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FAST-XPD: XFEL Photon Pulses Database For Modeling XFEL Experiments

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Abstract. Knowledge of different properties of the radiation from X-ray FEL is very important for planning experiments. An understanding of such properties can come from start-to-end simulations of experiments: modern FEL simulation allows to reliably predict the output radiation pulses from X-ray FEL. We present a web accessible XFEL photon pulses simulation database showing data calculated with the FAST simulation framework.

INTRODUCTION

Knowledge of temporal, spatial, spectral and coherence properties of the radiation from X-ray FEL are of key importance for planning user experiments. An understanding of these properties can come from performing start-to-end simulations of user experiments tracing radiation pulses from its origin (undulator) through a beamline (mirrors, monochromators, etc.) to a target, simulation of physical processes of the radiation interaction with a sample, and simulation of detection process of related debris (photon, electrons, ions, etc.) by detectors.

Modern FEL simulation codes allow to predict all the details of the output radiation pulses from x-ray FEL (3D maps of radiation fields for the fundamental and higher frequency harmonics) with a high degree of reliability. We present an XFEL photon pulses simulation database accessible through public web-server that allows the access to data calculated with the FAST simulation framework. FAST is generic name for a set of codes for analysis of the FEL amplification process in the framework of 1-D and 3-D models using multiple modeling techniques [1–4]. The delivered data are expected to be very similar to the real radiation to be produced by X-ray free electron lasers. In particular, start-up from the shot noise in the electron beam can be simulated in FAST with tracing actual number of electrons in the beam, so that the simulation procedure corresponds to real electrons randomly distributed in full 6D phase space.

A web application allows to pick up a selected photon pulse data in the HDF5 format for any given XFEL operation mode (electron energy, charge/photon pulse duration, active undulator range etc) suitable for statistical analysis, propagating through the optical system, interaction with the sample, etc. The pulses post processing data, including the gain curve, time structure, source size and far field angular divergence are also provided as data sets in HDF5 file for the pulse.

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Baseline Parameters of the European XFEL and FEL Simulations

European XFEL is driven by superconducting accelerator with maximum energy of electrons of 17.5 GeV [5, 6]. It operates in the burst mode with 10 Hz repetition rate of 0.6 ms pulse duration. Each pulse brings train of up to 2700 electron bunches (up to 4.5 MHz repetition rate). Five operating points for the bunch charge have been fixed: 20 pC, 100 pC, 250 pC, 500 pC, and 1 nC [7]. Electron bunches with different bunch charges will generate radiation pulses with different radiation pulse duration, from about 1 fs at 20 pC to about 100 fs at 1 nC bunch charge.

Three undulators are installed in the first stage of the project: SASE1, SASE2, and SASE3. All undulators have similar mechanical design. Length of the undulator module is equal to 5 meters. Length of undulator intersection is equal to 1.1 m. Undulators SASE1 and SASE2 are identical: period length is 40 mm, number of modules is 35, the range of the gap variation is 10 to 20 mm, range of undulator parameter $K = 3.9 - 1.65$. SASE3 undulator consists of 21 modules, the period is 68 mm, the gap tunability range is 10 to 25 mm, range of undulator parameter $K = 9 - 4.08$ [8].

Requirements by users are summarized and analyzed for providing maximum opportunities for every instrument and experiment simultaneously. Tunability ranges of the undulators ($\lambda_{\max}/\lambda_{\min} = 3.7$ for SASE1/2 and $\lambda_{\max}/\lambda_{\min} = 4.4$ for SASE3) are not sufficient to cover required wavelength ranges at one fixed electron beam energy, and four electron beam energies have been defined: 8.5 GeV, 12 GeV, 14 GeV, and 17.5 GeV (see Table 1) [6, 9].

TABLE 1. Energy and wavelength ranges

E [GeV]	Photon energy range [keV]		Photon wavelength range [nm]	
	SASE1/2	SASE3	SASE1/2	SASE3
8.5	1.99-7.27	0.24-1.08	0.171-0.622	1.15-5.10
12.0	3.97-14.48	0.48-2.16	0.086-0.312	0.57-2.56
14.0	5.41-19.71	0.66-2.94	0.063-0.229	0.42-1.88
17.5	8.45-30.80	1.03-4.59	0.40-0.147	0.27-1.20

Radiation properties for defined set of baseline parameters have been described in ref. [10], and an current update is under preparation. These reports present general description of the FEL process, and contain extended set of tables of the radiation properties in the saturation regime:

- Pulse energy;
- Peak power;
- Average power;
- FWHM spot size;
- FWHM angular divergence;
- Coherence time;
- FWHM spectrum width;
- Degree of transverse coherence;
- Radiation pulse duration;
- Number of longitudinal modes;
- Fluctuations of the pulse energy;
- Degeneracy parameter;
- Number of photons per pulse;
- Average flux of photons;
- Peak brilliance;
- Average brilliance.

This information is important to perform an overview of parameter space and to choose correct strategy for planning of user experiment. An example for parameter space is shown in Fig. 1. However, many user experiments require more detailed information like spatial and temporal structure of the radiation fields. These information is also required for correct design of focusing optics in the beamlines. That was the main reason for creating photon data base described in this paper. Simulations are performed with three-dimensional, time-dependent FEL simulation code FAST capable to trace actual number of electrons in the electron beam [1–4, 11–14]. In our simulation procedure particles correspond to real electrons randomly distributed in full 6D phase space according to parameters of the electron bunch at the undulator entrance [7]. This technique allows us to avoid any artificial effects which may arise from standard procedures of macroparticle loading [15, 16]. Simulation code solves self-consistent equations of the particle motion and electromagnetic fields taking into account all important physical effects: diffraction of radiation, effects of betatron motion, energy spread, slippage effect, undulator tapering and higher harmonic generation. Output of the simulation code are 3D arrays containing complex values of the radiation field amplitudes on a 3D mesh (x-y-z) for fundamental an higher odd harmonics at different undulator length (end of exponential gain regime, saturation, and post-saturation). Post-processing of the output of simulation code allows to trace radiation properties beyond the saturation point as it is shown in Fig. 2.

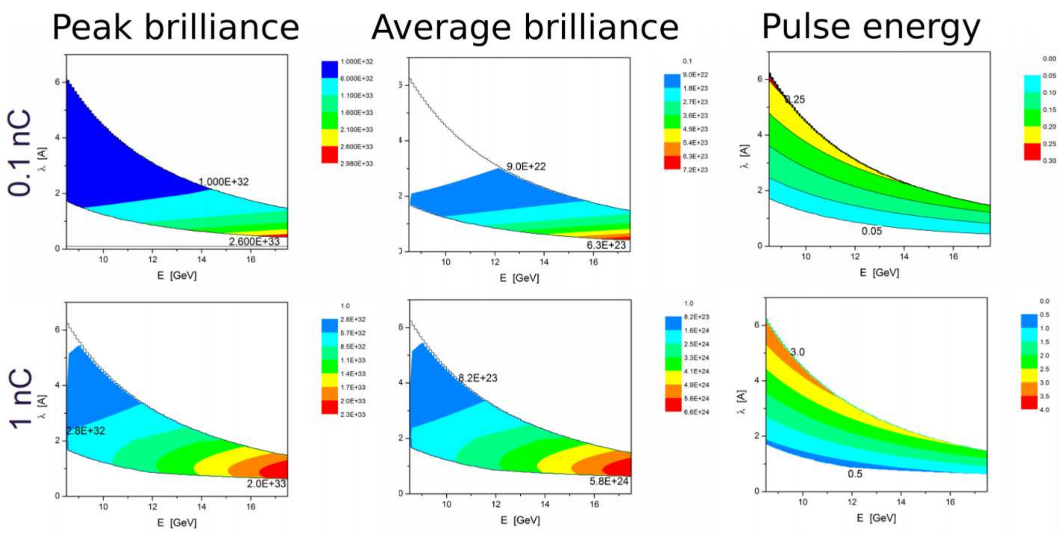

FIGURE 1. SASE1 operating range for available wavelength bands

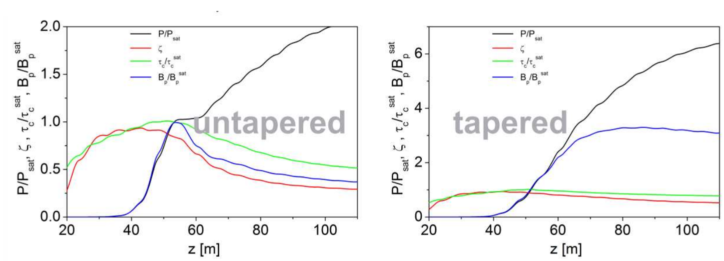

FIGURE 2. Radiation power, degree of transverse coherence, coherence time and brilliance

How to access and use FEL data

The structured HDF5 files (Fig. 3) contain all information about FEL simulation including input parameters and post-processing data. The files implement common interface with other software for waverfront propagation and start-to-end simulation of the XFEL experiments. The interactive simulation software for wave optics propagation [17] is fully integrated with FAST-XPD output. It has been used within strart-to-end frameworks [18, 19] and for detailed analysis of XFEL beamlines [20, 21].

The web application

The Fast-XPD web application published at https://in.xfel.eu/fastxpd/ allows to download a selected photon pulse data in the HDF5 format.

Since data is not immediately available for download but needs to be processed, users need to issue a request selecting the desired operation mode (electron energy, charge/photon pulse duration, active undulator range, etc.), start and end time of extracted range (in fs), dimension of XY mesh, slices sampling, point of output in z, required runs. Users are also required to provide an email address.

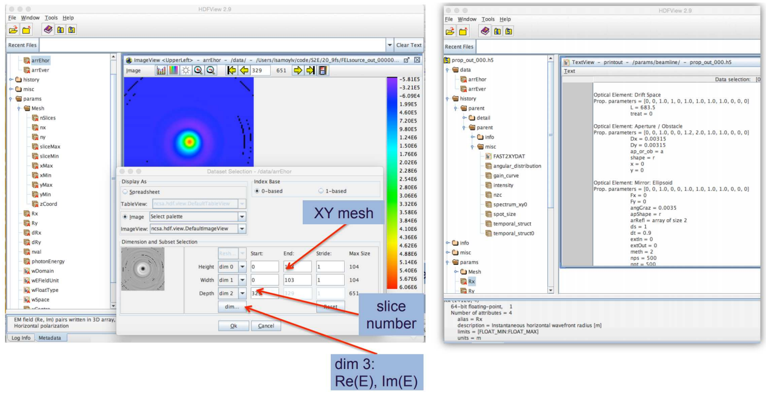

FIGURE 3. HDF5 file structure: wavefront glossary

After the request has been submitted, the system will provide to the user a URL where the status of the request can be monitored and where the data can be downloaded after it has been processed. From the same web page users will also have the possibility to abort the request for any reason (wrong parameters provided, time too long to complete, etc.). Users do not need to annotate the URL: providing their email address from the menu link "Where are my request?" they will be able to access to the lists of all their requests.

Once the request has been completed the system will inform the user by email. Processed data will be available for download up to 72 hours after completion (Fig. 4).

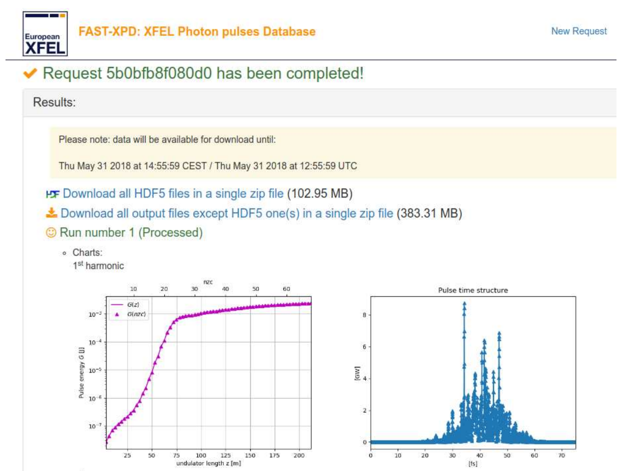

FIGURE 4. Result web page of processed request submission

The architecture of the complete application includes a web server, a database server and a processing machine with access to dCache, where the raw data are stored (Fig. 5).

Wavefront simulations

An example of treating the mirror imperfection influence on the XFEL beam quality is the simulation of the KB system intended to focus the beam into ~200 nm spot for bio-molecules imaging at SPB/SFX instrument at European XFEL [21]. The specified KB parameters, plane elliptical mirrors with a clear aperture 0.95 m and <2nm peak-to-valley (PV) residual height errors, are pushing to the limits of the modern mirror manufacturing technology. The beamline optics consists of a pair of the 0.8 m long offset mirrors located at 245 m from the SASE1 undulator source, with an incidence angle of 2 mrad and the focusing KB system of two plane elliptical focusing mirrors located at 955 m from

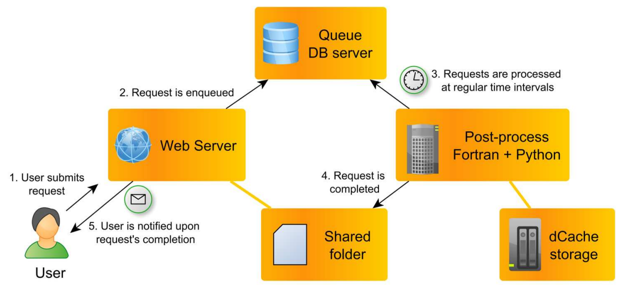

FIGURE 5. FAST-XPD backend architecture

the source: horizontal mirror with focal distance 3 m, and vertical mirror with focal distance 1.9 m, incidence angle 3.6 mrad. The calculations were done using FAST-XPD data for 3 fs SASE pulse at 4.96 keV photon energy. The simulation results that analyze the impact of active undulator length on focus quality are shown in Fig.6.

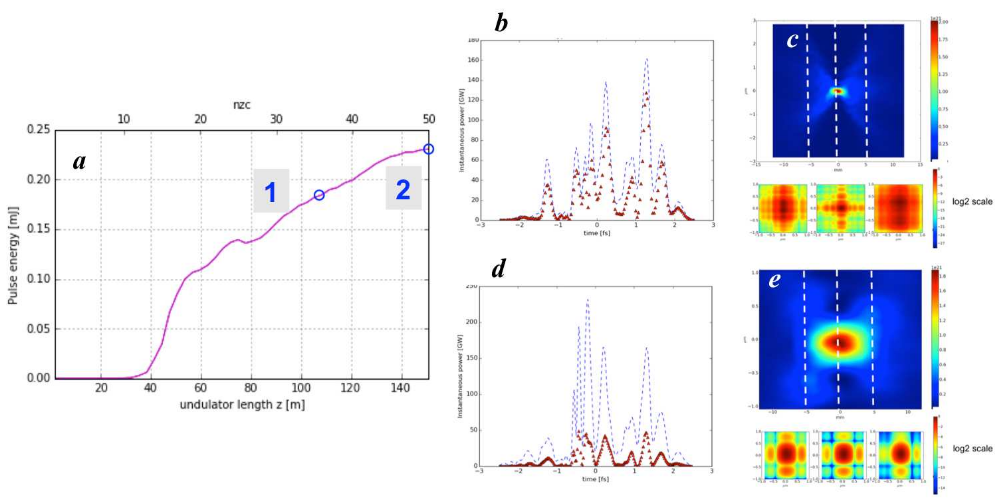

FIGURE 6. a: Gain curve for SASE1 undulator source of European XFEL for a 20 pC electron bunch charge, electron energy 14 GeV, an average photon energy of 4.96 keV. Two different active undulator lengths of 105 m and 145 m were used in simulations, shown as two circles at the curve. b-e: Simulated intensity distribution of the SPB/SFX 100 nm scale focus (see main text for details). b: time structure of the propagated pulse for active undulator length 105 m (point 1 at (a)), dash line corresponds to time structure before propagaion; c: Top: intensity distribution for active undulator length 105 m in the instrument “xz” plane (through focus), normalised to the highest intensity observed in the simulation. Propagation direction is left to right. Lower panel: intensity distribution in the plane perpendicular to the direction of propagation, normalised to the highest intensity observed in the simulation and displayed as a percentage of that maximum. Cuts of the intensity distribution are shown at 5 mm upstream of the focus (left), in the focal plane (centre), and 5 mm downstream of the focus (right) in log2 scale; d: the same as (b) for active undulator length 145 m (point 2 at (a)); e: the same as (c) for active undulator length 145 m.

Pioneer users of XPD

Photon data base has been used intensively used for optimization of the photon beam transport and imaging experiment [22, 23]. Realistic simulations of experiments at large scale photon facilities, such as optical laser laboratories, synchrotrons, and free electron lasers, are of vital importance for the successful preparation, execution, and analysis of these experiments investigating ever more complex physical systems, e.g. biomolecules, complex materials, and ultra-short lived states of highly excited matter. Traditional photon science modelling takes into account only isolated aspects of an experiment, such as the beam propagation, the photon-matter interaction, or the scattering process, making idealized assumptions about the remaining parts, e.g. the source spectrum, temporal structure and coherence properties of the photon beam, or the detector response. The authors of [22, 23] implemented a platform for complete start-to-end simulations, following the radiation from the source, through the beam transport optics to the sample or target under investigation, its interaction with and scattering from the sample, and its registration in a photon detector, including a realistic model of the detector response to the radiation. Such an approach allows researchers to simulate their experiments and instruments in real life scenarios, identify promising and unattainable regions of the parameter space and ultimately make better use of valuable beamtime.

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