XFEL Photon pulses Database (XPD) for modeling XFEL experiments

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XPD Website

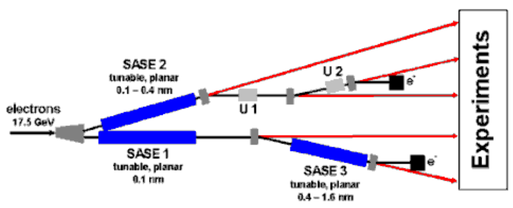
Abstract

Knowledge of temporal, spatial, spectral, and coherence properties of the radiation from x-ray FEL are of key importance for planning user experiments. The best way to do this would be 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 modelling techniques. 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.

FEL Simulations



Technical Design Report of the European XFEL (2006) assumed operation with the bunch charge of 1 nC and the value of the normalized emittance 1.4 mm-mrad. It has been planned to operate XFEL at fixed energy of 17.5 GeV and cover wavelength range from 0.1 nm to 1.6 nm in three undulators.

Revision of April, 2010 included extension of the range for bunch charges, change of the period of all SASE undulators (4 cm for SASE1 (SASE2) and 6.8 cm for SASE3), and extension of operating wavelength range from 0.05 nm to 5 nm by means of operation at three electron energies 17.5 GeV, 14 GeV, and 10.5 GeV. Safety margin for emittance has been reduced, and baseline values are between 0.32 mm-mrad and 0.97 mm-mrad when bunch charge changes from 20 pC to 1 nC.

Revision of November, 2013 has been driven by two reasons. The first reason is defined by the results of magnetic measurements of undulators which led to the reduction of wavelength tunability ranges with undulator gap. The second reason was next turn of collection of user requirements in terms of photon properties at different user beam lines. As a result, a concept of four operating energies has been accepted:

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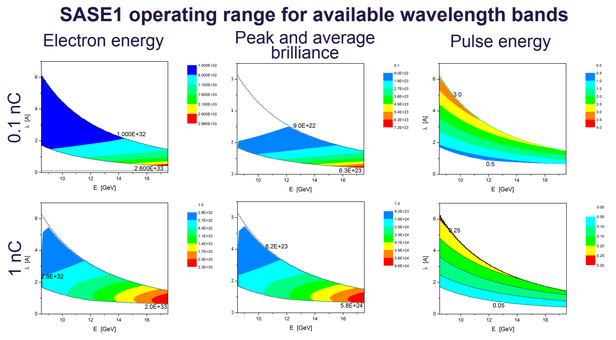
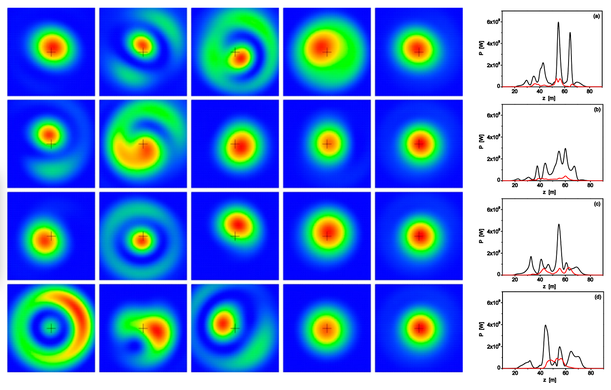
SASE1/2: gap = 10 mm ... 20 mm   K = 3.9 ... 1.65
SASE3:   gap = 10 mm ... 25 mm   K = 9 ... 4.08
Tunability range at fixed energy for SASE1/2:     3.7
Tunability range at fixed energy for SASE3:       4.5
        E [GeV]          SASE3              SASE1/2
Photon energy range [keV]:
          8.5          0.24- 1.08         1.99- 7.27
         12.0          0.48- 2.16        3.97-14.48
         14.0          0.66- 2.94        5.41-19.71
         17.5          1.03- 4.59        8.45-30.80
Photon wavelength range [nm]
         8.50           1.15- 5.10         0.171-0.622
        12.00           0.57- 2.56         0.086-0.312
        14.00           0.42- 1.88         0.063-0.229
        17.50           0.27- 1.20         0.040-0.147
```

Electron beam at the undulator entrance

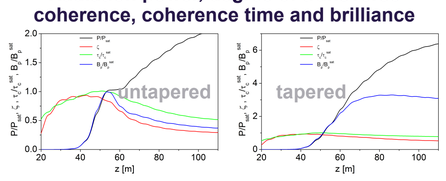
Bunch charge	nC	0.02	0.1	0.25	0.5	1
Peak beam current	kA	4.5	5	5	5	5
Normalized rms emittance	mm-mrad	0.32	0.39	0.6	0.7	0.97
rms energy spread	MeV	4.1	2.9	2.5	2.2	2
rms pulse duration	fs	1.2	6.4	16.6	30.6	76.6

SASE1 operating range for available wavelength bands

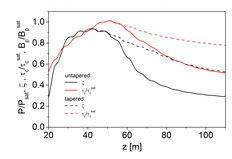




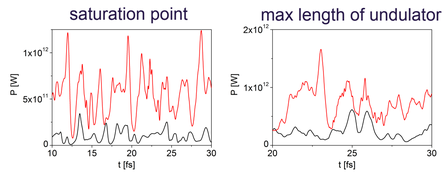
Radiation power, degree of transverse coherence, coherence time and brilliance



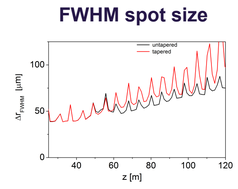
Coherence time and degree of transverse coherence



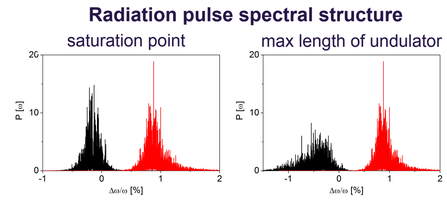
Radiation pulse temporal structure



FWHM spot size

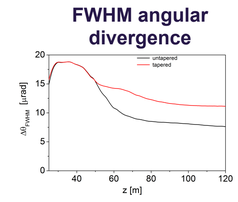


Radiation pulse spectral structure



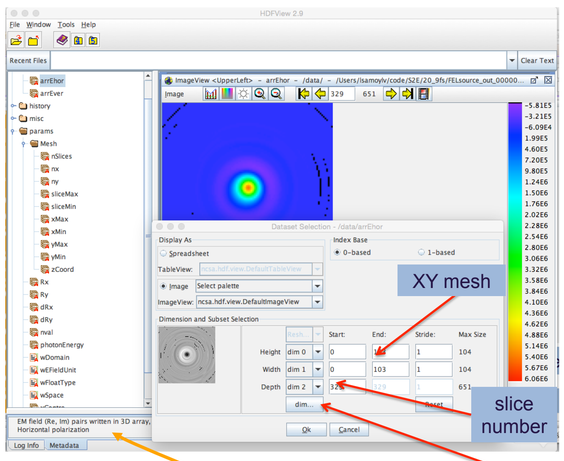
untapered (black)
tapered (red)

FWHM angular divergence

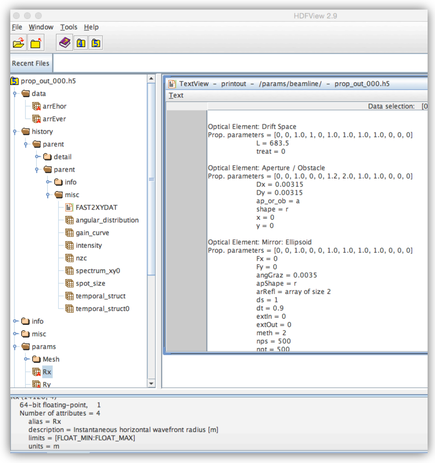


How to access and use FEL data

HDF5 file structure: Wavefront glossary



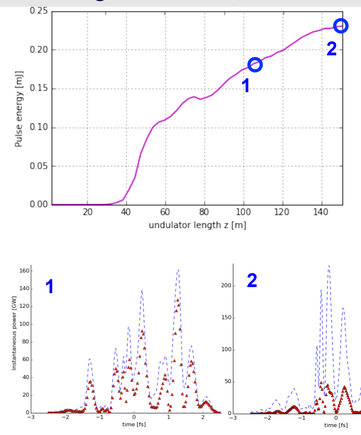
The structured HDF5 files contain all information about FEL simulation including input parameters and post-processing data. The files provide interface with other software for waverfront propagation and start-to-end simulation of the XFEL experiments.

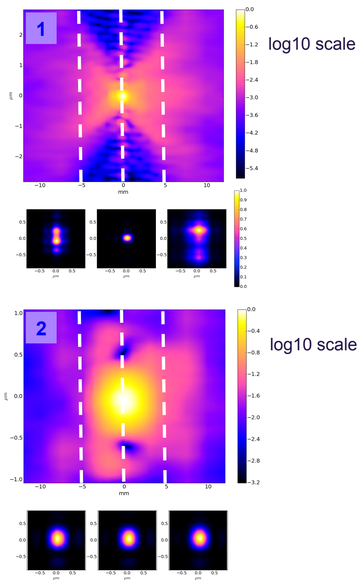


The interactive simulation framework for coherent X-ray wavefront propagation is available at **https://github.com/samoylv/WPG/**

Wavefront propagation

Simulated SASE pulse intensity distribution around focus of 100 nm scale focusing Kirkpatrick-Baez mirrors of the SPB/SFX instrument [3]. Active undulator length corresponds to point (1) and full length (2). Wavelength 0.25 nm, bunch charge 20 pC.

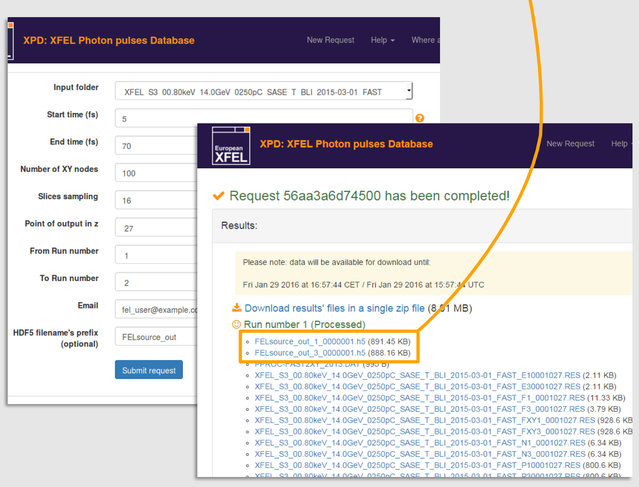




XPD web application

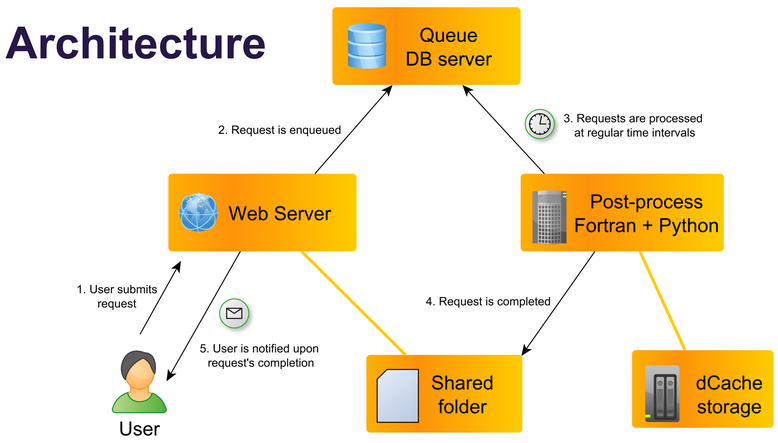
XPD Web application

https://in.xfel.eu/xpd/



- Web application is available at **https://in.xfel.eu/xpd/**
- Responsive web application's layout allows usage from any modern device (e.g. smartphones)
- Pick up a selected photon pulse data in the hdf5 format for any given XFEL operation mode
- Submit your request and wait for completion
- Requests are enqueued and data is post processed
- You'll get an email when request has been completed
- Data will be available for download up to 24 hours after completion

Architecture



References

[1] E.A. Schneidmiller, M.V. Yurkov, “Statistical properties of the radiation from SASE FEL operating in a post-saturation regime with and without undulator tapering”, J. of Modern Optics (2016) **63(4)**, p. 288

[2] L.Samoylova, A.Buzmakov, O.Chubar, H.Sinn, “WavePropaGator: Interactive framework for X-ray FEL optics design and simulations”, *in preparation*
see also *http://wpg.readthedocs.org/en/latest/index.html*

[3] R. Bean, A. Aquila, L. Samoylova and A. Mancuso, “Design of the mirror optical systems for coherent diffractive imaging at the SPB/SFX instrument of the European XFEL”, J. of Optics (2016), *submitted*