# Letter of Interest: Application of Machine Learning to Particle Accelerator Simulations

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Machine learning and neural networks have been used with great success in many areas of physics. First attempts have been made to utilize these powerful computational tools for simulations of particle accelerators. In this Letter of Interest, we briefly summarize the ongoing efforts and describe planned uses of machine learning for optimization, uncertainty quantification and tuning assistance in the realms of particle accelerator design and operation.

## I MOTIVATION

Machine Learning (ML) has seen massive progress in the past decades. Its successful application in computer vision and the establishment of many software packages that are widely available and standardized has led to attempts to use ML in almost all fields of science. ML has become a staple of modern computing and particle accelerator physics should benefit from this progress. In Section II we will briefly describe some of the ongoing efforts to utilize ML in the simulation, design, optimization, and tuning of particle accelerators. In Section III, we outline some of the necessary steps forward to make ML more accessible and applicable to particle accelerator physics. Finally, we present IsoDAR as a project where we plan to use ML to optimize the design, perform a thorough error analysis, and assist with machine tuning.

## II CURRENT EFFORTS

The current uses of ML in accelerator physics can loosely be divided in several groups, either by application or technique. Techniques are: surrogate models, computer vision and Bayesian optimization (using Gaussian processes or neural networks). Applications are then in design optimization, (virtual) diagnostics, online tuning, anomaly detection, error analysis, etc.

### A. Surrogate models

Surrogate models can be built by training a neural network on a smaller (compared to other optimization techniques) set of high fidelity simulations (often particle-in-cell) that coarsely maps out the hyperspace of possible input parameters. Non-simulated sets of input parameters can then be approximated by the surrogate model. This can be highly useful for optimization and online feedback about the accelerator. Some examples of successful use of surrogate models in particle accelerator optimization are [1–4]. A speedup of one to several orders of magnitude compared to conventional techniques has been observed in these cases.

### B. Computer vision

Arguably, the best established use of ML is image analysis using convolutional neural networks. These methods can also be used in the analysis of beam diagnostic devices like optical fibers, emittance scanners, and residual gas monitors or reconstruction of beam pulse structure [5].

### C. Bayesian Optimization

Bayesian optimization is a tool for global optimization with noisy evaluations. An example of successful use of this technique is the tuning of SwissFEL [6, 7]. Another example of Bayesian optimization, using Gaussian Process models is given in [8] for the Linac Coherent Light Source (LCLS).

## III THE PATH FORWARD

### A. Surrogate Models

Important steps forward to make surrogate models widely usable have been identified in a separate LOI [9]. The main paths forward are *finding the best practices* for various different accelerator systems and modeling needs thereof, and *developing a robust and flexible framework* for surrogate modeling.

### B. Other

In the ML community, there is research ongoing to create inverse ML models. If successful, a high fidelity inverse model can replace complex and time consuming multi objective optimisation. This would pave the way for high fidelity and on-line based optimisation.

Creation of ML toolboxes geared towards particle accelerators that are accessible, relatively easy to use and compatible with the well-established simulation codes. One such effort is ongoing at RadiaSoft [10].

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## IV PLANNED APPLICATION OF ML IN ISODAR

IsoDAR [11] is a proposed search for sterile neutrinos using a decay-at-rest $\bar{\nu}_e$ source in close proximity to a kiloton scale scintillator detector. In order for the experiment to be decisive within 5 years, a primary proton current of 10 mA cw is needed on target. The situation is further complicated by the necessity to install the driver and target ($\bar{\nu}_e$ production) underground. A compact cyclotron with RFQ injection [12] has been designed, that accelerates $H_2^+$ instead of protons to alleviate space charge effects, utilizing *vortex motion* to keep the bunches compact during acceleration [13]. This has to be carefully simulated and all aspects of the system benefit from optimization. The IsoDAR collaboration plans to augment their design and simulation effort with ML techniques similar to those described in [4]. Specifically, these systems are going to be optimized using ML:

- Ion source LEBT and coupling to RFQ (proof-of-principle for ML in IsoDAR).
- Cyclotron central region and RFQ matching to cyclotron.
- Cyclotron acceleration to 60 MeV/amu and vortex motion

It is envisioned that surrogate models will then be available for online feedback during commissioning and tuning up of the system. Feedback from measured beam data will enhance these models, which will then be available to the operators during production runs.

By augmenting ML models with data from real machine such as IsoDAR, the community at large will gain understanding of fidelity and accuracy of such ML models. The non-trivial topology of the cyclotrons will serve as a complex real world example (template). In this unique setup, techniques such as transfer-learning can be studied. Such a research project has the potential to lead to an *universal machine leaning inspired surrogate model* for a wide range of accelerators: linear accelerators, synchrotrons and complex beam lines such as therapeutic gantries.

## V CONCLUSION

We have presented a small glimpse into the ongoing efforts of incorporating ML into particle accelerator physics through surrogate models, optimization, computer vision, and anomaly detection. Though these studies are exciting and highly encouraging, there is a lot to be learned about making these models stable and reliable, as well as approachable also for scientists not well versed in computational physics and ML. We have identified a few paths forward to incorporate ML more into the day-to-day work of accelerator design and operation. We believe, that a mid-scale project like IsoDAR could be a test-bed for incorporating ML into the design process at an early stage and use various aspects of it, all the way through from the early prototype testing to running the full machine.


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