COMPUTATIONAL NEEDS FOR XFELS

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Abstract

X-ray Free Electron Lasers (FEL) make use of the principle of Self-Amplified-Spontaneous-Emission (SASE) where electron bunches interact in an undulator with their own co-propagating radiation. They do not require optical resonators and their frequency is therefore not limited by material properties as the reflectivity of mirrors.

The performance of X-ray SASE FELs depends exponentially on the beam quality of the electron bunch. Therefore effects in the beam-line before the undulator are as important as particle-field interactions of the FEL-SASE process. Critical components are the low emittance electron source, accelerating sections, the bunch compression system and the undulator. Due to the high peak currents and small beam dimensions space charge (SC) effects have to be considered up to energies in the GeV range. Coherent synchrotron radiation (CSR) drives not only the FEL but is also emitted in dispersive sections as bunch compressors. SC, CSR, and wake fields affect significantly longitudinal beam parameters (peak current, correlated and uncorrelated energy spread) and the transverse emittance. Start-to-end simulations use a sequence of various tracking codes (with or without SC, CSR and wake fields) and FEL programs. Usually the particle or phase space information has to be carefully converted for each transition from one tool to another. Parameter studies need many simulations of the complete system or a part of it and beyond that, calculations with several random seeds are necessary to consider the stochastic nature of SASE-FEL process.

THE FEL AND SASE PROCESS

Usually the interaction of ultra relativistic charged particles with plane electromagnetic waves in free space is weak and cancels over a period. This is changed by a device called undulator that creates a periodical magnetic field perpendicular to its axis. An electron that moves on a cosine like trajectory in the symmetry plane of that device, for instance the horizontal plane, can exchange systematically energy with a horizontally polarized wave. This happens if the slippage λ_s between the electron motion and the phase front of the light wave per undulator period λ_u is identical to the wavelength λ_l of the light wave.

The **resonance condition** for the wavelength and the slippage length is

$$\lambda_l = \lambda_s = \frac{\lambda_u}{2\gamma^2}\left(1+\frac{K^2}{2}\right), \qquad (1)$$

with γ the relativistic factor of the particle and K the undulator parameter proportional to the periodic magnetostatic field.

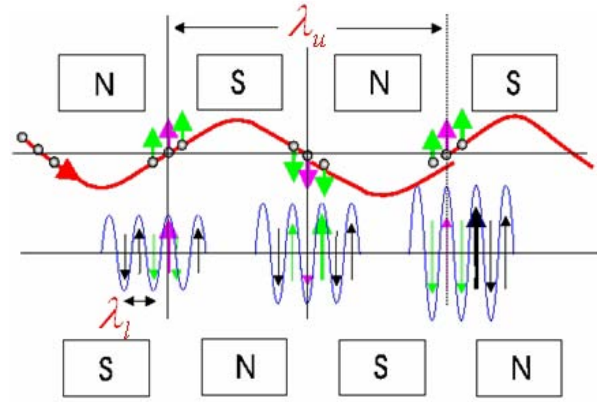

Fig. 1: Resonant particle-wave interaction in an undulator.

Fig. 1 shows the resonant interaction between particles and an electromagnetic wave. A particle, that observes an accelerating or de-accelerating electric field at a certain point of its trajectory, observes the same acceleration or de-acceleration half a period and multiples of half periods later.

Beam energy: In usual XFEL undulator designs K is of the order one (about two) and the geometrical periodicity λ_u is few centimetres. This determines the required energy for XFELs: today facilities, for instance FLASH [1] reach wavelengths down to 10 nm with beam energies of about 1GeV. The Linac Coherent Light Source (LCLS) is currently under construction at SLAC. It is planned for wavelengths from 15 down to 1.5 Å with an 15 GeV electron beam [2]. The European XFEL is in an advanced planning and technical preparation stage and its construction will start in 2007. The multi user facility will provide photons from 1 to 50 Å with maximal beam energy of 20 GeV [3].

μ bunching: The radiation of conventional electron synchrotron light sources is incoherent which means each electron radiates independent and the output power is proportional to the number of particles N. If it would be possible to organize the electrons in micro bunches with a spacing equal to λ_l, than all forward waves would be in constructive interference with an output power that is increased by many orders of magnitude. (The factor by which the output power is increased is the number of particles that radiate coherently.) The micro bunching as well as the stimulation or amplification of electromagnetic waves is caused by the collective instability of the FEL process. On the one hand, micro bunching is caused by the periodic energy modulation (which is induced by the wave) and by the longitudinal dispersion in the undulator. On the other hand, micro bunching drives electromagnetic waves.

SASE: Even the shot noise of a beam without micro modulation and incoherent synchrotron radiation are sufficient to start the bunching process, which is then called '**S**elf **A**mplifying **S**pontaneous **E**mission'. Of course this 'start up from noise' process is subject of numerical simulations with controlled seeded numerical noise.

Gain Length: In conventional lasers the electromagnetic wave propagates many times through the active medium and is reflected on both ends by mirrors that build an optical resonator. In the wavelength regime below 100 nm it is increasingly difficult to realize such mirrors. Therefore a SASE XFEL needs a very long active part, the undulator, where the photon-electron interaction takes place. (The multiple propagation through a short active element is replaced by a single path through a long active part.) A key parameter of SASE FEL design is the gain length L_g on which the radiated power is increased by the factor *e*. The saturation length is typically a dozen times larger and the total undulator length includes a safety margin. For Å-XFELs undulator length above 100 m are foreseen. It is a challenging task is to analyze and compute a process whose length scales (wavelength λ_l, correlation length, bunch length, undulator period λ_u, gain length L_g and saturation length) cover twelve orders of magnitude.

PHYSICAL CHALLENGES

Physical challenges for the electron beam concern a reasonably short gain length, the geometrical overlap of the electron and photon beam and the resonance condition of the electromagnetic wave with real particle beams that have transverse emittance and uncorrelated energy spread.

According to 1d FEL theory [4] the **gain length** is given by

$$L_g = \frac{1}{\sqrt{3}} \sqrt[3]{\frac{2mc}{\mu_0 e} \cdot \frac{\gamma^3 \lambda_u}{K^2} \cdot \frac{\sigma_r^2}{\hat{I}}} \qquad (2)$$

with $\hat{I}$ and σ_r the beam current and radius. (Empirical 3d extensions can be found in [5, 6].) The parameters γ, λ_u and K of the second factor in the root are defined by undulator design and required photon wavelength. The last term is inverse proportional to the current density.

To **overlap** the electron and laser beams their transverse dimensions should be similar as well as the Rayley length $L_r = \pi\sigma_r^2/\lambda_l$ and the gain length L_g. This sets a restriction for the electron beam radius:

$$\sigma_r \approx \sqrt{L_g \lambda_l / \pi} \, . \qquad (3)$$

The **resonance condition** for a particle with energy offset ($\delta\gamma = \gamma - \gamma_0$) and with transverse slope (x', y') is

$$\lambda_l = \frac{\lambda_u}{2(\gamma_0 + \delta\gamma)^2}\left(1 + \frac{K^2}{2}\right) + \frac{\lambda_u}{2}\left(x'^2 + y'^2\right). \qquad (4)$$

To fulfill this condition with sufficient accuracy, the relative uncorrelated energy spread σ_γ should be smaller than half of the relative FEL bandwidth

$$\sigma_\gamma < \frac{1}{2}\frac{\Delta\lambda_l}{\lambda_l} = \frac{1}{4\pi\sqrt{3}}\frac{\lambda_u}{L_g} \, . \qquad (5)$$

(The relative FEL bandwidth is proportional to the ratio λ_u/L_g.)

The divergence of a beam with finite emittance $\langle x'^2 \rangle, \langle y'^2 \rangle$ interferes with the resonance condition in a similar manner as the uncorrelated energy spread. The constraints for the beam radius σ_r and the divergence result in a criterion for the emittance [4, 7]:

$$\varepsilon < \lambda_l / 4\pi \, . \qquad (6)$$

The criterion is not fulfilled for the planned Å –XFELs. For instance a normalized emittance of 0.3 µm would be needed for 1Å@20GeV. This leads to increased gain and undulator lengths.

SASE FELs require electron beams with peak currents of several kilo Amperes, normalized emittances below 1.5 µm and uncorrelated energy spreads of about 1 MeV. Design of and beam dynamics in components before the undulator (electron source, accelerator and bunch compression system) are an important precondition for SASE FELs and the bigger part of the computational challenge.

INJECTOR AND ACCELERATOR

A schematic layout of the European XFEL is shown in Fig. 2. The basic elements are the same in the LCLS. A low emittance bunch (~1 nC, 50 A) is created at a photo cathode and is accelerated in the 1.5 cell cavity of the gun and the consecutive TESLA module to 130 MeV [9]. The bunch is further accelerated in the bunch compression system and the main linac and is collimated before the beam distribution to the undulators (compare Fig. 6).

Bunch Compression System

A two stage bunch compression system with magnetic chicanes is used to shrink the bunch length and to increase the peak current by two orders of magnitude to ~5 kA. The principle of dispersive compression is shown in Fig. 3. The upper row of diagrams shows an electron bunch in the horizontal Cartesian plane. An off crest acceleration was used to induce an energy chirp which is expressed by the color of the particles. 'Head' particles with less energy observe a stronger deflection in the first magnet of the chicane and travel on a longer trajectory to the exit where all particles come back to the axis. 'Tail' particles with higher energy can catch up or even overtake 'head' particles. A variety of effects as space charge (SC) fields, coherent synchrotron radiation (CSR), wakes and non-linearities of the chirp or of the longitudinal transfer function of a chicane complicate the beam dynamic considerably. For instance the lower row of diagrams in Fig. 3 demonstrate an extreme case of beam dilution due to CSR. The particles in the core of the bunch lose energy to radiation and are too strong deflected in the last magnets so that the transverse emittance is increased. A new class of beam dynamics codes is required (and developing) for such systems with non-linear trajectories and shape variant distributions where coherent radiation effects are not negligible and the length scale of transients is of the same order as the length scale on which shape variations take place [8]. These codes are usually called CSR codes although the name stands only for one of several physical mechanisms that have to be considered.

The qualitative behavior of the longitudinal phase space without (red) and with (blue) compensation of non-linear effects is shown in Fig. 4. Non-linear effects are caused by the cosine time dependency of the rf and by higher order dispersion in the chicane. This leads to a rollover in phase space and a sharp spike in the current distribution for the uncompensated case. The current is increased by a factor inverse proportional to the uncorrelated energy spread. The blue phase space distribution in the left diagram has a positive 2^{nd} derivative and differs less from the linear correlation (in black). The overcompensation is achieved with a higher harmonic rf system and leads to a more uniform compression. If a rollover is avoided, the compression factor depends sensitively on the shape of the energy-length correlation and therefore even on self fields as wakes, SC and CSR. On a scale that is short compared to the bunch length the sensitivity of the bunch shape to self fields by SC and CSR is known as μ-bunch instability.

μ-bunch "instability"

The μ-bunch instability has a *physical* aspect related to the typically 10^{10} particles in a bunch and a *numerical* aspect that is determined by their representation by much less macro particles. Physical is the problem of shot noise in the electron distribution that can be amplified by many orders of magnitude. A small modulation in density is converted by longitudinal SC and/or CSR impedances to a small energy modulation which causes longitudinal displacements in dispersive sections. This leads for a certain range of wavelength to a *μ-bunching amplification*. The real effect is controlled by additional hardware (the "laser heater") that increases the uncorrelated energy spread.

A numerical simulation of μ-bunching effects is still beyond the resolution of most tracking programs. Therefore the problem is split into a separate investigation of μ-bunching effects [10, 11, 12] and of pure macroscopic effects. *Noise suppression* strategies are important for the numerical field calculations and the treatment of particle distributions [8].

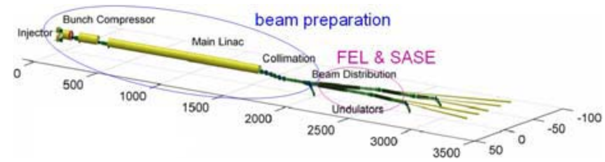

Fig. 2: Layout of the European XFEL.

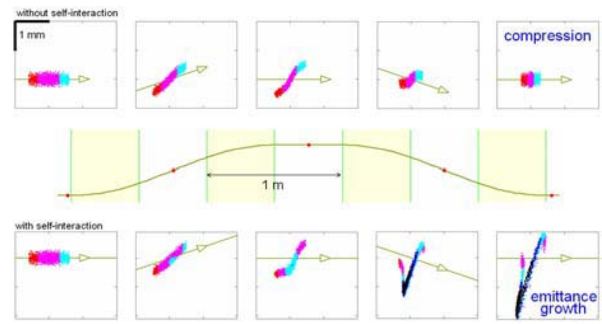

Fig. 3: Shape variation during compression.

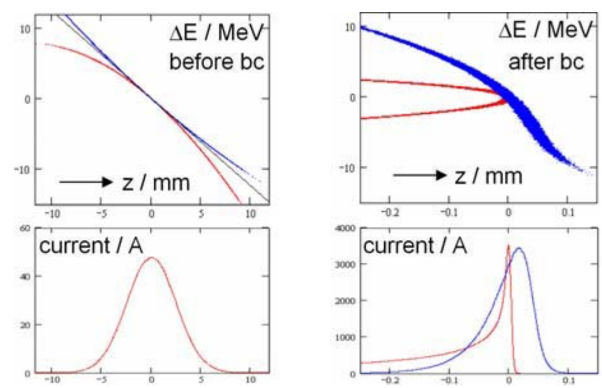

Fig. 4: Controlled- (blue) and rollover- (red) compression. (Idealized example without self-effects.)

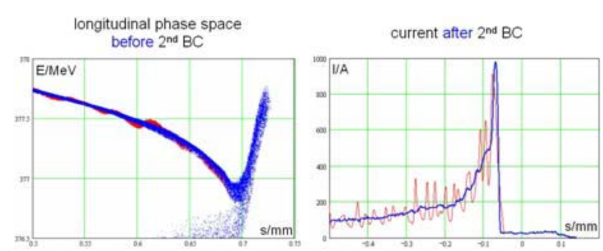

Fig. 5: Numerical μ-bunch instability caused by the shot noise of macro particles in a simulation of the 2^{nd} bunch compressor of FLASH.

Fig. 5 gives an example of numerical μ-bunching in a simulation of the FLASH bunch compression system. The left diagram shows longitudinal phase space distribution at the entrance of the second bunch compressor. In a first chicane the chirped distribution was compressed close to the rollover case (compare Fig. 4). The longitudinal density increases to the head and drops on few 10 μm to zero. The particles in the head of the distribution gained their energy due to the space charge field related to that drop. The space charge calculation was done with two different meshing strategies of the Poisson solver: the red distribution shows a slight energy modulation due to numerical noise caused by too few particles per mesh step. The bunch compressor converts this energy fluctuation into a significant density modulation.

Gun to undulator tracking for the Eurpn. XFEL

The simulation of the gun, accelerating sections and bunch compressor chicanes involves the use of several codes and tools for the calculation of linear and dispersive sections and for phase space conversions. Fig. 6 shows the segmentation of the European XFEL and Fig. 7 describes two approaches to track a particle distribution through these sections.

The approach 'method 1' uses the space charge tracking program ASTRA [13] for the injector, the one-dimensional CSR model of CSRtrack [14] for all dispersive sections and simple matrix transformations for the rest. Wake fields and a longitudinal semi analytic space charge (SASC) correction are added by interface utilities. This approach is fast and models the longitudinal compression accurately. The main effort is the ASTRA calculation of the injector, which needs several hours on a PC (Pentium 4, 3GHz). The CSR calculations need about half an hour.

The approach 'method 2' uses precise and time consuming models to validate the results of 'method 1'. It uses space charge tracking with ASTRA up to 3 GeV, the sub-bunch model of CSRtrack for dispersive sections and the program ELEGANT [15] together with a SASC correction for the rest. The computation on a LINUX cluster with twenty 64-bit cpus takes about 40h for the CSR part and about ~10h for SC sections.

Fig. 8 shows the current profile and the longitudinal phase space at the undulator entrance calculated by 'method 1'. The result of 'method 2' is nearly identical. The energy jump in the core of the bunch is caused by space charge effects after the second compressor.

The differences in the transverse phase space are noticeable [16]: 'method 1' underestimates the variation of optical parameters along the bunch and gets a few percent slice emittance growth. The slice emittance growth by 'method 2' is approximately 15% (compare Fig. 9).

FEL SIMUALTIONS

Approximations

Most FEL codes are based on the following approximations. The particle motion and the wave-particle interaction are *averaged over one or more undulator wavelengths*. For instance the particle energy is estimated by

$$\frac{d\gamma}{dz} = -\frac{e}{mc^2}\left\langle \frac{\mathbf{E}\cdot\mathbf{v}}{v} \right\rangle. \qquad (7)$$

The electromagnetic field computation uses a *slowly varying amplitude approximation*

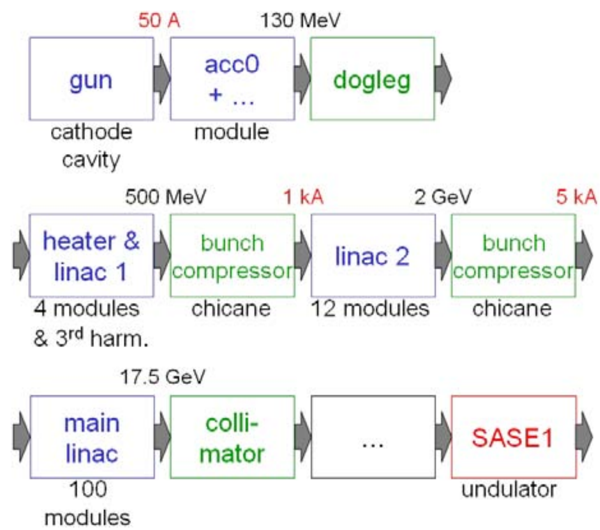

Fig. 6: European XFEL: segmentation for gun to undulator tracking

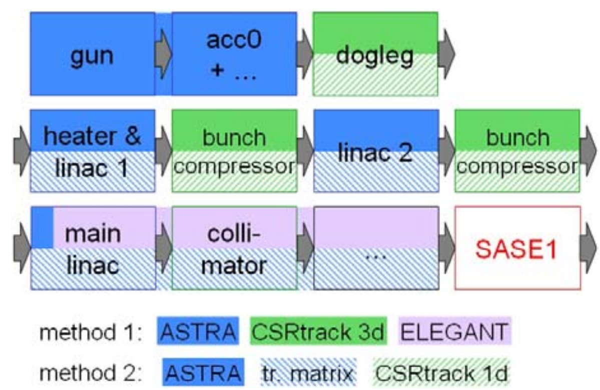

Fig. 7: European XFEL: Tracking codes used for gun to undulator tracking

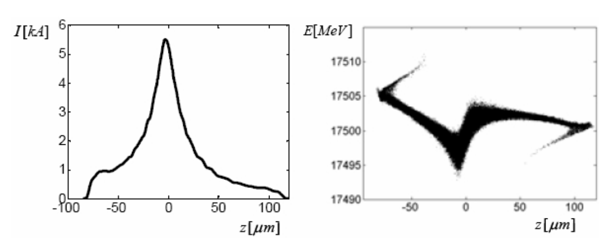

Fig. 8: European XFEL, Current profile and longitudinal phase space at the undulator entrance (1nC, 17.5 GeV).

$$\mathbf{E} \approx \mathrm{Re}\left\{\tilde{\mathbf{E}}_{\perp}(\mathbf{r},t)\exp\left(ik_l(z-t/c)\right)\right\} + E_z\mathbf{e}_z\,, \qquad (8)$$

with $k_l = 2\pi/\lambda_l$ the wave number of the fundamental mode and $\tilde{\mathbf{E}}_{\perp}$ the slowly varying amplitude of the trans-verse field. Some FEL codes take into account higher harmonics. The effort for the numerical integration of

Maxwell's equations can be dramatically reduced by the parabolic *paraxial approximation*

$$\left(\nabla_\perp^2 + 2ik_l\left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right)\right)\tilde{\mathbf{E}}_\perp = -i\mu_0\omega\tilde{\mathbf{J}}_\perp . \qquad (9)$$

The paraxial approximation neglects fast variations of the slowly varying amplitude: $\left|\partial^2\tilde{\mathbf{E}}_\perp / \partial z^2\right| << k_l\left|\partial\tilde{\mathbf{E}}_\perp / \partial z\right|$. It allows integration steps of one or more undulator period length.

The electron bunch with typically 10^{10} particles is replaced by a set of *macro particles with controlled artificial noise*. The macro particles and the electropmagnetic field are organized in slices of the length λ_l. Particle and field slices slip to each other by λ_l per undulator period. The particle motion is integrated in steps $\Delta_z = M\lambda_u$ of one or several undulator periods. The step size is limited by the gain length $\Delta_z << L_g$. The longitudinal discretization of the bunch can be incomplete which means *it not necessary to simulate all slices*. The slice spacing has to be short compared to the correlation length or $\Delta_s << L_g\,\lambda_l/\lambda_u$. Many effects on the FEL process can be studied with much less effort by the 'steady state model' that assumes an infinite periodic bunch: the particle dynamics and field propagation are calculated for one slice between periodic boundaries.

SASE Simulation for European XFEL

The effect of various undulator wakefields to the output power at 1 Å has been investigated in [17]. The input data for the FEL code GENESIS 1.3 have been prepared as follows: The macro particle distribution at the undulator entrance was cut into longitudinal slices. The mean energy, rms energy spread, current and rms emittance were calculated for each slice. A new macro particle distribution with ~10^4 slices of one wavelength and ~10^4 particles per slice was created, that has the same properties. (The number of macro particles per slice is comparable to the real number of electrons). All slices were perfectly matched to the undulator entrance and all centroids placed on the ideal orbit. The SASE process was calculated along 140 m of the undulator in ~10^3 steps. The computation of 150 SASE runs with different random seeds took 10 days on a LINUX cluster with twenty 64-bit cpus. The shape of bunch and undulator wakes and the output power with and without wakes or tapering are shown in Fig. 10. The simulation shows that it is possible to compensate the energy loss of the beam along the undulator by tapering.

Gap tolerances

The 'steady state model' was used in [17] to investigate the influence of tolerances of the (tapered) undulator gap on the output power, see Fig. 11. A steady state calculation of the European XFEL with the same parameters as described above (but with only one slice) needs about 30 seconds on a conventional PC (Pentium 4, 3GHz). The computation of Fig. 11 with 100 seeds for the undulator tolerances and for 30 values of the rms tolerance took lees than one day.

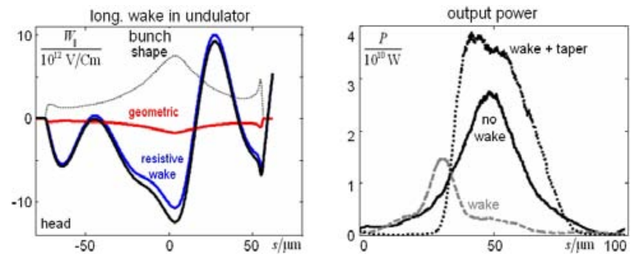

Fig. 10: Wakes and SASE output power of European XFEL without and with tapered undulator.

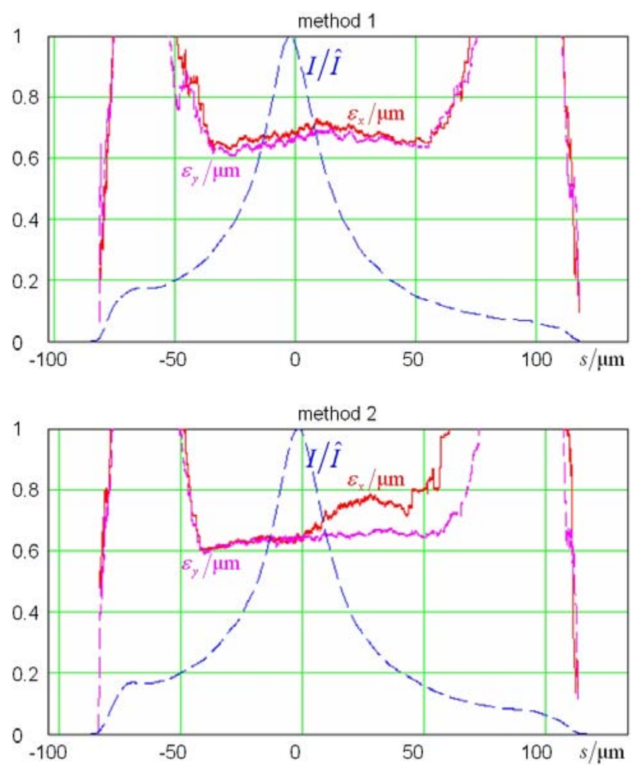

Fig. 9: Normalized current and transverse emittance at entrance of undulator of European XFEL.

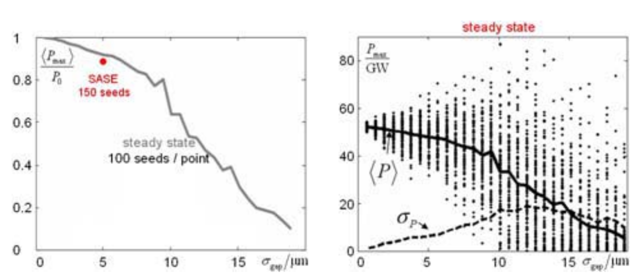

Fig. 11: Impact of undulator gap tolerance.

SUMMARY

XFELs require beams with kA peak currents and µm normalized emittances. The beam dynamics before the undulator is complicated to model especially in and after the gun and in bunch compression chicanes. Gun-to-undulator-tracking needs the use of different programs (SC, CSR) and the conversion of different phase space descriptions. Automated multi-method computations have been done: they need experience and careful inspection of intermediate results. Fast approaches are known for several particular problems (f.i., parameter sensitivity and µ-bunch instability).

SASE simulations rely on the preceding beam dynamics and need input from other investigations as surface properties and wakes. SASE simulations for many random seeds are used to investigate tolerances or statistical properties of the radiation. They are time consuming and need parallel computing. The "steady state" model allows a time efficient estimation of various FEL effects.

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