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ACHIEVING DIVERSE BEAM MODES WITH MODELLING AND OPTIMISATION FOR THE VERSATILE SRF PHOTOELECTRON GUN AT SEALAB

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Abstract

The SEALab facility in Berlin is home to an R&D superconducting radio-frequency (SRF)photoinjector and electron diagnostics beamline. Designed to support multiple varied applications - ranging from Energy Recovery Linac (ERL) to Ultrafast Electron Diffraction (UED) and Electron-Beam Water Treatment (EBWT) - the photoinjector requires flexible, high-precision tuning to support these diverse beam modes. These applications span over three orders of magnitude in bunch charge, emittance, and current, alongside picosecond to sub-picosecond pulse lengths. This makes the accelerator setup and tuning a significant challenge. With the world's first beam achieved at a SRF photoinjector from a Na-K-Sb cathode, a suite of analytical and computer-aided models have been developed to support understanding of the beam dynamics in the injector, even where no observations are possible through virtual diagnostics, and to support the commissioning process. These models include a first-order analytical model based on equations of motion, particle tracking simulations with the ASTRA code, and a machine-learning surrogate model trained for achievable operation ranges during commissioning. These models are coupled with a Multi-Objective Bayesian Optimisation (MOBO) algorithm to enable rapid tuning across multiple beam modes. This combination of surrogate modelling and optimisation algorithm reduces optimisation timescales from hundreds of hours to minutes, allowing near-real-time tuning for the accelerator. This paper presents the modelling framework, its validation, and its application to photoinjector multi-mode optimisation.

INTRODUCTION

SEALab is an accelerator R&D faciilty aiming to study Superconducting Radio-Frequency (SRF) photoinjector designs for future applications. The aim is to develop a photoinjector platform which could serve diverse applications such as Energy Recovery Linac (ERL) technology [1], Ultrafast Electron Diffraction (UED) [2], or Electron Beam Water Treatment (EBWT) [3]. These applications require highly diverse beam parameters spanning orders of magnitude (see Table 1) whilst maintaining high quality and stability. Since downstream beam properties are limited by the properties of the beam generated in the photoinjector, achieving such a range of parameters is contingent on efficient and precise control of the electron beam qualities produced by the gun.

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The beam parameters required for different applications are often competing (for example, bunch length and transverse emittance are coupled with the peak current). This requires identifying trade-offs during optimisation runs of these beam modes. This has previously been achieved through Multi-Objective Genetic Algorithms (MOGA) which are time consuming and not applicable for near real-time optimisations [4]. A faster and more efficient approach is required to reach this goal, for which Multi-Objective Bayesian Optimisation (MOBO) presents a promising option [5]. MOBO is more sample-efficient and better suited for online tuning with large parameter spaces.

This paper presents first a linear analytical model of the gun and solenoid, secondly a machine learning-based surrogate model trained on Particle-In-Cell (PIC) simulations generated using A Space Charge Tracking Algorithm (ASTRA), and thirdly a MOBO algorithm which, when paired with the machine learning surrogate model, efficiently identifies optimal injector settings for the varying beam modes.

The SRF photoinjector, schematically shown in Fig. 1, consists of a normal-conducting Na-K-Sb photocathode embedded in a 1.4-cell SRF cavity, initiated by a 522 nm drive laser [1]. The standard setup considered for the basis of this model reflects the machine at the time of commissioning with a beam of 7 pC bunches at a current and emittance of 1 μA and 1 mm mrad respectively, and to operate with electric field strengths between 10 MV/m and 40 MV/m.

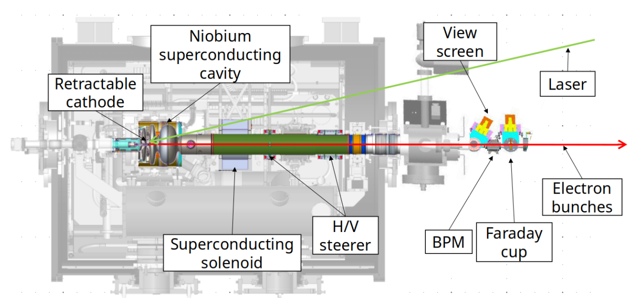

Figure 1: The SEALab photoinjector consists of a 1.4-cell Nb cavity housing an Na-K-Sb photocathode, an emittance-compensation solenoid and horizontal and vertical kicker magnets.

MODELLING

In this section, an analytical model and a machine learning surrogate model are introduced. ASTRA tracking simulations are used as the high-fidelity benchmark for these

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Table 1: Design Parameters for SEALab Applications

Parameter	ERL	UED	EBWT	Models
Bunch charge	77 pC	0.1 pC	77-500 pC	7 pC
Emittance	<1 μm	10^{-3} μm	1-6 μm	1 μm
Pulse length	2-3 ps	1 fs	2-10 ps	10 ms
Kinetic energy	50 MeV	6-10 MeV	<10 MeV	2.5 MeV
Repetition rate	1.3 GHz	100 kHz	1.3 GHz	1.4 kHz
Average current	100 mA	100 nA	20-100 mA	10 nA

models, since ASTRA simulations, including space-charge effects, themselves are too time-consuming to be used for online optimisation.

Analytical Model

For generation of rapid insights into first-order beam dependencies and beam parameter propagation in the SRF photoinjector itself, an analytical model has been developed, shown in Fig. 1. This model is useful during the early stages of commissioning when beam diagnostics are limited and fast estimates of parameter corrections are required.

This model treats the beamline as a series of linear optical elements, approximating the SRF gun as a drift space followed by a thin lens approximation for the cavity, a solenoid, and a second drift section to the screen. This formalism follows the transfer matrix approach outlined by [6].

The total beamline is therefore represented by a linear transfer matrix which determines the information for the longitudinal and transverse phase space. This method retains closed-form solutions, enabling fast propagation of parameters. This is achieved by making several assumptions. Namely, no higher-order effects, like space charge, are included, the solenoid focussing is linearised, and an ideal, monoenergetic beam is assumed to travel through ideally aligned beamline elements. These assumptions break down at low accelerating gradients. In addition to this, the cavity field is modelled as a purely sinusoidal standing wave, which neglects discrepancies in field shape at the location of the iris, the amplitude of the second peak, and the location of the second peak. These are caused by the uniques features of the photoinjector. The emission are is not located in in the backwall of a 0.5cell idealised cavity but slightly retracted inside a 0.4cell real cavity. These differences produce difficulties in modelling this field.

Nonetheless the analytical model provides valuable insights into beam dynamics through fast, closed-form solutions to the first-order, linear transfer matrices. The speed of these insights makes this model useful for initial commissioning and tolerance studies where the sensitivity of the beam to each control parameter can be estimated and initial parameters values can be suggested. This model is fast, but lacks the accuracy of other models. Therefore, it cannot be used for detailed studies, beyond first-order approximations, or for any online beam-based machine corrections.

Surrogate Model via Neural Network

In order to develop a model for the beam dynamics which has increased accuracy to the analytical model and a reduced running time to the ASTRA simulations, a neural network-based surrogate model is developed for the SRF photoinjector beamline. This model can then also include realistic field distributions inside the SRF gun caviy and the solenoidal field.

The surrogate model developed here builds on previous work to build a machine-learning surrogate model for this machine [7]. The model in this paper uses a fully-connected multilayer perceptron, trained on 400,000 ASTRA simulations, and takes in six input parameters (bunch charge, laser pulse length, laser spot size, emission phase, gun gradient, solenoid strength) and gives predictions for sevem output parameters (longitudinal and transverse emittances, bunch length, kinetic energy, energy spread, transverse divergence and spot size). The resulting predictions are accurate within 6.6% of the ASTRA simulation. Once trained, this neural network replaces ASTRA simulations as a look-up table and predictions about beam characteristics can be made almost immediately, reducing the time taken from minutes to less than a second.

The speed and accuracy of the predictions from this model makes it ideal for online use and integration into optimisation algorithms and virtual machines.

MULTI-OBJECTIVE BAYESIAN OPTIMISATION

In order to achieve high-quality machine performance in all required machine modes, simultaneous optimisation of many beam parameters needs to be conducted. Optimising many of these parameters is a conflicting endeavour and requires identifying a trade-off which is most appropriate for the situation at hand, such as minimising bunch length and transverse emittance for UED applications. To address this problem, Multi-Objective Bayesian Optimisation (MOBO) is employed.

MOBO is a class of machine learning-based algorithms which use a Bayesian interpretation of statistical Gaussian-Process models to identify the set of optimal trade-off solutions between multiple objectives: the Pareto set. The Pareto set of solutions is then passed to a human operator that can make an informed decision on which solution to put onto the machine.

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MOBO aims to solve for the vector which optimises the objective function $f(x)$ [8]. In this case, $f(x)$ is a vector of objectives (minimise bunch length, minimise transverse emittance). For SEALab optimisations, the Upper Confidence Bound Hyper Volume Improvement (UCB-HVI) acquisition function is used, similar to work undertaken by Ji [9], allowing control over the exploration-vs-exploitation parameter. This acquisition function maximises the dominated hypervolume between the current Pareto front and a defined reference point. In addition to this, a kth-nearest-neighbour penalty is applied to further mitigate local optima.

MOBO works by iteratively sampling the parameter space and improving its search, based on the performance of the results of previous iterations. The exploration of the parameter space is guided by Gaussian Process (GP) models, which act as surrogate models for the real accelerator's behavior, enabling faster optimisations with fewer time-consuming measurements from either the machine itself or computationally-expensive simulations. MOBO balances the exploration of new, unprobed parameter space and exploitation of known optima in parameter space, allowing for efficient navigation through high-dimensional parameter spaces. This makes MOBO well-suited for problems in high-dimensional space where the objective functions are not known and where few initial data points are available, such as the optimisation of beam modes of the SRF photoinjector.

Measurements for the MOBO algorithm are taken from the machine learning surrogate model in lieu of the physical machine, but will migrate to the machine in the coming weeks. An example of the results of MOBO with the surrogate model are shown in Fig. 2, demonstrating the active searching for the Pareto set to optimise the trade-off for setup of a UED mode as mentioned above.

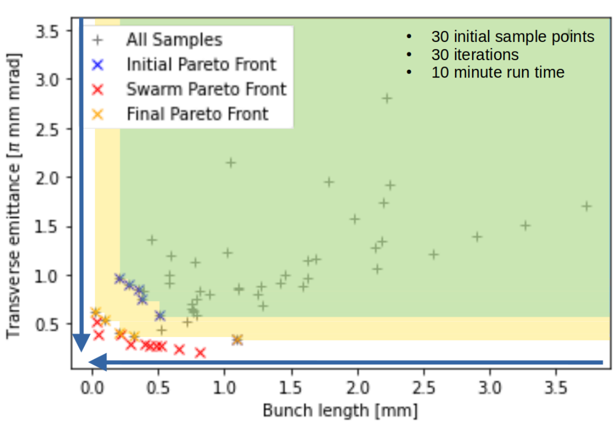

Figure 2: An example of the MOBO algorithm minimising bunch length and transverse emittance simultaneously. The dominated hypervolume is shaded for the initial (blue) and final (gold) Pareto fronts.

Figure 2 shows how the initial Pareto front in blue has evolved after only 30 iterations to find the reference Pareto front (found using a swarm optimisation) in 10 minutes. In an equivalent MOGA optimisation, 22 iterations are needed to find this Pareto front, each taking 10s of minutes. This shows the efficiency of the MOBO algorithm at finding the true Pareto front and exploring along the curve, avoiding local optima. The algorithm is initiated with only 30 samples, demonstrating the sample-efficiency that MOBO provides.

MOBO is efficient for multi-dimensional space. However, for each iteration a GP model is built for each input dimension. This causes the computational time to increase exponentially when dimension space becomes very large (around 2 dimensions). This effect is already noted from around 6 dimensions onward. Thus, it is appropriate for the optimisation of the gun using the 6-input parameter space chosen for the surrogate model, but dimension reduction techniques will need to be employed for higher dimensional problems.

The integration of MOBO with a surrogate model significantly reduces the time required for identifying initial, optimal solutions at the start of each operation, enabling more efficient commissioning and operation of the SRF photoinjector. Machine operation envisioned at SEALab requires many beam modes for many applications and therefore frequent machine reconfiguration. Optimising important parameters at each machine setup is essential to ensuring this can be done swiftly and reliably. Currently, MOBO is validated on ASTRA simulations and indicates good agreement. This optimisation scheme will be implemented on the accelerator in the coming months.

CONCLUSIONS

In order to achieve fast and accurate control of the SRF photoinjector and produce high-quality beam across multiple beam modes, a comprehensive understanding of beam dynamics is required. This paper demonstrates three beam dynamics models: an analytical model, particle tracking simulations and a machine learning-based surrogate model. Each model provides essential information about beam behaviours and plays a distinct role in the practical commissioning of the machine.

Multi-Objective Bayesian Optimisation (MOBO) has been implemented using a surrogate model for offline evaluation of each iteration of the algorithm. MOBO is proven to be effective for optimising conflicting machine parameters in high-dimensional space with a limited quantity of initial data points and reduces optimisation time from tens of hours to 10 minutes.

The combination of beam dynamics modeling techniques and optimisation algorithms helps to streamline SEALab's commissioning process and enhances operational efficiency. These tools will be critical as the facility progresses toward delivering high-quality beams tailored to various scientific and industrial applications.

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