SIMULATION STUDY ON A VIRTUAL DIAGNOSTICS CONCEPT FOR X-RAY PULSE CHARACTERISATION

F. Jafarinia*, C. Grech, M. Guetg, Deutsches Elektronen-Synchrotron DESY, Germany
G. A. Geloni, European XFEL, Germany

Abstract

In this study we investigate simulation results for a virtual diagnostics concept that is planned for the SASE1 beam-line at the European XFEL. These virtual diagnostics will be used to predict photon beam properties like pointing and divergence. We first use the GENESIS simulation framework to compute different lasing conditions in the undulator beam-line, and then use Artificial Neural Networks (ANN) to predict the pulse properties. The final model will be able to estimate X-ray pulse characteristics based on properties like electron beam trajectories inside the undulator sections along with other diagnostics data. This study will provide insight towards the development of online virtual diagnostics in the real machine.

INTRODUCTION

Free Electron Lasers (FELs) are powerful sources of intense and coherent radiation that have become essential tools for a wide range of scientific and industrial applications [1]. However, FELs are complex machines that require careful tuning and optimization to achieve the desired output. This is where Machine learning (ML)-based virtual diagnostics can play a crucial role. Virtual diagnostics refer to the use of ML algorithms to analyze data from various beam-line components and predict the properties of the beam.

One area where machine learning has been applied in FELs is in the prediction of the output properties of the FEL, such as the intensity, energy, and polarization of the emitted radiation [2, 3]. By analyzing data from various beam-line components, such as undulators and beam-line diagnostics, machine learning algorithms can predict the properties of the FEL output, allowing for real-time optimization of the FEL performance [4, 5].

This paper provides an overview of our virtual diagnostics concept for the XFEL machine at the Deutsches Elektronen-Synchrotron (DESY). We present simulation results and the predicted radiation beam properties using our ML model in the following sections. Finally, we discuss the necessary steps for implementing the ML model in the XFEL beam-line at DESY.

MACHINE LEARNING MODEL

Simulation

The aim of this study is to create a ML based model for prediction of electron and radiation beam properties. For this reason, a series of GENESIS [6] simulations were done and required parameters to train the model and desired outputs for the training and prediction were extracted. Regarding the simulations the beam-line is composed of 30 undulator cells of the length of 5 meters with focusing elements between these cells.

Table 1: Simulated Beam Properties

Parameter	Value	Unit
Energy	14	GeV
Normalized Emittance(X/Y)	0.5	µm
Bunch Length	20	µm
Current (Flattop)	4	kA
Radiation Wavelength	0.1	nm

The beam energy is 14 GeV and a flat-top current profile of 4 kA for a bunch length of 20 micron is considered here. The Twiss parameters are matched to the initial cell in order to have minimum beam size variation along the undulators. Table 1, shows the beam parameters used in the simulations. For this study the electron beam trajectory along the undulator cells is used as an input for our ML model and the radiation properties like radiation pointing, divergence and spectral intensity regarded as outputs.

Electron beam trajectory can be recorded by using beam position monitors (BPMs) in a real machine. Therefore, the horizontal and vertical electron beam offset after each undulator section was recorded in the simulation. Furthermore, the electron beam trajectories were disturbed by introducing initial offsets in position and momentum and as a result, the electron bunch performs transverse oscillations in the external focusing field imposed by quadrupoles between the undulator sections. The offset range was chosen such that the radiation intensity dropped by a maximum of 50 percent.

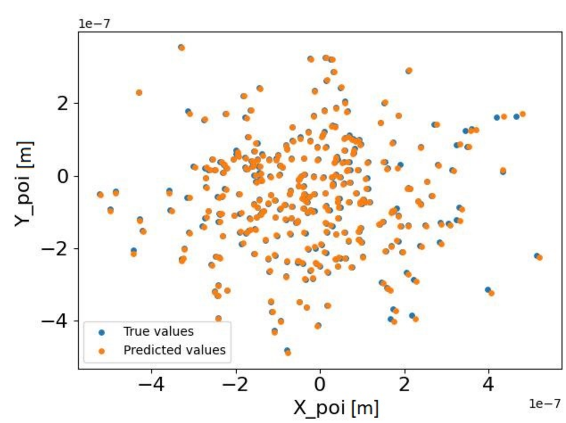

Figure 1: Radiation pointing prediction.

* farzad.jafarinia@desy.de

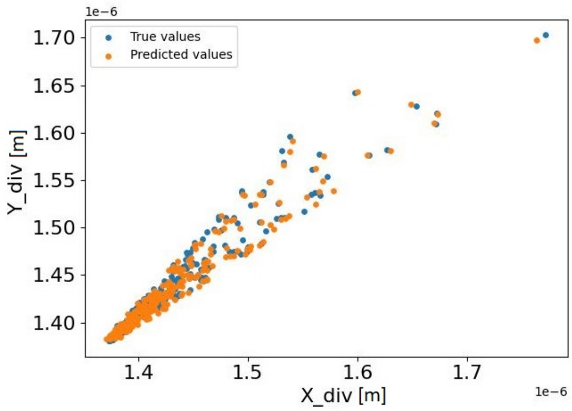

Figure 2: Radiation divergence prediction.

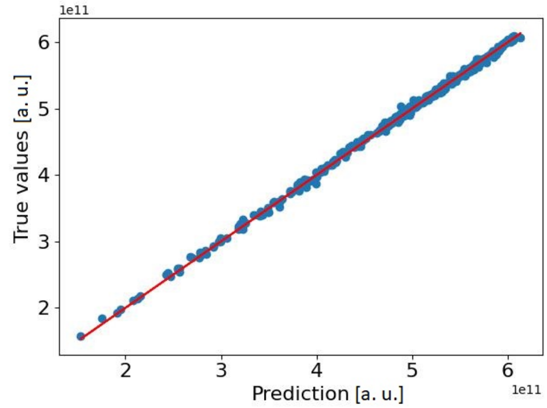

Figure 3: Spectral intensity prediction.

Pointing Prediction

We utilized horizontal and vertical electron beam offset after each undulator section as inputs and radiation pointing as outputs to train the machine learning model. The dataset consisted of 300 data points, and we employed a grid search approach to identify the optimal hyperparameters for the neural network (NN) model. The optimized model consisted of two hidden layers with 8 and 4 neurons, a batch size of 32, a learning rate of 10^{-3}, and an epsilon value of 10^{-7}.

The model's performance was evaluated by calculating the root mean squared error (RMSE), resulting in an approximate value of 2.5×10^{-3}, indicating a high degree of accuracy in predicting the radiation pointing. Furthermore, we evaluated the performance of the model using the R^2 score, which measures the goodness of fit between the predicted and actual values, was found to be 0.998, indicating an excellent correlation between the predicted and actual values.

The results of the prediction are depicted in Fig. 1, where the true and predicted values of the horizontal and vertical radiation pointing at the end of the beam-line are plotted.

Divergence and Spectral Intensity Prediction

In addition to predicting radiation pointing based on electron beam trajectory data, we also explored the prediction of other critical radiation properties such as radiation divergence and spectral intensity. To optimize the ML models, we conducted a grid search, which resulted in the selection of the same neural network architecture for both cases. The selected model consisted of two hidden layers with 64 and 32 nodes, a batch size of 8, a learning rate of 10^{-3}, and an epsilon value of 5×10^{-7}.

The accuracy of the predicted radiation divergence and spectral intensity was assessed using the RMSE metric, which was found to be approximately 6.1×10^{-3} and 6.6×10^{-3}, respectively. The R^2 score for predicted radiation divergence was 0.996, and for spectral intensity, it was 0.998.

The results of the prediction for radiation divergence and spectral intensity are plotted in Fig. 2 and 3, respectively. The plots illustrate the accuracy of the ML models in predicting these radiation properties, demonstrating the potential of ML models to accurately predict various critical properties of X-ray pulses.

TRANSITIONING TO MEASUREMENTS

Based on our analysis, it is evident that the electron beam trajectory data alone can accurately predict the most critical properties of X-ray pulses. However, it is important to consider various degrading effects such as undulator detuning, field error, and beam yaw that can potentially impact the radiation properties. While our simulations did not account for these effects, it is crucial to incorporate them while training the ML models to ensure their accuracy in real-world scenarios.

Furthermore, our investigation revealed that the ML models were unable to accurately predict the final output when there was an initial correlation in the X-Z beam phase space ($R15 > 0$). This highlights the importance of training the ML models with data that includes cases with errors and expected effects that may arise during real measurements.

Therefore, to optimize the performance of ML models in predicting X-ray pulse properties, it is essential to consider the impact of degrading effects and train the models using data that reflects real-world scenarios, including cases with errors and expected effects. By doing so, we can ensure the accuracy and reliability of ML models in predicting X-ray pulse properties.

Toward an Online ML Model

The European XFEL is able to provide X-rays with energies ranging from 0.25 keV to 25 keV using three SASE undulators. These undulators are powered by a superconducting linear accelerator that uses TESLA technology. The electron beams are allocated to three distinct beamlines in each pulse, allowing for simultaneous operation of three experiments [7, 8].

The implementation of an online ML model for predicting X-ray pulse properties as a virtual diagnostics involves three stages: data acquisition, feature extraction, and model training. Here we briefly describe each stage, including the necessary requirements in developing this concept for the XFEL beamlines at DESY.

BPMs installed in the beam-lines allow the recording of the electron beam trajectory as it travels through the undulator sections. The generation of angular and spatial offsets can be achieved by using orbit correctors located upstream of the initial cell. The impact of these offsets on the electron beam properties and final radiation, such as radiation pointing, divergence, and intensity, can be analyzed using appropriate downstream diagnostics. The X-ray Gas Monitor Detector (XGMD) measures the total pulse energy of each individual FEL pulse and FEL imagers can be used to measure the FEL beam position, shape and pointing.

In the data conversion and feature extraction phase the recorded data (electron and photon data) are merged and processed to extract the necessary features and parameters required for model training. One such feature is the center-of-mass (COM) of the radiation on the FEL imager screen, which serves as a proxy for radiation pointing and is used as the output target in our ML model. Additionally, other radiation properties such as skewness, kurtosis, and beam size can be computed from the image on the FEL imager screen by fitting the data to a Gaussian distribution. To improve the prediction accuracy, we include XGMD values as an additional input along with the BPMs data in our model.

After the feature extraction phase, the combined data is split into training and validation sets for model training and evaluation. In the training stage neural networks algorithm is used to build the model and the performance of the model is evaluated using metrics such as mean squared error (MSE), RMSE, and R^2 score.

To optimize the performance of the model, we perform a grid search for hyperparameter tuning, such as the number of hidden layers and nodes. By systematically exploring different hyperparameter combinations, we can find the best set of hyperparameters that yield the most accurate predictions. Once the model is trained and validated, it can be implemented in real-time to optimize the FEL performance and improve experimental outcomes.

CONCLUSION

In this study, we have presented our preliminary work on developing virtual diagnostics for the XFEL machine at DESY using machine learning techniques. Our ML model, which is based on simulation data, shows accurate predictions of radiation properties, such as radiation pointing, divergence and spectral intensity, using electron beam trajectory data as inputs. We have also discussed the potential implementation of a virtual diagnostics system and the necessary steps for its integration into the beamlines of the XFEL facility at DESY.

Overall, our study highlights the potential of machine learning in developing virtual diagnostics for XFEL machines, which can lead to more efficient and reliable operation of these complex instruments. We envision that our work will pave the way for further developments in the field of virtual diagnostics, and ultimately contribute to the scientific community by enabling more precise and efficient experiments at XFEL facilities

REFERENCES

[1] Z. Huang, K-J. Kim, "A review of x-ray free-electron laser theory", *Phys. Rev. Spec. Top Accel Beams*, vol. 10, p. 034801, 2007. `doi:10.1103/PhysRevSTAB.10.034801`

[2] A. Hanuka et al., "Accurate and confident prediction of electron beam longitudinal properties using spectral virtual diagnostics", *Sci. Rep.*, vol. 11, no. 1, pp. 1–10, 2021.

[3] A. E. Pollard, D. J. Dunning, and M. Maheshwari, "Learning to Lase: Machine Learning Prediction of FEL Beam Properties", in *Proc. ICALEPCS'21*, Shanghai, China, Oct. 2021, pp. 677–680. `doi:10.18429/JACoW-ICALEPCS2021-WEPV020`

[4] J. Zhu, Y. Chen, F. Brinker, W. Decking, S. Tomin, andH. Schlarb, "High-fidelity prediction of megapixel longitudinal phase-space images of electron beams using encoder-decoder neural networks", *Phys. Rev. Appl.*, vol. 16, p. 024005, 2021. `doi:10.1103/PhysRevApplied.16.024005`

[5] A. Edelen, N. Neveu, C. Emma, D. Ratner, and C. Mayes, "Machine learning models for optimization and control of x- ray free electron lasers", in *Proc. NeurIPS Machine Learning for the Physical Sciences Workshop (NeurlPS2019)* , Vancouver, Canada, 2019.

[6] S. Reiche, "GENESIS 1.3: a fully 3D time-dependent FEL simulation code, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, Vol. 429, Issues 1–3, pp. 243-248, 1999. `doi:10.1016/S0168-9002(99)00114-X`

[7] W. Decking *et al.*, "Status of the European XFEL", in *Proc. IPAC'19*, Melbourne, Australia, May 2019, pp. 1721–1723. `doi:10.18429/JACoW-IPAC2019-TUPRB020`

[8] L. Frohlich *et al.*, "Multi-Beamline Operation at the European XFEL", in *Proc. FEL'19*, Hamburg, Germany, Aug. 2019, pp. 335–338. `doi:10.18429/JACoW-FEL2019-WEP008`