OCELOT: a software framework for synchrotron light source and FEL studies

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Abstract

OCELOT is a novel multiphysics simulation toolkit, which has been in development at European XFEL in collaboration with NRC Kurchatov Institute and DESY since 2011. In this paper we describe its architecture, implementation, and applications in the area of synchrotron light sources and FELs.

Keywords: Accelerators, Synchrotron radiation, Free Electron Lasers, Software

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1. Introduction

OCELOT is a novel multiphysics simulation toolkit which has been in development at European XFEL in collaboration with NRC Kurchatov Institute and DESY since 2011. It is partially based on solutions from previous accelerator physics software [1, 2]. It has already been used for calculating spontaneous and SASE radiation characteristics for the European XFEL [3], [4], and for other purposes [5]. The code is MPI- enabled and utilizes the power of the supercomputing platform at DESY [6]. The motivation was to have a consistent and easily extensible set of tools covering the whole range of physics and having features relevant for design and optimization of synchrotron radiation and FEL facilities. In such facilities electron beam dynamics, radiation production and radiation transport share technical infrastructure and need to be studied together in order to deliver the optimal photon beam quality to the experiments. Software covering this range of physics can thus facilitate such studies considerably. The emphasis on extensibilty is driven by fast advances in FEL and light source technology in recent years that call for new software features. Based on previous experience, a number of architecture solutions was used, e.g.

- 'Soft' model. Different sets of attributes might be needed in different types of calculations. For example, for electron beam optics calculations the bending angle of a dipole magnet may be sufficient, for on-line use its transfer function is required, and for calculating the emitted synchrotron radiation its exact field distribution is sometimes important; other applications might require its aperture discription, material and so on. It is counterproductive to try to standardize all potential information in advance. In our approach the level of standardization is minimal, and the model can be augmented with additional information when necessary.

- Model as Python code. Although the choice of model as Python code is restrictive, we think it is the only reasonable way to represent the 'soft' model effectively. Using language-independent technologies such as XML would create prohibitively large overheads. Moreover, as Python is becoming more widely used in scientific and engineering communities, advanced visualization, data processing, and numerical analysis packages are now available [7].

- Scripting and data are interleaved and implemented as a high-level code. Problem-specific input languages [8, 9] are restrictive with respect to scripting, since it is hard to decouple data and code on the one hand, and designing a high-level programming language is beyond the scope of almost any software project on the other hand. As an example, in accelerator physics calculations all magnet settings are almost always rematched as a first calculation step. If necessary, converters between an OCELOT model and e.g. the Accelerator Markup Language (AML) can be implemented.

- 'Apps'. The software package provides basic functionality. Concrete functionality is implemented in 'apps',

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which could be a simulation script, a web-based access to simulation data, an on-line control tool and so on.

- Abstract layer for controls interface. This allows to work with objects such as Orbit or Magnet using getters and setters for various properties. Concrete implementation of such getters and setters is control system specific and implemented as an additional module for each control system.
- Framework for single-particle and collective physics processes.

The code is open source and the latest development version is publicly available at `https://github.com/iagapov/ocelot`. The design objective was to enable all types of possible physics processes and applications. However, the implementation was following the lines necessary for the R&D of existing facilities, European XFEL [10] and Siberia-2 [11]. The currently available modules are listed in Tab. 1. In the next section we demonstrate the potential of the code on several examples. They include: spontaneous radiation calculation with long segmented undulators, where a detailed model of the electron transport is also necessary; FEL calculations, where the 'multiphysics' functionality is important; beam dynamics in synchrotrons, demonstrating the features of the electron beam dynamics module; and finally, the application as a lightweight high-level control tool.

Module	**Description**
cpbd	Charged particle beam dynamics, including: linear and nonlinear tracking, Twiss parameter calculation and matching, dynamic aperture calculation
fel	Estimates for ρ, gain length and other basic FEL parameters, 1D FEL simulations
rad	Synchrotron radiation calculations
optics	Optics (photon), ray tracing and Fourier wave methods
xio	IO based on hdf5 (`http://www.hdfgroup.org/HDF5/`)
math	Optimization and peak finding
gui	Graphical user interface utilities
adaptors	Adaptors to Genesis and SRW

Table 1: Currently available modules

2. Applications

2.1. Synchrotron radiation

An electromagnetic field solver for single-particle synchrotron radiation written in C++ and interfaced through Python was introduced into OCELOT. Moreover, a well-known undulator and synchrotron radiation code SRW [12] was interfaced. Undulator radiation parameters for the European XFEL were calculated and benchmarks performed [3] showing good agreement. Calculations taking into account emittance and energy spread are accomplished with a Monte-Carlo method. It was shown that when taking into account the combined effect of electron beam focusing, emittance, energy spread, quantum fluctuations in the electron energy and the trajectory misalignment, the peak spectral brightness of undulator radiation in the X-ray wavelength range is noticably decreased. The exact value depends on the wavelength, the length and the undulator K parameter. It can reach an order of magnitude in the case of European XFEL. Some examples are shown in Figs. 1 and 2. A more practical application of spontaneous synchrotron radiation calculations is the photon-beam-based alignment (PBBA) of the undulators [13]. OCELOT includes an app with a graphical user interface for performing such alignment. For both applications it is essential to take into account detailed description of electron optics, including focusing quadrupoles, phase shifter magnets, trajectory errors and optics beating.

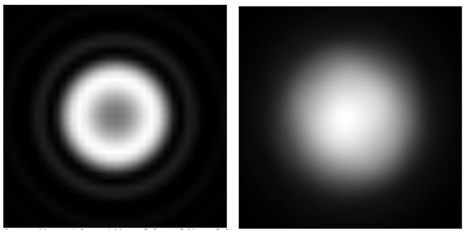

Figure 1: Right:effect of emittance (1.7×10^{-11}) on an off-resonance monochromatized undulator radiation image (24KeV), 2 undulator sections. Left: image without the emittance effect.

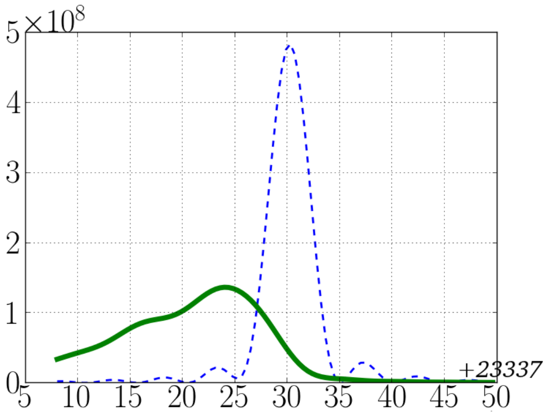

Figure 2: Effect of emittance (1.7×10^{-11}) on spectrum (solid green), 34 undulator sections, hard x-ray undulator SASE1. Dashed blue line corresponds to zero emittance. Horizontal axis is in eV, vertical in A.U.

2.2. FEL calculations

The primary objective of the code is the effective FEL calculations for the European XFEL. Whereas many topics of X-ray FEL physics can be studied analytically [14], quantitative analysis is possible only numerically. Numerical methods of FEL simulations have been in development for many years [15, 16, 17], and are now well understood. OCELOT features some numerical modules for FEL calculations. However, to predict performance characteristics with confidence, the particular implementation needs extensive testing and benchmarking. This is in particular true for more subtle questions like the transverse field profile and higher harmonics, which start playing a more important role with advanced radiation production schemes. To increase confidence, it was decided to interface a widely-used open FEL code Genesis 1.3 [18] to OCELOT. Compared to the basic Genesis functionality many additional features become available, such as optimization tools, beam electron optics matching, field transmission through crystals and some others. Moreover, the standard input description and output post-processing are readily available. The calculations of optimized radiation parameters over the whole wavelength range of the European XFEL was thus possible [4]. Such calculations involve electron beam optics matching, FEL process calculation and propagation of the resulting photon pulse through the X-ray optics to check for the photon beam quality at the experimental station. OCELOT allows for effectively automating such procedures. While full linac simulations are currently not possible with OCELOT, groundwork for collective effect simulation is present, such as numerical geometrical wakefield calculations [19], focusing effect of accelerating RF structures and the framework for collective effect calculations; implementation of space charge and Coherent Synchrotron Radiation (CSR) solvers are to be included in the future.

2.3. Beam dynamics in synchrotrons

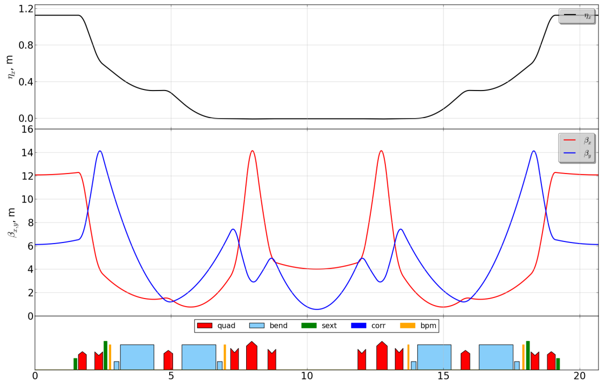

Figure 3: Siberia-2 optics

OCELOT features the full range of functionality needed for electron beam dynamics analysis in the latest generation of syncnhrotron light sources. The linear and nonlinear optics calculations were cross-checked with widely used tools MAD-X [20] and Six-Track [21] on the example of PETRAIII light source in operation at DESY among others, and showed good agreement. OCELOT has been widely used for optics studies at Siberia-2 (see e.g. Fig.3).

Dynamic aperture, the region of particle stability in phase space, is important for injection and beam lifetime. Influence of insertion devices on dynamic aperture has been analyzed for Siberia-2 [23]

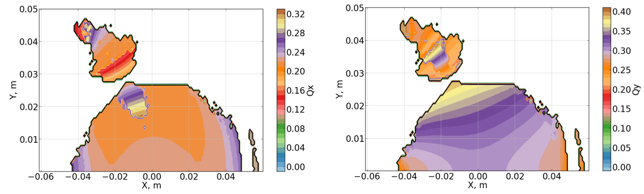

Figure 4: Dynamic aperture and dependence of horizontal (left) and vertical (right) betatron tunes on amplitude, without insertion devices.

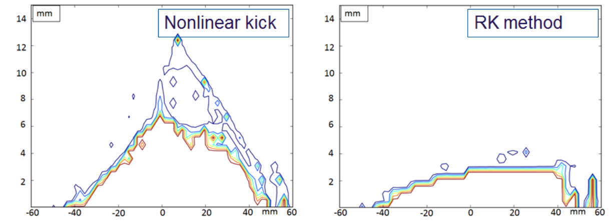

Figure 5: Siberia-2 dynamic aperture with a 7mm-period undulator, comparison of tracking with Runge-Kutta and nonlinear kick methods for the undulator

Siberia-2 runs at 2.5 GeV with a 7.5 T wiggler, installation of two additional 3T wigglers and a short period (7mm) undulator is considered. The influence of these insertion devices on the dynamic aperture was calculated with OCELOT, using both non-linear maps and Runge-Kutta methods for trajectory calculation. A significant decrease in the available vertical dynamic aperture due to the undulator was found (see Figs. 4, 5).

A new injection system for Siberia-2 has been recently introduced and commissioned [24, 25]. Design of the injection process from the perspective of beam dynamics was carried out with OCELOT. The pecularity of the new injection system is that the kicker pulse duration is long (1 μs), which exceeds the electron revolution period in the ring (412 ns). This allows to reduce the pulse generator voltage from 50KV to 10 KV, thus making it possible to significantly simplify the pulse generator design and improve the injection stability. The problem is to keep both the stored and the newly injected beam in the ring acceptance while the kicker magnets affect them on several successive revolutions. Due to large oscillations of the injected beam, the nonlinear dynamics is to be modelled accurately. The possibility of effective injection (up to 96% efficiency) with such kicker pulses was demonstrated in simulations and later experimentally. In Fig.6 trajectories of injected and stored beams are shown. The horizontal phase space during the first 4 turns for the injected beam is shown in Fig.7.

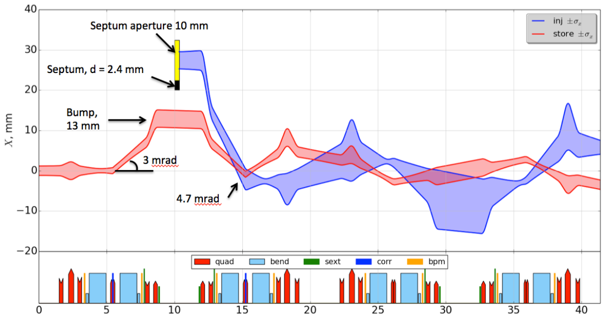

Figure 6: Siberia-2, trajectories of injected and stored beams

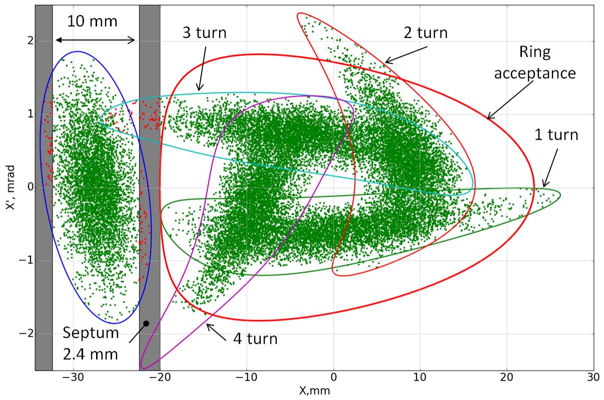

Figure 7: Phase space of injected beams on the septum magnet azimuth. The ellipse is at $\pm 3(\sigma_x, \sigma_x)$. In vertical dimension no aperture limitations are present.

2.4. On-line usage

Bridging simulations with operation and measurements is important in accelerator facilities. The architecture allows for the possibility of model description in a close-to-hardware manner. A software layer allows to switch between working with a simulation model and real hardware. It allows for running various tools, mostly foreseen for correction and tuning, in a flight simulator mode, thus reducing the time spent working on software with the real beam. Moreover, consolidating high level controls and simulation software reduces the amount of required modules. Recently, OCELOT was integrated into the control system of Siberia-2 and is being used for orbit correction, among other purposes [26], Figs. 8, 9. Device interfaces for BPMs running under EPICS [28] and correctors running under NAMU [27] were implemented, and an orbit correction algorithm based on singular value decomposition (SVD) was used. The software was debugged in a flight simulator mode and the actual software commissioning with beam took about one hour. Integration prototyping and tests were also performed to work with devices using the accelerator control system at DESY [29]. It is foreseen that the software can be used for some high-level tuning purposes during the commissioning of the European XFEL, e.g. for the photon-beam-based alignment.

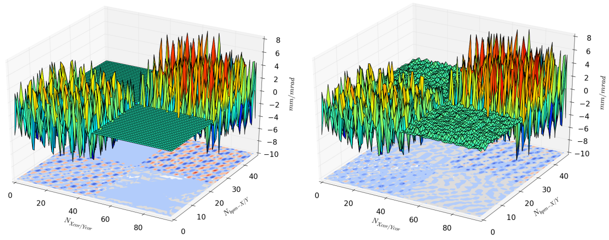

Figure 8: Calculated and measured response matrices of the Siberia-2 model.

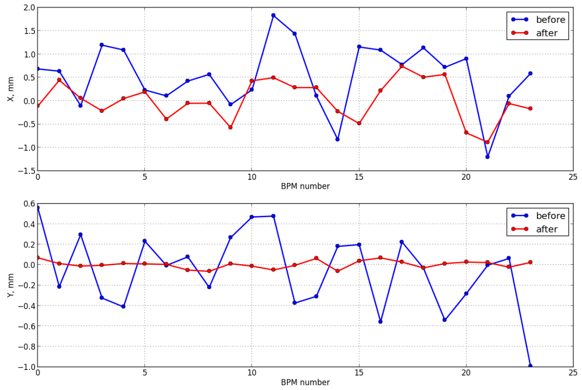

Figure 9: Orbit correction of Siberia-2 at 2.5 GeV (measurement). Horizontal correction is less effective mainly due to misalignment and limitations in BPM and corrector performance.

3. Conclusion and outlook

We presented new software which has been successfully used for various studies related to synchrotron light sources and FELs. Several directions of improvement are now being actively pursued. First, the low energy electron beam transport in linear accelerators requires more accurate models for space charge and CSR effects, which is the subject of current development. At the moment for European XFEL calculations we have to rely on low energy transport caclulations performed with third party codes [30]. Second, OCELOT features an X-ray optics module, including ray tracing and wave optics, capable of propagating time-dependent optical pulses (such as XFEL) through several types of elements, e.g. mirrors. Wave optics calculations can be effectively and relatively simply implemented in the framework of Fourier optics [31]. The module can be already used to e.g. assess the photon beam quality. Work is in progress to include the whole spectrum of optical elements relevant to synchrotron radiation and XFEL facilities with the appropriate level of detail and reliablilty as to enable the photon beamline studies.

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