OCELOT AS A FRAMEWORK FOR BEAM DYNAMICS SIMULATIONS OF X-RAY SOURCES*

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Abstract

We describe the OCELOT open source project focusing on new beam dynamics simulation capabilities of the whole machine in modern electron-based x-ray sources. Numerical approaches for particle tracking and field calculations are discussed. In developing of the full-dimensional numerical modeling we pursue two important competitive aspects: the simulation has to be fast and has to include accurate estimations of collective effects. The simulation results for the European XFEL [1] are presented. The results have been benchmarked agains other codes and some of such benchmarks are shown.

INTRODUCTION

OCELOT is a multiphysics simulation toolkit and an on-line control framework for FEL- and storage-ring-based light sources [2]. The code is written in Python and includes native modules for beam dynamics and (spontaneous) synchrotron radiation calculations. Simulation of FEL physics is based on an external code Genesis 1.3 [3] which is interfaced to OCELOT. Modules for online beam control [4] and machine performance optimization [5-7] are available.

In this paper, we will focus on the features of the code related to design and beam dynamic simulations of linear accelerators (first steps in this direction were discussed in [8]). Single-particle dynamics can be modelled in several ways (the transfer maps are configurable and can even be user-defined), for linacs the matrix formalism up to the second order [9] is typically used (thick-lens non-symplectic integrators). The code allows to include asymmetric field effects in radiofrequency (RF) cavities. Collective effects include coherent synchrotron radiation (CSR), space charge (SC) and wakefields. Solvers for single-particle and collective effects are briefly described in what follows.

One of the most important and time-consuming stages of the beam dynamics code development is the cross-checking of simulation results with existing codes (e.g. Astra, CSRtrack, Elegant). Here the cross-checking results for the European XFEL linac will be presented.

COLLECTIVE EFFECTS

The tracking of particles is done in the same way as, for example, in Elegant [10]. Quadrupoles, dipoles, sextupoles, RF cavities and other lattice elements are modelled by linear and second order maps. The focusing effect of RF cavities is taken into account according to the Rosenzweig-Serafini model [11].

In order to cross-check the code with codes ASTRA [12] and CSRtrack [13] we use the European XFEL lattice (Fig.1).

Space charge and RF focusing effects are strongest for the low energy beam in the booster (the first TESLA cryomodule, A1 in Fig. 1). Hence we consider the part of injector from 3.2 m up to 14.45 m to cross-check OCELOT with ASTRA. The CSR effects are strongest in the last bunch compressor (BC2 in Fig.1) and it was chosen to cross-check OCELOT with CSRtrack.

To cross-check wakefield effects we consider the beam dynamics in the corrugated structure [14]; when installed, it will be the strongest compact source of wakefields at the European XFEL.
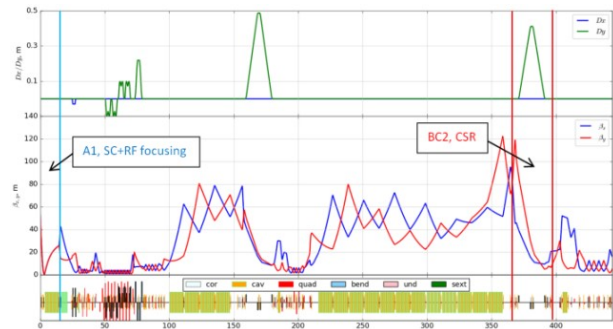

Figure 1: European XFEL lattice up to BC2.

Space Charge Effect

The space charge forces are calculated by solving the Poisson equation in the bunch frame. Then the Lorentz-transformed electromagnetic field is applied as a kick in the laboratory frame. For the solution of the Poisson equation we use an integral representation of the electrostatic potential by convolution of the free-space Green's function with the charge distribution. The convolution equation is solved with the help of the Fast Fourier Transform (FFT). The same algorithm for the solution of the 3D Poisson equation is used, for example, in ASTRA. However, ASTRA solves the equations of motion directly with the Runge-Kutta method, while in OCELOT particles are tracked using maps up to the second order.

The cross-checking was performed for the beam distribution with the following parameters: 200 000 particles, 250 pC, initial reference particle energy 6.55 MeV. Each of the 8 RF cavities has phase of 18.73 grad and amplitude of 19.54 MV. Because of the axial symmetry of the beam and accelerator lattice (up to the first quadrupole), the vertical and horizontal beam envelope (beta) functions are the same. Only the horizontal beta functions are shown in the Fig.2. The beta functions were calculated at each tracking step from the beam distribution. The beta

functions with space charge effect are in good agreement with ASTRA. To estimate the SC effect strength the beta function without space charge effect is also shown (dashed line, Fig.2). Note that the ideal linear map (with RF focusing) was used in OCELOT for particles tracking through the cavities while tracking through drift was performed up to second order. ASTRA uses the Runge-Kutta tracking with calculated 3D field profile. The RF coupler kicks are not considered here. The calculation speed in OCELOT for this setup is a few minutes (3-10 mins, depending on step size) on an Intel i7 CPU.
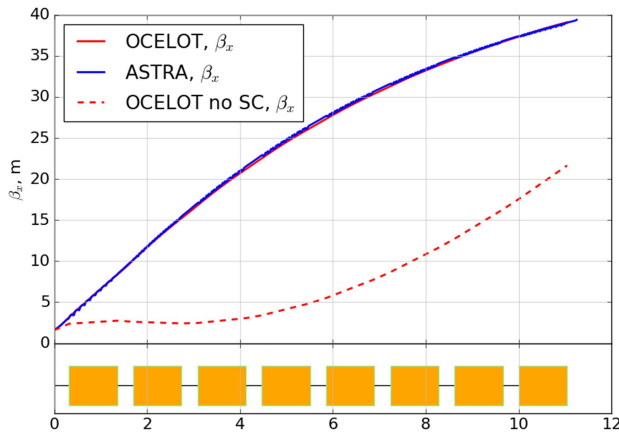

Figure 2: Beta-functions with and without SC.

CSR Effect

The CSR module uses a fast 'projected' 1-D method from CSRtrack code and follows the approach presented in [15-17]. The particle tracking uses matrices up to the second order. CSR wake is calculated continuously through beam lines of arbitrary flat geometry. The transverse self-forces are neglected completely. The method calculates the longitudinal self-field of a one-dimensional beam that is obtained by a projection of the 'real' three-dimensional beam onto a reference trajectory. A smooth one-dimensional charge density is calculated by binning and filtering, which is crucial for the stability and accuracy of the simulation, since the instability is sensitive to high frequency components in the charge density.
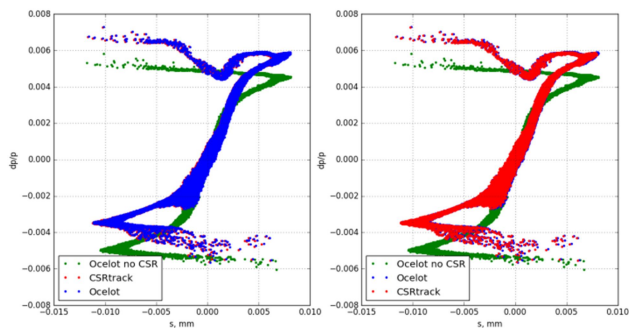

Figure 3: Longitudinal phase space after BC: OCELOT without CSR (green), OCELOT with CSR (blue), CSRtrack with CSR (red).

As mentioned above, the bunch compressor BC2 was chosen for CSR effect cross-checking with CSRtrack. The

setup has the following parameters: the beam distribution of 200 000 particles, bunch charge of 100 pC, reference energy of 2400 MeV and bending magnet angle of 0.0336 rad. The longitudinal phase space is shown in Fig.3 and is in good agreement with that of CSRtrack. Despite the absence of nonlinearities of higher than second order, we do not see a large difference compared to CSRtrack which uses Runge-Kutta tracking. The calculation speed in OCELOT is of the same order as in CSRtrack (a few minutes for this setup on Intel i7 PC).

Wakefields Effect

In order to take into account the impact of the wake field on the beam we represent the longitudinal wake function through the second order Taylor expansion. In general case we use 13 one-dimensional functions to represent the longitudinal component of the wake function for arbitrary offsets of the source and the wittness particles near to the reference axis. The transverse components of the wake function are calculated with the help of Panofsky-Wenzel theorem. The wake field impact on the beam is included as a series of kicks. The implementation of the wakefields follows closely the approach described in [18,19].

For cross-checking of wakefield we consider the corrugated structure setup with parameters of corrugations suggested at SLAC [20]. Our setup contains 6 planar corrugated structures (3 in the vertical plane (V) and 3 in horizontal one (H), see Fig. 6) and one quadrupole. Simulation for this setup was described in details in [14], where a comparison of the simulation results with analytical expressions are shown as well. In Fig.4 the beam envelope functions calculated from the beam distribution with and without wakefield effects are shown. Other results and the effect on SASE radiation are discussed in [14].
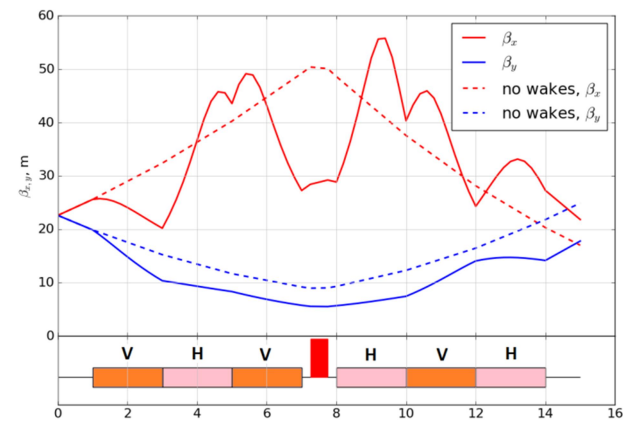

Figure 4: Beta-functions calculated from beam distribution with energy chirper.

COUPLER KICK

The input coupler and the higher order mode couplers of the RF cavities distort the axial symmetry of the electromagnetic (EM) field and affect the electron beam. This effect can be calculated by direct tracking of the particles

in the asymmetric (due to the couplers) 3D EM field using a tracking code (e.g. ASTRA). For fast estimation of the coupler effect a discrete coupler model (as described, for example in [21]) was implemented in OCELOT. The 1st order part of the model includes time and offset dependency; the offset dependency has a skew component. To include effect of all couplers, the kicks are applied at the entrance and the exit of each cavity.

As an example of the coupler effect, we consider the beam dynamics at Linac 1 (L1) of the European XFEL. The beta functions with and without the coupler kick effect are shown in Fig.5. The phase advance differences ($\Delta\mu = \mu_{ck} - \mu_{wo}$) for L1 in the horizontal and vertical planes are 0.044 and –0.023 rad, correspondingly. The coefficients of the coupler kick were calculated assuming 8 mm penetration depth of the coupler antenna. The beam is "on-crest" and the RF voltage of each of 32 modules is 14.68 MV.
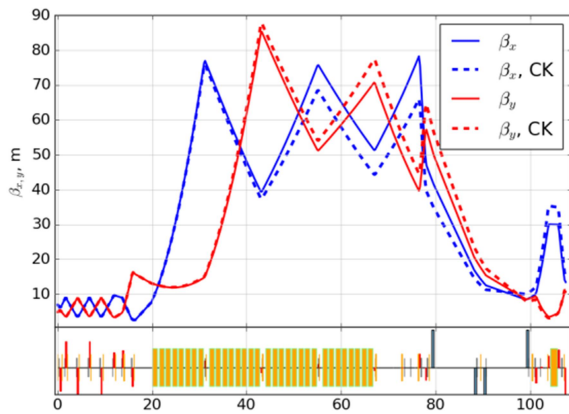

Figure 5: Coupler kick. First-order effect (offset dependancy with a skew component).

The influence of the coupler effect on the trajectory in the L1 is shown in the Fig.6. As it can be seen, the amplitude of the zero order kick (independent of the particle offset) is large (especially in horizontal plane) and should be compensated by orbit correction.
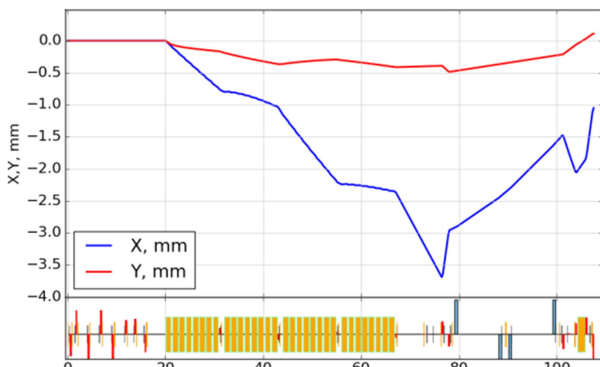

Figure 6: Coupler kick, 0th-order effect.

SUMMARY AND OUTLOOK

We described the implementation of collective effects in OCELOT as well as the cross-checking results with existing codes (ASTRA, CSRtrack). The coupler effect

was also implemented as an important effect for the European XFEL which uses TESLA-type cavities. Now all major collective effects to be taken into account for simulations of XFEL driver linacs have been implemented and the calculation results cross-checked. This opens up several possibilities for future applications, e.g. optimization of accelerator performance and beam properties (e.g. using genetic algorithms which were recently implemented in OCELOT [22]). Code optimization for multicore architectures is an important line of future work.

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