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ON-LINE OPTIMIZATION OF EUROPEAN XFEL WITH OCELOT

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Abstract

FEL tuning and optimization within the OCELOT framework [1, 2] has been implemented in 2015 and has been since used for SASE pulse energy optimization at FLASH [3] and later at LCLS [4], as well as injection efficiency maximization in the Siberia-1 storage ring [5]. For the European XFEL [6] commissioning purposes the code was considerably improved and additional set of tools has been introduced. Here these tools and experience of their use during the European XFEL commissioning and initial operation will be presented. Future development directions will be outlined.

INTRODUCTION

Tuning of performance parameters such as photon pulse energy, beam pointing, or spectral width, are a considerable part of daily FEL operation. When done manually, such tuning is lengthy as tedious. Moreover, it has to be repeated often due to limited machine reproducibility. While tuning the whole machine might require human expertise, tuning a particular subsystem using a limited number of actuators can be done automatically by maximizing or minimizaing a certain objective function with standard functional minimization methods. Such approach was implemented for SASE tuning ([3,5,7]). The diffuculty in this approach lies primarily with processing (averaging) of detector data, defining hardware parameter limits, identifying the most effective control parameters, and selecting the objective function. This approach was extended to minimizing arbitrary objective functions, and an appropriate GUI was created. Examples of use of such a generic optimizer are given below.

Optimization based on function minimization typically results in significant changes of the objective function during the optimization process. So, a Nelder-Mead optimization of the SASE pulse energy usually leads to a significant signal drop before the optimum level is reached. This approach is thus not compatible with beam delivery to the users. It turned out that the method proposed in [8] (also implemented in OCELOT under the name ‘adaptive feedback’), based on the slow adjustment of the orbit based on recent pulse energy history, can work simultaneously with user operation and results in significant pulse energy improvement.

Other tools – dispersion and orbit correction, generic correlation tool, and an on-line optics model, were also added to the software suite and are briefly discussed in what follows.

All the examples are drawn from the operation of the European XFEL (see Fig. 1), which has been successfully commissioned and is now in operation in Hamburg [9].

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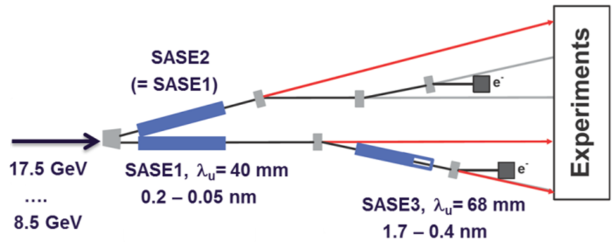

Figure 1: Schematic layout of the European XFEL beam distribution.

THE GENERIC OPTIMIZER

The Generic Optimizer is the next generation of the SASE optimizer developed for FLASH [7], and is described in this section. While initially the functionality of running through a sequence of minimization steps automatically and deciding on the stopping criteria was envisaged, presently the functionality is limited to a single optimization step, but an advanced GUI for setting that optimization is provided. Deciding on the sequence of steps is presently left to the operator. Command-line-based fully automated optimization tool is available, but rarely used. The optimizer was specifically designed to facilitate ad-hoc tuning and optimization of arbitrary subsystems, which could be expected during commissioning.

Interface to Control Systems

The architecture of OCELOT allows easy interfacing to different control systems by inheriting from the MachineIterface class and implementing the desirable API (getting and setting of scalar and vector data, definition of the photon pulse energy readout, definition of beam position and beam loss measurements). Implementations using pyDOOCS [10] and PyEpics [11] are available.

Optimization Algorithm and Noise Reduction

OCELOT extensively uses Python's NumPy (Numerical Python) [12] and SciPy (Scientific Python) [13] libraries, which enables efficient numerical computations within Python and gives access to various mathematical and optimization methods. The Generic Optimizer extensively uses the Nelder-Mead algorithm [14], which is included in the SciPy package. To deal with the photon pulse energy signal fluctuation which can “confuse” the optimization method, two steps are taken. First is averaging of the objective function. The GUI allows to choose the number of objective function readouts and time delay between

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readouts. Most of the signals at the European XFEL accelerator are available with a 10 Hz repetition rate, so averaging over 10 readings takes 1 s. This approach is used for SASE optimization. In other cases the objective function signal is usually more stable and does not require averaging. Second, setting the initial simplex size well above the noise level helps the optimization to converge to the proper value. This situation is illustrated in Fig. 2, where a simulation of a noisy Gaussian signal minimization is shown. Nelder-Mead method with a small initial simplex size (red curve) fails to find the minimum, in contrast to the method that uses a larger initial simplex (green curve). Generic Optimizer allows to define the size of the multidimensional simplex (i.e. initial step for each device) in each dimention individually.

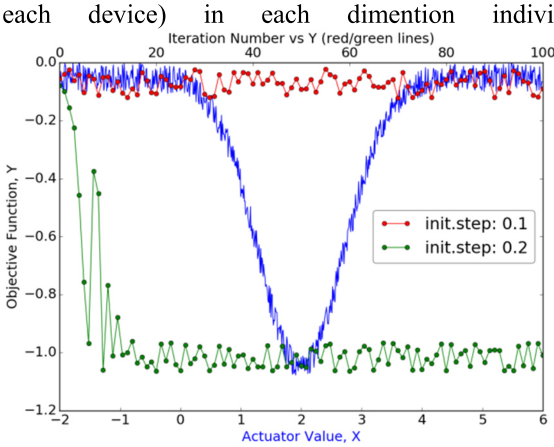

Figure 2: Objective function vs. actuator (blue curve, lower axis). Objective function vs. iteration number for different initial steps (red and green curves, upper axis).

GUI and the Objective Function Selection

The Generic Optimizer GUI is shown in Figs. 3 and 4. Device names can be added to the actuator panel via drag-and-drop. Device limits are important to provide initial guess on the parameter range where the optimum is sought. Fig. 4 shows the objective function and alarm setup panel. The alarm signal pauses the optimization if the corresponding value is out of range. In most cases, the alarm signal is generated by a charge monitor in a beam dump section. If the machine protection system (MPS) blocks the beam, the optimization will be automatically paused until the charge monitor is in the allowed range. Two options for creating objective functions are available: GUI-based and script-based. In the GUI-based approach he operator can set up to 5 devices/signals as input parameters (drag-and-drop functionality is supported as well) and write an expression for objective function. Vector signals are also supported. In the script-based approach, a text editor opens from the optimizer GUI and the objective function can be coded in Python with PyDOOCS or the OCELOT machine interface API, without any limitations.

Saving and loading configuration files (objective function, set of knobs, device limits and so on) is possible. Examples of using the Generic Optimizer for various taks are given in what follows.

Dispersion Minimization

In additional to standard dispersion correction approaches (e.g. response-matrix-based), the dispersion minimization can be performed with the Generic Optimizer, especially if the correction in a small part of the machine is desired.The objective function is then as follows:

1. Read the beam position in selected BPMs
2. Change the beam energy
3. Read the new beam position
4. Restore the beam energy
5. Calculate the dispersion, return the rms value

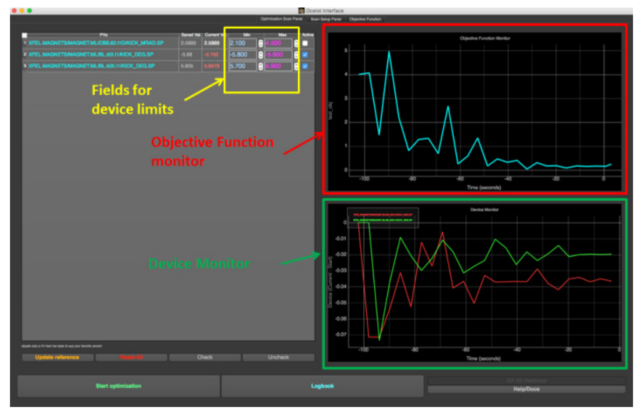

Figure 3: The generic optimizer GUI and dispersion optimization after the laser heater.

In Fig. 3 an example of dispersion minimization after the laser heater (LH) using two dipoles is shown. The correction time is approximately 1 minute.

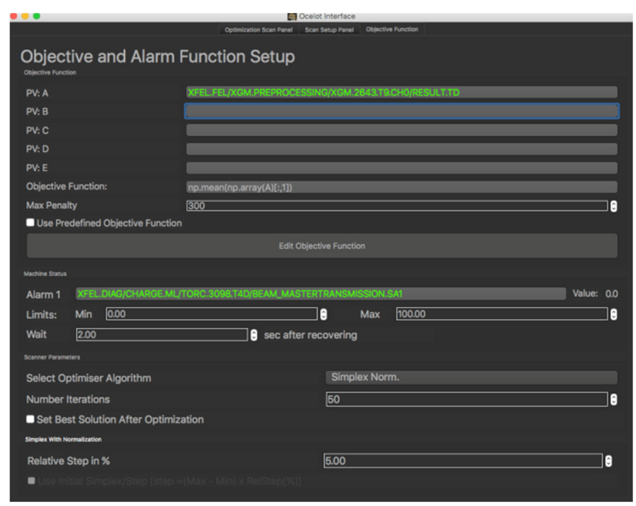

Figure 4: Objective function and alarm selection.

Orbit Distortion Compensation with Aircoils

The so-called aircoils in the undulator section compensate residual undulator field integrals, which depend on the undulator gaps. Magnetic measurements on a stand give good but often insufficient accuracy of the integrals compensation, and beam-based orbit distortion compensation with aircoils is needed. Before a tool for updating aircoil tables with beam-based measurements was in op-

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eration, such correction was done with the generic optimizer.

Beam Loss Minimization

As a part of the MPS, the Beam Loss Monitor (BLM) system ([15]) detects the electron beam losses, and the beam delivery is inhibited if a certain threshold is exceeded. Reduction of the beam losses is an important step during the accelerator start-up. For the European XFEL, even in commissioning stage the beam losses could be reduced relatively easily by manual steering of the orbit. In some cases, such task was easier to accomplish with the optimizer. The objective function, in that case, is a combination of the BLM and the BPM signals so that the optimizer tries to reduce the losses keeping a reasonable orbit.

Photon Pulse Energy Maximization

The photon pulse energy maximization is the primary goal of the Generic Optimizrer, and is extensively used for the European XFEL. Fig. 5 shows an example of SASE tuning using 4 quadrupoles in the so-called Injector DogLeg section. To make the software more generic, a minimization problem is always assumed, so the signal inversely proportional to the photon detector readout is used. The SASE level in the case shown in Fig. 5 increased from 100 μJ to 240 μJ. Generally, arbitrary photon pulse energy units are shown since several readout channels from several detectors with potentially changing calibration could in principle be used. This makes later statistical analysis of tuning data complicated and should be avoided in the future.

Figure 5: SASE tuning with 4 quads in the injector dogleg section. SASE level increased from 100 uJ to 240 uJ. Many inactive devices are seen in the actuator panel.

The most frequently used optimization procedure is the photon pulse energy maximization with orbit launch conditions in the undulators. Fig. 6 shows a SASE tuning example with 4 correctors. In the examples shown averaging over 50 SASE detector readings was used with a time delay of 0.1 s between readings.

Figure 6: SASE tuning with 4 correctors in front of the undulator section.

ADAPTIVE FEEDBACK

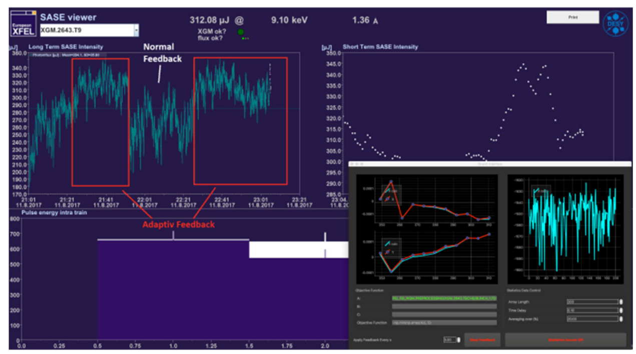

Figure 7: Example of adaptive feedback during European XFEL operation. Lower right corner shows the GUI featuring the current reference and measured orbit, and the photon pulse energy monitor.

A typical optimization of the photon pulse energy with a Nelder-Mead simplex method results in large variation of the SASE signal and is generally not compatible with beam delivery to the users. To provide optimization simultaneously with the beam delivery, and especially to address the need to periodically retune the machine during the beam delivery (since the parameter drifts cause the photon pulse energy to drop with time), we implemented the "adaptive feedback" method described in [8]. When such feedback is running, the photon pulse energy and the orbits are stored, and the orbit corresponding to the best photon pulse energy is taken as reference (more specifically, the average over orbits above 90s percentile photon pulse energy level, over 300 to 500 latest pulse energy measurements). The orbit correction to that reference orbit is then periodically performed (with a standard response-matrix-based method), usually with the 4 launch correctors only. Such feedback proved very useful in the initial stage of the European XFEL operation. An example is shown in Fig. 7.

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CORRELATION TOOL

In the spirit of data-centric control software, a generic correlation tool was introduced. So, on-line plot of orbit correlation with energy gives a real-time dispersion display (Fig. 8).

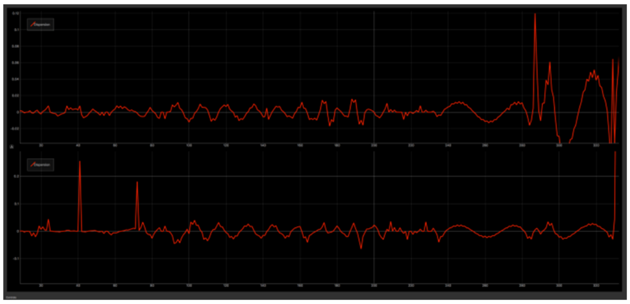

Figure 8: Correlation tool showing orbit-energy correlation (dispersion).

ORBIT AND DISPERSION CORRECTION

For the sake of providing a complete set of control tools within OCELOT, an orbit and dispersion correction tool following a standard response-matrix-based approach was developed and is in operation at the European XFEL (see Fig. 9.).

Figure 9: Orbit and dispersion correction tool.

ON-LINE OPTICS MODEL

An on-line optics model (currently using design single-particle optics, calculated with OCELOT) was introduced. The machine parameters – magnet strengths, accelerating voltages and phases – are read out on-line from the control system and fed into the OCELOT optics model. Model or measured Twiss parameters at selected locations can be used, and the optics is calculated. Then, magnet and other settings can be changed in the GUI, and projected optics changes seen (see Fig. 10). Such a tool could be of some use to operators or machine physicists to get the impression of how various knobs influence the machine, but the real long-term goal of this development is towards bridging the gap between simulation and operation, so that the amount of empirical tuning is minimized and beam physics models can be increasingly employed in machine set-up . The first step in this direction is to identify where the simulations diverge from measurements delivered by diagnostics (emittance, bunch length, optics). Steps towards advanced high-fidelity on-line simulations with all physics effects included are being taken (see [16]).

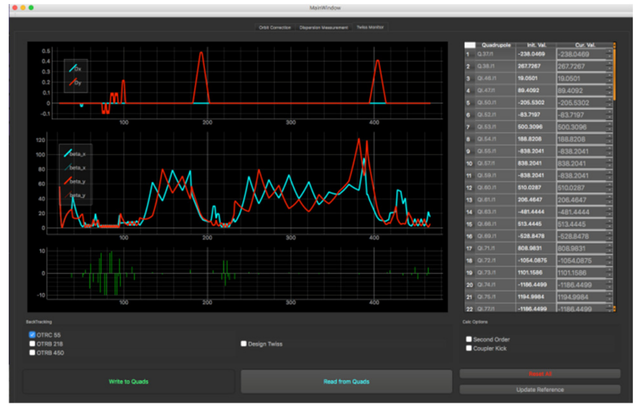

Figure 10: On-line optics monitor.

OUTLOOK

Empirical optimization methods have been extensively used during commissioning and initial operation of the European XFEL. A mixture of model-free and model-based methods such as the adaptive orbit/photon pulse feedback proves extremely useful and more advantageous compared to purely empirical methods. Boosting both statistical methods and accelerator model fidelity for operation purposes with the goal of fullest possible automation of XFEL operation is the focus of ongoing developments. Controls infrastructure issues – specifically handling of increasingly large amounts of data – has to be addressed too. Statistical or machine learning (ML) methods are to be better exploited. Such methods are better understood for pattern recognition-type problems such as image and speech recognition, spam classification, medical treatment or economic behaviour analysis, rather than control-type problems. The ML methods have advanced greatly in the past decades, benefiting from growing computing power. ML approaches are translatable to the field of physics data analysis, and have to some extent been pioneered in physics applications. Especially Astronomy and Particle Physics benefit from such methods greatly ([17,18]), where obscure patterns (faint objects, tracks of decaying particles) are searched for in a vast amount of data delivered by experimental instruments. With increasing data rates, X-ray science such as single-particle imaging also heavily relies on advanced statistical methods ([19]). ML methods for accelerator controls are gaining popularity (see e.g. [20]), with the focus on more efficient dealing with huge amounts of sensor data. In the context of control, ML methods could be used for decision-making (e.g. based on the decision tree approach [21]), but the hurdle of making ML systems more efficient than human operators is difficult to take. The usual drawback of many ML methods is that algorithms are trained to produce “black box” models that give little insight into physic and often need retraining

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when the context changes. Sometimes statistical analysis produces results which could be trivially arrived at by other means such as talking to a human expert. Some statistical analysis of FEL performance data illustrating these issues is presented in [6]. Our point of view is that for XFEL operations ML methods are probably unavoidable to reach ultimate facility performance, but should be employed on the parameter space restricted by beam physics models. To this end, both high-fidelity high-performance accelerator physics models and advanced ML methods should be pursued. It is also not to be forgotten that advanced control methods can not replace sound hardware and software engineering.

Another important direction is looking for synergies between XFEL and synchrotron light source tuning approaches ([22]), which has significance at DESY in connection with the Petra IV upgrade activities [23].

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