over a given number of turns. Understanding the features of dynamic aperture is crucial for the design and operation of such accelerators, as it provides insights into nonlinear effects and the possibility of optimising beam lifetime. The standard approach to calculate the dynamic aperture requires numerical simulations of several initial conditions densely distributed in phase space for a sufficient number of turns to probe the time scale corresponding to machine operations. This process is very computationally intensive and practically outside the range of today's computers. In our study, we introduced a novel method to estimate dynamic aperture rapidly and accurately by utilising a Deep Neural Network model. This model was trained with simulated tracking data from the CERN Large Hadron Collider and takes into account variations in accelerator parameters such as betatron tune, chromaticity, and the strength of the Landau octupoles. To enhance its performance, we integrate the model into an innovative Active Learning framework. This framework not only enables retraining and updating of the computed model, but also facilitates efficient data generation through smart sampling Since chaotic motion cannot be predicted, traditional tracking simulations are incorporated into the Active Learning framework to deal with the chaotic nature of some initial conditions. The results demonstrate that the use of the Active Learning framework allows faster scanning of the configuration parameters without compromising the accuracy of the dynamic aperture estimates.

KEYWORDS: Accelerator modelling and simulations (multi-particle dynamics, single-particle dynamics); Beam dynamics; Simulation methods and program

\*Corresponding author

https://doi.org/10.1088/1748-0221/19/04/P0400

DOI 10.1088/1748-0221/19/04/P04004

Interface with tracking tools is crucial for assessing chaotic dynamics whenever the estimate errors are significant

N

N <sup>1</sup>

# **ACTIVE LEARNING FRAMEWORK**

To test the effectiveness of smart sampling, we compared the performance of the model when trained with two different data sets: random search of machine configuration input and with the AL framework.



- The AL framework allows to explore machine configurations more efficiently where the model has not yet learnt the features of the underlying physics.
- By adding 1000 synthetic machine configurations (predicted errors < 0.1 beam  $\sigma$ ), MAE improved to 0.20 beam  $\sigma$



Ability to refine the model's prediction while waiting for the acquisition of new simulated data.

### CONCLUSION

- Improving beam dynamics simulations with ML for optimization and design of accelerators:
  - Faster simulations and good predictions within uncertainty.
  - Models based on physics variables offer adaptability across various optics setups, a crucial advantage when dealing with unknown optics, such as in accelerator design.
  - Incorporating accelerator tools like MAD-X and Xsuite empowers models to learn physics and enhances the tools themselves.
  - Active Learning to efficiently generate datasets containing relevant physics.
  - Preserving accelerator knowledge, eliminating the need for redundant simulations.

