FREE ELECTRON LASER SIMULATION TOOL BASED ON FDTD/PIC IN THE LORENTZ BOOSTED FRAME*

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Abstract

Free Electron Lasers (FELs) are the only radiation sources generating electromagnetic from THz to hard X-rays. Therefore, it is crucial to develop rigorous simulation tools. Our work is motivated by the desire to develop compact X-ray sources based on radiation generated with optical undulators. The currently existing softwares are usually written to tackle special cases allowing for particular approximations, such as 1D FEL theory, steady state, slow wave and forward wave approximation, wiggler-averaged electron motion and slice approximation. Many of the above approximations are hardly valid when sub-femtosecond bunches interact with intense optical lasers. The presented software aims at the analysis of an FEL interaction without using any of the above approximations. The developed tool apparently suffers from a long computation time but offers a more accurate picture of the radiation process. In order to overcome the problem of multiple scales, we exploit the Lorentz boosted coordinate system and implement a Finite Difference Time Domain (FDTD) method combined with a Particle in Cell (PIC) simulation in this frame.

INTRODUCTION

Free Electron Laser (FEL) concept as the only solution for providing hard X-ray radiation offers valuable devices enabling the study of materials, crystallography and chemical reactions [1]. The high operation costs of hard X-ray FEL machines adds considerable importance to the prediction of their performance based on accurate simulations. Optimizing a complete FEL facility and the investigation of important effects in the FEL process are enabled by these simulation tools. Our main motivation for pursuing a complete and precise numerical analysis of FEL operation is the simulation of FEL radiation in an optical undulator. This technique has recently gained attention owing to its promise in the development of compact X-ray sources. The currently existing simulation tools for predicting the FEL dynamics are usually written to tackle special cases and therefore particular assumptions or approximations are considered in their formulations. However, the accuracy of these approximations may fail when FELs based on optical undulators are being studied.

These assumptions were often indispensable steps in a FEL simulation because of the multiple length scales involved in the process. Typical values encountered in a FEL are ~ 100 fs or 300 μm for the bunch length, ~ 1 cm for the undulator period, ~ 10 – 500 m for the undulator length and ~ 1 – 100 nm for the radiation wavelength. Comparing the typical undulator lengths with radiation wavelengths immediately communicates the very wide range of length scales involved in FEL interactions. This makes the accurate FEL simulation very challenging and calls the need for very high computation costs to resolve all physical phenomena, which is not practical even with existing supercomputer technology. In order to overcome this problem, we exploit the Lorentz coordinate system transformation into the bunch rest frame and implement a Finite Difference Time Domain (FDTD) method combined with Particle in Cell (PIC) simulation in this frame. The use of a Lorentz boosted coordinate system causes the very different length scales to transform into values with the same order of magnitudes, thereby considerably reducing the computation cost. Consequently, the size of the computational domain is reduced to slightly more than the bunch size making the full-wave simulation numerically feasible. We comment that the simulation of particle interaction with an electromagnetic wave in a Lorentz boosted framework is not a new concept. The advantage of this technique is already demonstrated and widely used in the simulation of plasma-wakefield acceleration. However, to the best of our knowledge, this technique has never been used to simulate the FEL process, which is the main goal of our study.

NUMERICAL IMPLEMENTATION

The Finite Difference Time Domain method is used for the time domain solution of Maxwell's equations. The equation of motion is simultaneously updated using a Particle In Cell (FDTD/PIC) method leading to the well-known FDTD/PIC algorithm. There are several important considerations to obtain reliable results converging to the real values. Examples are the method for electron bunch generation, particle pusher algorithm and computational mesh truncation, which need particular attention. For the sake of brevity, we do not explain these features in this contribution and discuss their precise implementation in another paper.

Finite Difference Time Domain-Particle In Cell (FDTD/PIC)

FDTD is a superior choice for the time domain solution of the electromagnetic fields due to its inherent properties for explicit time update and zero DC fields in the solution [2]. As usual in a FEL solution, we solve the Helmholtz equations extracted from Maxwell's equations for electromagnetic waves propagating in free space. It is well-known that

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the proper definition of the vector potential ($\boldsymbol{A}$) and scalar electric potential (φ) recast Maxwell's equations for $\boldsymbol{E}, \boldsymbol{B}$ into two uncoupled equations, namely vector Helmholtz equation for $\boldsymbol{A}$ and scalar Helmholtz equation for φ:

$$\nabla^2 \boldsymbol{A} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\boldsymbol{A} = -\mu_0 \boldsymbol{J} \quad (1)$$

$$\nabla^2 \varphi - \frac{1}{c^2}\frac{\partial^2 \varphi}{\partial t^2} = -\frac{\rho}{\varepsilon_0} \quad (2)$$

$c = 1/\sqrt{\mu_0 \varepsilon_0}$ is the light velocity in vacuum. In the derivation of above equation the Lorenz gauge condition $\nabla \cdot \boldsymbol{A} = -\frac{1}{c}\frac{\partial \varphi}{\partial t}$ is used. The original $\boldsymbol{E}$ and $\boldsymbol{B}$ vectors are obtained from $\boldsymbol{A}$ and φ as:

$$\boldsymbol{B} = \nabla \times \boldsymbol{A} \quad (3)$$

$$\boldsymbol{E} = -\frac{\partial}{\partial t}\boldsymbol{A} - \nabla \varphi \quad (4)$$

In addition to the above equations, the charge conservation law written as

$$\nabla \cdot \boldsymbol{J} + \frac{\partial \rho}{\partial t} = 0 \quad (5)$$

should not be violated in the employed computational algorithm. It is immediately observed that the Equations (1), (2), (5) and the Lorentz gauge introduce an over-determined system of equations. In a numerical solution algorithm, one needs to neglect one of the equations and try to implement the numerical solution such that minimizes the error is minimized. Due to the space-time discretization and the interpolation of quantities to the grids, a suitable algorithm that maintains charge conservation without violating energy and momentum conservation does not exist. The approach that we follow is using the discretized form of (1) with electron currents (i.e. macro-particles) as the source and solving for the scalar potential using the Lorentz gauge. To obtain the fields $\boldsymbol{E}$ and $\boldsymbol{B}$ at the grid points, we use momentum conserving interpolation, which interpolates the field values to the grid points. The Lorentz gauge $\nabla \cdot \boldsymbol{A} = -\frac{1}{c}\frac{\partial \varphi}{\partial t}$ is solved similar to the Helmholtz equation through the discretization using the central finite differences.

Particle in cell (PIC) method is the standard algorithm to solve for the motion of particles within an electromagnetic field distribution. The method takes the time domain data of the fields $\boldsymbol{E}$ and $\boldsymbol{B}$ and updates positions and momenta according to the relativistic equation of motion for macro-particles:

$$\frac{\partial}{\partial t}(\gamma m \boldsymbol{v}) = -e(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}), \quad \text{and} \quad \frac{\partial \boldsymbol{r}}{\partial t} = \boldsymbol{v}, \quad (6)$$

where $\boldsymbol{r}$ and $\boldsymbol{v}$ are the position and velocity vectors of the macro-particles, e is the electron charge and m is its rest mass. γ stands for the Lorentz factor of the moving particle.

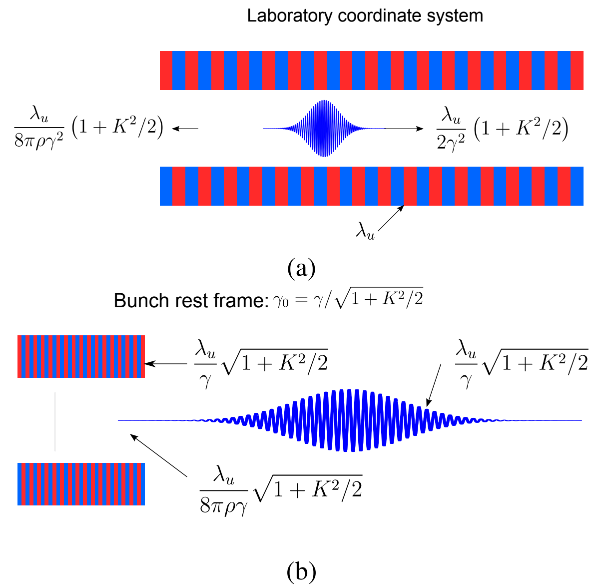


Figure 1: Schematic illustration of the Lorentz boosting to transform the problem from the laboratory frame to the bunch rest frame.

Lorentz Transformation

A novelty of the implemented technique is the solution of Maxwell's equations in the bunch rest frame. Based on the already developed and matured FEL theory, it can be demonstrated that coordinate transformation into the bunch rest frame causes all the involved parameters such as bunch length, undulator period, undulator length, and radiation wavelength converge from widely different length scales into values with the same orders of magnitude. In Fig. 1, we present a schematic illustration of how transformation into the bunch rest frame offers this advantage. In a typical FEL problem, the FEL parameter ρ_{FEL} is about 10^{-3}. Therefore, simulation of FEL interaction with a bunch equal to the cooperation length of the FEL ($L_c = \lambda_l/(4\pi\rho_{FEL})$, with λ_l being the radiation wavelength) requires a simulation domain only 100 times larger than the wavelength, which is completely feasible using present computer technology.

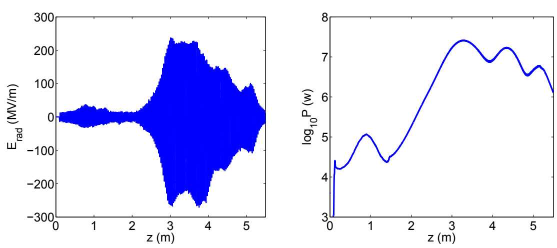
RESULTS

We benchmark the developed software by simulating an infrared FEL with the parameters tabulated in table 1 and comparing the results with the one-dimensional FEL theory. For this purpose, The bunch distribution is assumed to be uniform, the transverse energy spread is considered to be zero and a minimal longitudinal energy spread is assumed. Figure 2a shows the transverse electric field sampled at 55 µm in front of the bunch center. The logarithmic plot of the radiated power at different positions along the undulator (z) is also depicted in Fig. 2b. According to the 1D FEL theory the gain length of the considered SASE FEL configuration is $L_G = 22.4$ cm, which is calculated as $L_G = 22$ cm from the slope of the power curve in Fig. 2b. The beam energy according to the data in table 1 is 1.52 mJ which for the bunch

Table 1: Parameters of the Infrared FEL Configuration Considered as the First Example

FEL parameter	Value
Bunch type	Uniform cylinder
Bunch size	$(260 \times 260 \times 100)$ µm
Bunch charge	29.5 pC
Bunch energy	51.4 MeV
Bunch current	88.5 A
Longitudinal momentum spread	0.01%
Transverse momentum spread	0.0
Undulator period	3.0 cm
Magnetic field	0.5 T
Undulator parameter	1.4
Undulator length	5 m
Radiation wavelength	3 µm
Electron density	8.7×10^{18}
Gain length (1D)	22.4 cm
FEL parameter	0.006
Cooperation length	39.7 µm

length of 100 µm corresponds to $P_{beam} = 4.55$ GW beam power. The estimated saturation power according to the 1D theory is equal to $P_{sat} = \rho P_{beam} = 2.7$ GW. The saturation power computed by the FDTD/PIC code is 2.6 GW.



(a) (b)

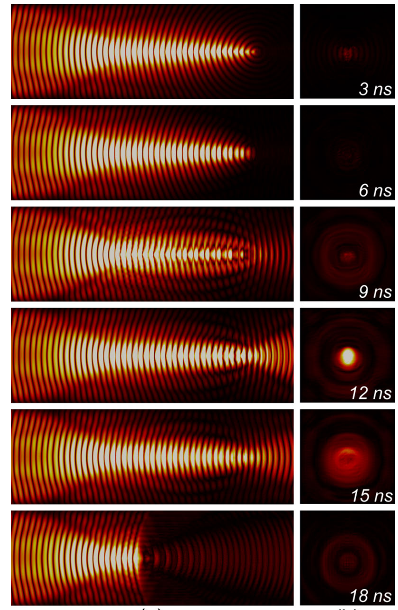
Figure 2: (a) The transverse field E_y at 55 µm distance from the bunch center and (b) the total radiated power measured at 55 µm distance from the bunch center in terms of the traveled undulator length.

In Fig. 3, snapshots of the radiated field profile at different time instants are illustrated. The emergence of lasing radiation at the end of the undulator motion is clearly observed in the field profile.

Furthermore, snapshots of the bunch profile are also presented in Fig. 4. The main FEL principle which is the lasing due to micro-bunching of the electron bunch is observed from the field and bunch profiles.

CONCLUSION

A full-wave simulation tool for the FEL process is presented. Maxwell equations together with relativistic equation of motion are solved using FDTD/PIC algorithm for the simulation of the underlying electron-wave interaction. In order to make the simulations feasible Lorentz boosted transformation into the bunch rest frame is applied. The simulation results for a typical Infrared FEL are in good agreement with those of the 1D FEL theory. Microbunching as the core basis for FEL coherent radiation as well as natural undulator focusing are clearly observed.



(a) (b)

Figure 3: Snapshots of the radiated field profile taken at (a) $y = 0$ and (b) $z = 55$ µm plane.

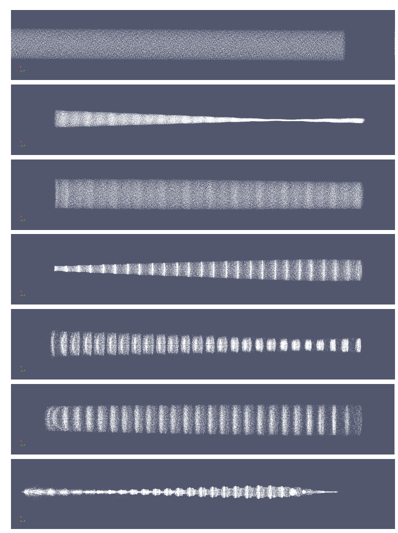


Figure 4: The bunch profile viewed from the y axis.

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