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FEL OPTIMIZATION: FROM MODEL-FREE TO MODEL-DEPENDENT APPROACHES AND ML PROSPECTS

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Abstract

Users beam-time at modern FEL sources is an extremely valuable commodity. Moreover, maximization of FEL up-time must always be performed accounting for stringent requirements on the photon pulse characteristics. These may vary widely depending on the Users requests, which poses challenges to parallel operation of high-repetition rate facilities like the European XFEL. Therefore, both model free or model-dependent optimization schemes, where the model might be given, or provided by machine-learning approaches, are of high importance for the overall efficiency of FEL facilities. In this contribution we review our previous activities and we report on current efforts and progress in FEL optimization schemes at the European XFEL. Finally, we provide an outlook of future developments.

INTRODUCTION

Automatic optimization of accelerator performance is part of the daily operation procedures at the European XFEL [1,2] and other FEL facilities, e.g. [3-5]. The dedicated tools help to tune machines performance faster and more efficient (multidimensional optimization) in comparison to manual tuning. However, the tuning of the large-scale facilities as the European XFEL remains a time-consuming procedure. Moreover, the best machine performance is usually achieved for the most explored operation modes, see Fig. 1, which also points to the importance of optimization procedures. Figure 1 shows dependence of the photon energy against the photon pulse energy for the hard X-Ray undulator SASE1. The colour shows number of machine files – a snapshot of the machine in a stable state. As it can be seen, one of the most frequently used photon energy is around 9–9.3 keV, where the maximum photon pulse energy was around 2.7 mJ. At longer wavelengths, for example 8 keV the maximum photon pulse energy was half as much.

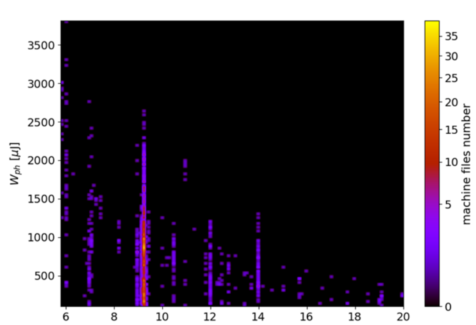

Figure 1: EuXFEL SASE1 performance statistics.

Taking into account high pressure on the machine availability for parallel multi-user operation, the European XFEL is looking for more automation of optimization procedures and new effective approaches to speed up the machine performance tuning.

The analysis of the collected optimization logs performed by OCELOT Optimizer [6] shows that one of the problems is the high dimensionality of parameter space that needs to be explored in the optimization process. For example, 446 unique devices have been used in optimizations at the European XFEL to maximize the SASE pulse energy within the last 2.5 years [2]. Although the frequency of use of a particular set of devices varies. It can still give an indication of how complex the tuning is. Another obstacle to fast and efficient machine tuning is that hyperparameters of optimization algorithms and set of devices which need to tune specific physical parameters, e.g. beam matching, are not always optimally selected, which also affect efficiency. In this paper we will consider the current state of optimization methods used in the European XFEL, and possible ways to overcome the problems discussed.

MODEL-FREE OPTIMIZATION

The main tool for a model-free SASE optimization in the European XFEL is the OCELOT Optimizer. It is the next generation of the SASE optimizer developed for FLASH [6] but with the possibility of creating/modifying an objective function by the operator. Each optimization is logged including an objective function and actuator changes during optimization and can be analyzed afterwards. The tool was deployed in the EuXFEL control room at the beginning of 2017. Since then we collected experience of more than 6000 optimizations (Fig. 2). More details of OCELOT optimizer statistics analysis can be found in [2].

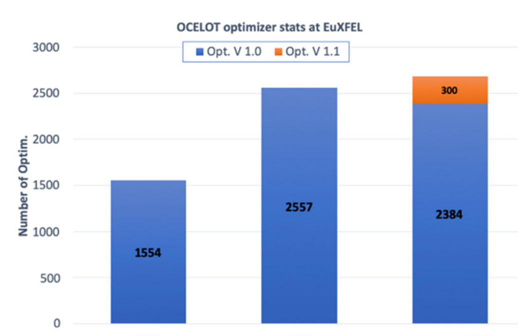

Figure 2: OCELOT optimizer statistics.

As it was mentioned above high dimensionality of the parameter space is one of the problems for fast FEL ma-

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chine tuning. Recently, the Extremum Seeking method [7, 8] was added to a family of other optimization algorithms in the OCELOT optimization toolbox [9]. One of the features of the algorithm from the optimizing point of view is the smooth change of actuator's parameters (this can be an essential advantage for tuning of mechanical devices) and the ability to find an extremum in parameter space with many (>10) dimensions, one of the examples of such an optimization is SASE maximization with 16 simultaneously tweaked phase-shifters (Fig. 3). More details and examples of optimizations at European XFEL can be found in [9].

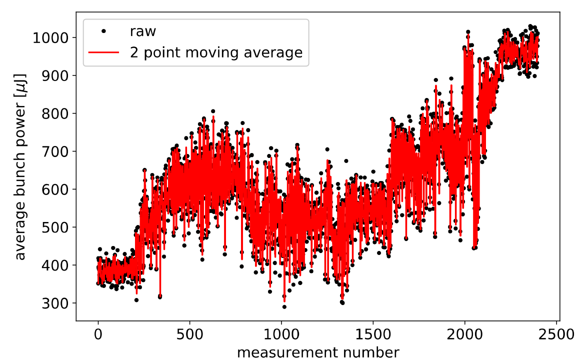

Figure 3: Extremum Seeking simultaneous optimization of 16 phase-shifters gaps [9].

A new version (v1.1) of the optimization toolbox was developed and deployed to the control room in June 2019, taking into account the proposals outlined in [2]. One of the main changes is the extension of command line interface (CLI) capabilities of the tool. The CLI offers a flexible way of using all the functions of the Optimizer without GUI restrictions. For example, the ability to connect a physical accelerator model to an optimization algorithm or run an optimization sequence. Also, the number of logged control channels in the new version was considerably increased mainly by adding channels about machine conditions to allow in the future to use ML methods for choosing the most effective optimization setups for particular machine condition.

Use of a Physics Model in Optimizations

FEL performance maximization in the European XFEL usually includes tuning of the orbit with correctors and optimizing bunch compression by tweaking RF settings as well as beam matching with quadrupoles in dedicated sections. One of the advantages of the model-independent optimization is the flexibility when an operator can apply optimization for any set of devices and any objective function. However, the flexibility has drawbacks: often chosen actuators as well as hyperparameters for the optimization algorithm (e.g. initial step size, number of iterations etc) to tune in particular the accelerator section is nearly random. In general, that affects the effectiveness of the optimization. From another side, a physical model of an accelerator can be used to define the most effective setup for the optimization, e.g. hyperparameters and/or most effective sets of actuators.

One example is the beam matching with help of the beta mismatch parameters [10] and mismatch phases tuning instead of tweaking quadrupoles directly. The advantage of this approach is that only 4 parameters with well-defined boundaries are required to tune a certain matching accelerator section with several quadrupoles. In this case, the optimization procedure looks as shown in Fig. 4. To convert the mismatch parameters into quadrupole strengths and vice versa, a physical accelerator model based on the OCELOT beam dynamics module is used [11, 12]. We tested this approach to tune a matching section in front of the SASE1 undulator. The result of such an optimization is shown on Fig. 5. The set of quadrupoles was chosen to cover a range of beta mismatch parameters $M_{x/y} = [1,\ 2]$ and phases $\psi_{x/y} = [-90, 90]$.

A similar approach can be applied for orbit tuning using the amplitude and angle of the orbit distortion instead of tweaking corrector's strengths.

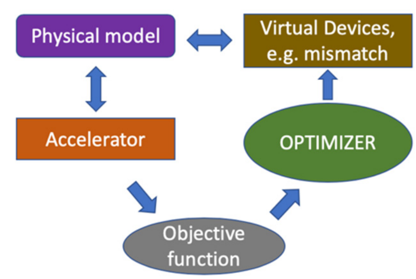

Figure 4: Optimization procedure for tuning beta mismatch parameters and phases.

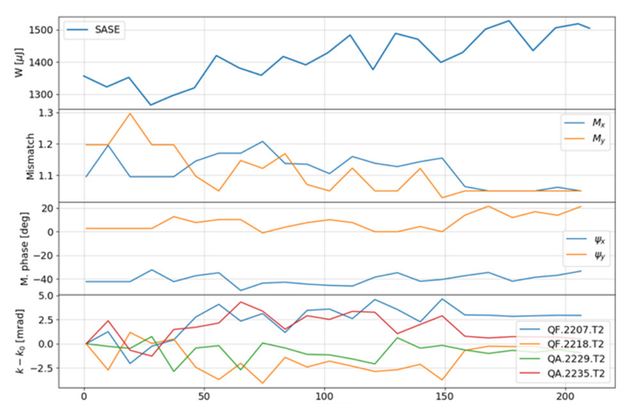

Figure 5: Optimization SASE pulse energy with beta-mismatch parameters $M_{x/y}$ and mismatch phases $\psi_{x/y}$ in matching section in front of SASE1 undulator, number iteration is 25.

Sequence of Optimizations

The ability to launch a sequence of optimizations (*Actions*) was proposed for the first time in [6]. But due to technical reasons it was not implemented but the efforts were aimed at a single optimization that affects the existing capabilities of the OCELOT graphical interface.

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Reliability and efficiency of the model-free optimizations have raised the question of applying optimization sequences without an operator intervention, increasing the level of automation of optimization procedures. As a first step we tested the capability of a new software to run predefined optimization sequence. One of the preliminary results is shown in Fig. 6, where two optimizations in a row were used to optimize the SASE pulse energy by aircoils. In addition, the software monitors the status of the machine, and in the event of a beam shutdown, the optimization is paused.

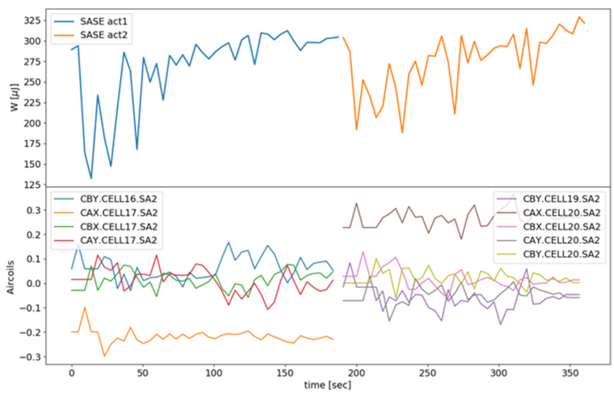

Figure 6: Sequence of optimization with aircoils in SASE2 undulator.

MODEL-DEPENDENT OPTIMIZATION

Model-based optimization methods use/build a regression model that predicts performance. The regression model may be provided, for example, either by a physical/mathematical model or by fitting the previously collected data, for example, with help of ML methods.

If the construction of a mathematical model to predict FEL performance on the real FEL facility with hundreds of free parameters - the task is extremely difficult, then a physical model of the multi-stage bunch formation system can be mathematically described [13]. This algorithm was implemented in OCELOT and was used in simulations to optimize compression scenarios with taking into account collective effects for the European XFEL accelerator [14]. The peculiarity of the algorithm is its fast convergence. Only a few iterations (<10) are required to obtain a compression scenario with the desired beam parameters. It is also planned to implement and test this approach on the accelerator.

Another example of a model-dependent optimization which is in operation at the European XFEL is a statistical optimization of the launch orbit to the SASE1 undulator. The method proposed in [15] was implemented in OCELOT under the name 'Adaptive Feedback'. Details can be found in [1]. Here, the regression model is not provided by physics or ML methods but rather by simple statistical analysis of synchronously collected data of the orbit and the SASE pulse energy. The best trajectories in terms of maximum pulse energy are averaged and used as a golden orbit by the orbit feedback. That moves the beam quickly to its best trajectory and thus it pushes the pulse energy to its maximum.

OUTLOOK AND ML METHODS

Model-free optimization methods were widely used during commissioning and further in daily operation of the European XFEL. A model-based method such as the adaptive orbit feedback proved to be extremely useful and more advantageous compared to purely empirical methods.

Recently, new approaches have been developed with the aim to reduce tuning time. One of them is the Bayesian optimization utilizing Gaussian process [4, 16, 17] that allows to find the extremum of an objective function faster than, for example, the Nelder-Mead algorithm [18]. The version of the Bayesian optimization described in [4] was included to a family of optimization methods of the Optimizer but not yet tested at the European XFEL.

The other approach uses a combination of two methods: a machine learning technique, which suggests a working point close to the global minimum based on the previously collected data, and a model-independent optimization, which explores the proposed area and makes final optimization [19].

A third approach, which we can note, is virtual diagnostics, which is not directly related to the optimization, but can be used to get additional information about the electron and/or photon beams properties, which in turn can be used for machine or experiment performance optimization [20,21].

The approaches described are promising, but the lack of infrastructure to collect, process, cleanse and analyse these large volumes of data is one of the main obstacles to integrating these methods into the accelerator control systems for daily use. The importance of the problem has been recognized and the high level control teams are making efforts to create a more user-friendly control room environment for machine learning applications, for example, see [22].

CONCLUSION

We present the status of the existing optimization procedures used at the European XFEL accelerator, as well as new approaches including test results.

A new version of the OCELOT Optimizer was recently launched. The main difference are the advanced features of the command line interface, which allow us to perform various types of optimizations in script mode. Thus, we are now able to run an optimization sequence without operator intervention and use the physical accelerator model to determine hyperparameters in some types of optimizations.

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