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FAST: a three-dimensional time-dependent FEL simulation code

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Abstract

In this report we briefly describe the three-dimensional, time-dependent FEL simulation code FAST. The equations of motion of the particles and Maxwell's equations are solved simultaneously taking into account the slippage effect. Radiation fields are calculated using an integral solution of Maxwell's equations. A special technique has been developed for fast calculations of the radiation field, drastically reducing the required CPU time. As a result, the developed code allows one to use a personal computer for time-dependent simulations. The code allows one to simulate the radiation from the electron bunch of any transverse and longitudinal bunch shape; to simulate simultaneously an external seed with superimposed noise in the electron beam; to take into account energy spread in the electron beam and the space charge fields; and to simulate a high-gain, high-efficiency FEL amplifier with a tapered undulator. It is important to note that there are no significant memory limitations in the developed code and an electron bunch of any length can be simulated.

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1. Introduction

Complete calculation of the parameters of an FEL amplifier can be performed only with numerical simulation codes. At present there are several numerical simulation codes calculating the amplification process in the FEL amplifier using the steady-state approximation. Such an approximation describes rather well the case when the FEL amplifier is seeded by monochromatic external radiation and when the slippage effect can be neglected. Such a simplification allows one to simulate the electron beam with one slice equal to the radiation wavelength, thus significantly reducing the requirements for computer resources. Nevertheless, the steady-state simulations do not provide a correct result when the slippage of the radiation is comparable with the length of the electron bunch. The steady-state code cannot be used in principle

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for the simulations of the FEL amplifier starting from the shot noise (SASE FELs), and a complete simulation of SASE FELs can be done only with a fully three-dimensional, time-dependent simulation code.

Recently, the development has been reported of one dimensional, time-dependent simulation codes which revealed the possibility to perform detailed investigation of the process of formation of the longitudinal coherence in the SASE FELs. Nevertheless, the one-dimensional approximation omits an essential effect of the diffraction of the radiation giving only a rough estimate of the SASE FEL parameters. Complete simulation of the physical process in the SASE FEL can be done only with a three dimensional, time-dependent simulation code. Unfortunately, the progress in this field is rather limited, and the main reason for this is due to limited possibilities of the computers.

In this paper we report on the development of a fast three dimensional, time-dependent simulation code FAST. The ideas implemented during the construction of this code allowed a significant reduction of the requirements on the computer, and the simulations of actual devices can be performed using a conventional personal computer.

2. General approach

Time-dependent simulations of the FEL amplifier should be performed by simultaneous solutions of Maxwell's equations and the equations of motion of the electrons. Nevertheless, the problem formulated in such a general form cannot be implemented in the simulation code and some physical approximation should be made. Here it is reasonable to remember that the free electron laser is a resonance device amplifying the radiation within a narrow bandwidth. Using this resonance approximation we present the transverse beam current density as $j_1(\boldsymbol{r},t)=\tilde{j}_1(\boldsymbol{r},t)\exp(\mathrm{i}\omega(z/c-t))+\mathrm{C.C.}$, where ω corresponds to the resonance FEL frequency and $\tilde{j}_1(\boldsymbol{r},t)$ is the slowly varying complex amplitude. The radiation field is also presented in the resonance approximation, $E(\boldsymbol{r},t)=\tilde{E}(\boldsymbol{r},t)\exp(\mathrm{i}\omega(z/c-t))+\mathrm{C.C.}$ with the slowly varying complex amplitude $\tilde{E}(\boldsymbol{r},t)$. Using paraxial approximation one can obtain the following expression for $\tilde{E}(\boldsymbol{r},t)$:

$$\tilde{E}(z,\boldsymbol{r}_\perp,t)=\mathrm{i}\frac{\omega}{c^2}\int_0^z\frac{\mathrm{d}z'}{z-z'}\int\mathrm{d}\boldsymbol{r}_\perp\tilde{j}_1\left(z',\boldsymbol{r}'_\perp,t-\frac{z-z'}{c}\right)\times\exp\left[\frac{\mathrm{i}\omega|\boldsymbol{r}_\perp-\boldsymbol{r}'_\perp|^2}{2c(z-z')}\right]. \quad (1)$$

The simulation code is organized as follows. We divide the electron beam in a large number of elementary volumes. The longitudinal size of each volume is equal to (or a multiple of) the radiation wavelength. Also, the electron beam is divided into a large number of divisions in the transverse direction. The FEL equations for the particle motion in each elementary volume are solved at each integration step. Then the radiation fields are calculated for each elementary volume using an integral solution (1). At the next integration step these fields are substituted into the FEL equations, etc. As a result, one can trace the evolution of the radiation field and the particle distribution when the electron beam passes the undulator. One can obtain from the integrals (1) that the radiation field at each point is defined only by the sources located closer than the slippage distance and it is not necessary to keep in the memory all the current sources. The procedure of the simulations begins from the tail slice of the electron bunch and the procedure of integration is performed over the whole undulator length. Then the equations of motion for the second slice are integrated taking into account the radiation field from the first slice, etc. As a result, the self-consistent FEL equations can be integrated for an electron bunch of any length. The memory requirements for the code are rather moderate. Our experience shows that a few tens of megabytes is sufficient to simulate most practical devices with sufficient accuracy.

The code is realized in two versions: linear and nonlinear. The linear simulation code is based on solution of the kinetic equation describing the evolution of the distribution function of the electron beam, and the nonlinear simulation code uses the traditional technique of macroparticles for the simulation of the distribution function of the electron beam.

3. Self-consistent equations

To be specific, in this section we present explicit formulae implemented in the code for the simulation of the FEL amplifier with an axially symmetric electron beam. The transverse distribution of the beam current density is assumed to be Gaussian; $j(r,z) = I(z)\exp(-r^2/2\sigma_r^2)/\sqrt{(2\pi\sigma_r^2)}$ with $\sigma_r = \sqrt{\varepsilon_n\beta/\gamma}$ where ε_n is the rms normalized emittance, β is the focusing beta function and $\gamma = \mathscr{E}_0/m_ec^2$ is the relativistic factor. The electron beam is divided into $L = l_b/k\lambda$ slices in the longitudinal direction (k is an integer), in M slices over the azimuthal angle ϕ, and in N divisions in the radial direction (we use the polar coordinate system (r,ϕ,z) here). As a result, we have $L\times M\times N$ elementary volumes. The self-consistent equations for the linear simulation code are as follows [2,3]:

$$\frac{d^2b_1}{d\hat{z}^2} + 2i\hat{C}\frac{db_1}{d\hat{z}} + [\hat{\Lambda}_p^2\alpha(\hat{r},\hat{z},t) - \hat{C}^2]b_1 = \sum_n \exp(in\phi)U_r^{(n)}(\hat{r},\hat{z},t) \tag{2}$$

where $b_1(\hat{r},\hat{z},\phi,t)$ is the beam bunching in the elementary volume, $\alpha(\hat{r},\hat{z},t) = I(\hat{z},t)\exp(-\hat{r}^2)/I_{max}$ and $U_r^{(n)}(\hat{z},\hat{r})$ is the nth azimuthal harmonic of the effective potential of interaction of the particle with the electromagnetic radiation

$$\begin{aligned} U_r^{(n)} &= U_{ext}^{(n)}(\hat{z},\hat{r},t) \\ &+ e^{in\pi/2}\int_0^{\hat{z}}\frac{d\hat{z}'}{\hat{z}-\hat{z}'}\int\hat{r}'d\hat{r}'\alpha(\hat{r}',\hat{z}',t-(z-z')/c) \\ &\times b_1^{(n)}(\hat{z}',\hat{r}',t-(z-z')/c)) \\ &\times J_n\left(\frac{B\hat{r}\hat{r}'}{\hat{z}-\hat{z}'}\right)\exp\left\{\frac{iB(\hat{r}^2+\hat{r}'^2)}{2(\hat{z}-\hat{z}')}\right\}. \end{aligned} \tag{3}$$

Here term $U_{ext}^{(n)}(\hat{z},\hat{r})$ corresponds to the external electromagnetic field, $b_1^{(n)}(\hat{r},\hat{z},t)$ are azimuthal harmonics of the beam bunching calculated using the values of $b_1(\hat{r},\hat{z},\phi,t)$ and J_n are the Bessel functions.

When writing down the normalized equations we used the following notations. The transverse coordinate is normalized as $\hat{r} = r/\sqrt{2\sigma_r^2}$. The corresponding reduced variables are as follows: $\hat{z} = \Gamma z$ is the reduced longitudinal coordinate, $\hat{C} = (2\pi/\lambda_w - \omega/(2c\gamma_z^2))/\Gamma$ is the detuning parameter, $\hat{\Lambda}_p^2 = \Lambda_p^2/\Gamma^2 = 4c^2(\theta_s\sigma_r\omega A_{JJ})^{-2}$ is the space charge parameter, $B = 2\Gamma\sigma_r^2\omega/c$ is the diffraction parameter, and the gain parameter Γ is

$$\Gamma = [I_{max}A_{JJ}^2\omega^2\theta_s^2/(2I_Ac^2\gamma_z^2\gamma)]^{1/2} \tag{4}$$

where $\omega = 2\pi c/\lambda$ is the frequency of the radiation field and $I_A = m_ec^3/e$. The undulator is assumed to be planar with magnetic field amplitude H_w and period λ_w. The undulator parameter K, the angle of electron oscillations θ_s, the longitudinal relativistic factor γ_z and the factor A_{JJ} are defined as follows: $K = eH_w\lambda_w/2\pi m_ec^2$, $\theta_s = K/\gamma$, $\gamma_z^2 = \gamma^2/(1+K^2/2)$ and $A_{JJ} = J_0(K^2/(4+2K^2)) - J_1(K^2/(4+2K^2))$, where J_0 and J_1 are the Bessel functions.

In the nonlinear simulation code, the electron beam distribution function is simulated with N_p macroparticles in each elementary volume. The equations of motion for the macroparticle written down in the "energy-phase" variables are as follows (for the low efficiency approximation):

$$\begin{aligned} \frac{d\hat{P}}{d\hat{z}} &= \mathrm{Re}\left[2ie^{i\psi}\sum_n\exp(in\phi)U_r^{(n)}(\hat{r},\hat{z})\right] + U_c \\ \frac{d\psi}{d\hat{z}} &= \hat{C} + \hat{P} \end{aligned} \tag{5}$$

where $\hat{P} = (\mathscr{E}-\mathscr{E}_0)/\rho\mathscr{E}_0$ is the reduced energy deviation, ψ is the phase of the macroparticle within the longitudinal slice and $\rho = c\gamma_z^2\Gamma/\omega$ is the efficiency parameter. The initial energy spread is simulated with the additional distribution of the particles according to the Gaussian law

$$dw = \frac{1}{\sqrt{2\pi\hat{\Lambda}_T^2}}\exp\left[-\frac{\hat{P}^2}{2\hat{\Lambda}_T^2}\right]d\hat{P}$$

where $\hat{\Lambda}_T^2 = \langle(\Delta\mathscr{E})^2\rangle/(\rho^2\mathscr{E}_0^2)$ is the energy spread parameter. An algorithm for the calculation of the space charge contribution, U_c, can be found in Ref. [3]. The complex amplitude of the beam bunching is calculated by averaging the macroparticle ensemble in the elementary volume, $b_1 = \langle\exp(i\psi_k)\rangle$, and is used for the calculations of the azimuthal harmonics of $b_1^{(n)}$. Eqs. (5) can be simply extended to the case of a high efficiency approximation and undulator tapering [3,4].

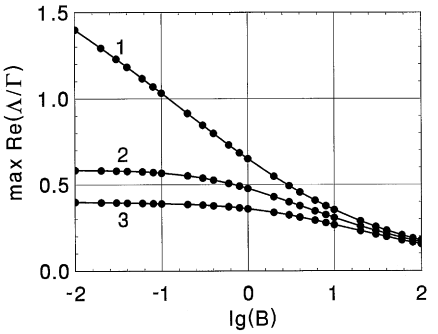

Fig. 1. The dependence of the maximal reduced field gain max $\mathrm{Re}(\Lambda/\Gamma)$ on the diffraction parameter B. Here $\hat{\Lambda}_{\mathrm{p}}^2 \to 0$, $\hat{\Lambda}_{\mathrm{T}}^2 = 0$. Curve (1): TEM_{00} mode, curve (2): TEM_{10} mode and curve (3): TEM_{01} mode.

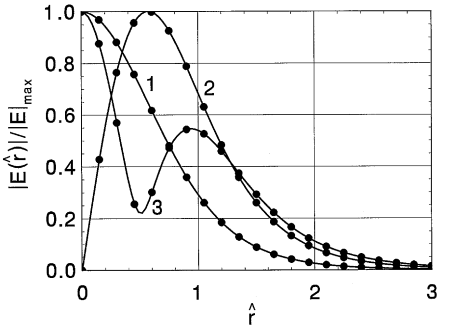

Fig. 2. Transverse distribution of the radiation field for TEM_{00}, TEM_{10} and TEM_{01}. Here $B = 10$, $\hat{\Lambda}_{\mathrm{p}}^2 \to 0$ and $\hat{\Lambda}_{\mathrm{T}}^2 = 0$. Curve (1): TEM_{00}, curve (2): TEM_{10} mode and curve (3): TEM_{01} mode. Solid curves are analytical results and the circles are the results of the numerical simulation code.

A complication for the case of the betatron oscillations and the undulator field errors to be taken into account is also straightforward [5].

Analysis of the integrals (3) shows that at the chosen radial mesh and at a fixed integration step Δz, calculations can be simplified significantly, since there is a finite set of the combination of the values $z - z'$, r and r'. The integrals over Δz for each of the combinations are calculated only once for the "unit" source term b_1. Then these data are transferred into the simulation code solving the self-consistent equations. Such a trick allows one to drastically reduce the required CPU time for the field calculations, since at each integration step the computer calculates simple sums weighted by the current sources.

The procedure for the solution of the self-consistent Eq. (5) has been described in the previous section. The accuracy of the calculations is controlled by changing the number of the axial, radial and azimuthal divisions, and the number of the azimuthal modes for the calculations of the radiation field. The criterium is that the final result is independent of the details of the simulations. Figs. 1 and 2 present the test results of the simulation code operating in a high gain, steady-state limit. It is seen that there is a good agreement between analytical [1] and simulation results. The relative accuracy for the calculation of the radiation field and the gain is about 0.1%.

At the exit the simulation code produces the matrices for the field values in the Fresnel diffraction zone. Then the post-processor programs are used to extract additional information for the field distribution in the far diffraction zone, for the spectrum, for the time, space and spectral correlation functions, and for the probability distributions of the radiation power and the radiation energy (see, e.g. Ref. [6]).

4. Initial conditions for the start-up from noise

The initial shot noise in the electron beam is simulated according to the algorithm presented in Ref. [6]. The number of particles per elementary volume N_{v} is large, so the bunching in each box is the sum of a large number of random phasors with fixed amplitudes and phases uniformly distributed on $(0, 2\pi)$. Using the central limit theorem, we can conclude that the phases of the bunching parameters are also distributed uniformly and the squared moduli of amplitudes, $|b_1|^2$, are distributed in accordance with the negative exponential distribution:

$$p(|b_1|^2) = \frac{1}{\langle |b_1|^2 \rangle} \exp\left(- \frac{|b_1|^2}{\langle |b_1|^2 \rangle} \right) \tag{6}$$

where $\langle |b_1|^2 \rangle = 1/N_{\mathrm{v}}$. The distribution of the modules, $|b_1|$, is the Rayleigh probability density function. So, we use the negative exponential random generator setting $1/N_{\mathrm{v}}$ as a mean value to extract

the values of $|b_1|^2$ for each box and then we extract the square root to find the values of $|b_1|$. The phases of b_1 are produced by a random generator of a uniform distribution from 0 to 2π. These values are directly used as input parameters for the linear simulation code. In the nonlinear simulation code the macroparticles are distributed in such a way that the resulting bunching corresponds to the target value of b_1 in each elementary volume.

5. Conclusion

In conclusion, we should notice that the speed of calculations is an essential parameter for the FEL code calculating the start-up from noise. The reason for this is that the most important characteristics of the SASE FEL (the spectrum, time, space and spectral correlation functions and the probability distributions of the radiation power and energy) can be calculated only with statistical analysis of a large number of simulation runs [6]. For instance, the number of the simulation runs required for the calculation of the probability distribution of the radiation energy in the pulse is about several thousands. The presented code allows one to calculate all the above-mentioned statistical parameters of the SASE FEL within a reasonable time. For instance, a typical simulation run with the linear simulation code for the parameters of the UCLA/LANL/RRCKI/SLAC SASE FEL [7] takes about 1 min on a VAX processor [8]. This is about two orders of magnitude less than the time required by other time-dependent codes (such as GINGER or GENESIS) to obtain the same physical result [9,10].

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