Nuclear Instruments and Methods in Physics Research A 768 (2014) 151–156

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

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

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ARTICLE INFO

Article history:
Received 18 June 2014
Received in revised form
22 September 2014
Accepted 22 September 2014
Available online 28 September 2014

Keywords:
Accelerators
Synchrotron radiation
Free Electron Lasers
Software

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.

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 extensibility 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 were 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 description, 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 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

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http://dx.doi.org/10.1016/j.nima.2014.09.057
0168-9002/

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', which could be a simulation script, a web-based access to simulation data, an online control tool and so on.
- *Abstract layer for controls interface*: This allows us 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 Table 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.

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 noticeably 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.

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 [15–17], 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

Table 1
Currently available modules.

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

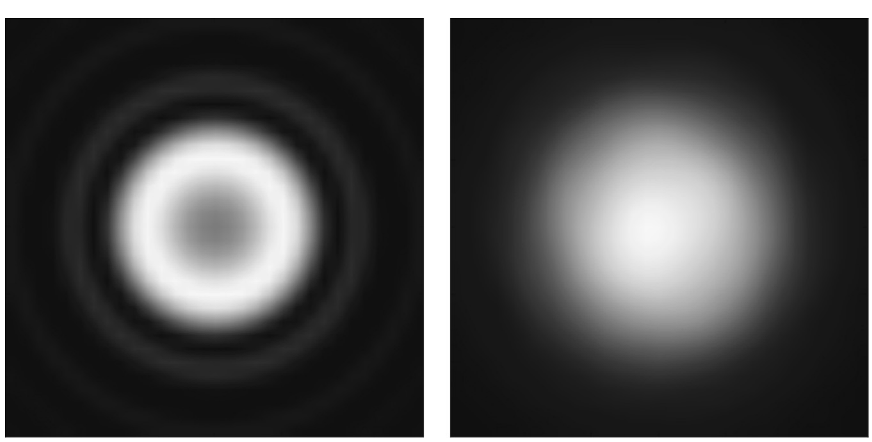

Fig. 1. Right: effect of emittance (1.7×10^{-11}) on an off-resonance monochromatized undulator radiation image (24 keV), 2 undulator sections. Left: image without the emittance effect.