UNAVERAGED THREE-DIMENSIONAL MODELLING OF THE FEL

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Abstract
A new three-dimensional model of the FEL is presented. A system of scaled, coupled Maxwell–Lorentz equations are derived in the paraxial limit. A minimal number of limiting assumptions are made and the equations are not averaged in the longitudinal direction of common radiation/electron beam propagation, allowing the effects of coherent spontaneous emission and non-localised electron propagation to be modelled. The equations are solved numerically using a parallel Fourier split-step method.

INTRODUCTION
A three-dimensional model of a helical wiggler Free Electron Laser (FEL) is presented that minimises the assumptions made. This model does not average the Maxwell–Lorentz equations describing the interaction between the electrons, wiggler and radiation fields. Furthermore, no relativistic approximations in the equations governing electron motion are made and transverse motion of the electrons is self-consistently driven by both the wigglers and radiation fields. Current 3D codes perform averaging over a radiation wavelength of the radiation and others also model 

3D MODEL
Following the method of previous studies for the one-dimensional FEL [1] [3] [2] the physics of the FEL may be described in three dimensions by the coupled Maxwell–Lorentz equations

\begin{equation}
\nabla^2 \mathbf{E}(\mathbf{r}, t) = \frac{1}{c^2} \frac{\partial^2 \mathbf{E}(\mathbf{r}, t)}{\partial t^2} + \mu_0 \frac{\partial \mathbf{J}_{\perp}(\mathbf{r}, t)}{\partial t}
\end{equation}

where \( \mathbf{J}_{\perp}(\mathbf{r}, t) = -\frac{e}{m} \sum_{j=1}^{N} \frac{\mathbf{p}_j}{\gamma_j} \delta(\mathbf{r} - \mathbf{r}_j(t)) \),

\begin{equation}
\frac{d\mathbf{p}_j}{dt} = -e \left( \mathbf{E}(\mathbf{r}, t) + \frac{\mathbf{p}_j}{\gamma_j m} \times \mathbf{B}(\mathbf{r}, t) \right)
\end{equation}

where \( \mathbf{m} \) is the electron rest mass. The helical wiggler and radiation electric field are assumed to be

\begin{align}
\mathbf{B}_w(\mathbf{r}) &= \frac{B_w}{\sqrt{2}} (\mathbf{e} e^{-ik_w z} + c.c.) \\
&+ \frac{B_w k_w}{2} [i x (e^{-ik_w z} - c.c.) + y (e^{ik_w z} + c.c.)] \hat{z}
\end{align}

where \( \mathbf{e} = (\mathbf{x} + i\mathbf{y})/\sqrt{2} \), \( \xi_0 \) is a slowly varying complex field envelope and \( B_w \) is the wiggler magnetic field strength of period \( \lambda_w = 2\pi/k_w \). The magnetic component of the radiation field \( \mathbf{B}(\mathbf{r}, t) \) is required in the Lorentz equation and may be calculated from Maxwell’s equations to give:

\begin{equation}
\mathbf{B}(\mathbf{r}, t) = -\frac{i}{\sqrt{2}} \left( \frac{\xi_0(\mathbf{r}, t)}{c} \mathbf{e} e^{ik_z(t-z)} - c.c. \right)
\end{equation}

where it has been assumed that any radiation that is counter-propagating the electron beam may be neglected.

The following scaling notation is now introduced:

\begin{align}
\xi &= \frac{1 - \beta_z}{\beta_z}, \xi_n = \frac{1 - \beta_z}{\beta_z}, \alpha = \left( \frac{2\gamma_r \rho}{\omega_w} \right)^2, \\
\rho_\perp &= \frac{p_x - ip_y}{mc}, \mathbf{A} = \frac{e\xi_0}{m c \omega_p \sqrt{\gamma_r \rho} c.c.} \mathbf{B}(\mathbf{r}, t), \\
\bar{\xi} &= 2k_w \rho z, \bar{z}_2 = 2k_w \rho \beta_z (ct - z), \\
\bar{x} &= \frac{x}{\sqrt{l_g c}}, \bar{y} = \frac{y}{\sqrt{l_g c}}
\end{align}

where \( \beta_z = v_z/c \) is the mean electron velocity on entering the interaction region, \( \gamma_r \) is the resonant electron energy and \( \rho \) is the fundamental FEL parameter, defined as

\[ \rho = \frac{1}{\gamma_r} \left( \frac{a_w \omega_p}{4 c k_w} \right)^{2/3} \]

where \( \omega_p = \sqrt{\varepsilon_0 n_p (\varepsilon_0 m)} \) is the plasma frequency for the peak electron number density of the electron pulse \( n_p \), and \( a_w = eB_w/(mc k_w) \) is the wiggler deflection parameter. The scaled electron density is defined as \( n_{\rho} = n_p l_y l_z^2 \), where \( l_y \) is the gain length and \( l_z \) the cooperation length. Note the scaling in the transverse plane is with respect to the physically relevant gain and cooperation lengths. This allows the equations above describing the FEL interaction to be written as

\begin{equation}
-\rho \left( \frac{\partial^2 A}{\partial \xi^2} + \frac{\partial^2 A}{\partial \bar{z}^2} \right) + \frac{\partial A}{\partial \bar{z}} + 2i \rho \frac{\partial^2 A}{\partial \xi \partial \bar{z}} = (7)
\end{equation}
\[
\frac{\gamma_r}{a_w \bar{n}_p} \sum_{j=1}^{N} \bar{\rho}_{1j}(\varepsilon Q_{j} + 2) \frac{1}{(1 + |\bar{\rho}_{1j}|^2)^{1/2}} \delta(\bar{r} - \bar{r}_j)e^{i\bar{z}_2}\]

\[
\frac{d\bar{\rho}_{1j}}{d\bar{z}} = \frac{a_w}{2\rho} \left[ ie^{-i\bar{z}} - \varepsilon Q_{j} A e^{-i\bar{z}_2} \right] - \frac{a_w^2 \varepsilon}{8\rho^2} \frac{Q_{j}(2 + \varepsilon Q_{j})(\bar{x} - i\bar{y}_{j})}{(1 + |\bar{\rho}_{1j}|^2) (1 + \varepsilon Q_{j})^2} \]

\[
\frac{dQ_{j}}{d\bar{z}} = \frac{a_w Q_{j}(\varepsilon Q_{j} + 2)}{4\rho + |\bar{\rho}_{1j}|^2} \times \left[ i(\varepsilon Q_{j} + 1)(\bar{\rho}_{1j}^* e^{-i\bar{z}} - c.c.) + \varepsilon Q_{j}(\bar{\rho}_{1j} A e^{-i\bar{z}_2} + c.c.) \right] \]

\[
\frac{d\bar{z}_2}{d\bar{z}} = Q_{j} \quad (10)
\]

\[
\frac{d\bar{x}}{d\bar{z}} = \Re(\bar{\rho}_{1j}) \left( \frac{Q_{j}(2 + \varepsilon Q_{j})}{1 + |\bar{\rho}_{1j}|^2} \right) \]

\[
\frac{d\bar{y}_{j}}{d\bar{z}} = -\Im(\bar{\rho}_{1j}) \left( \frac{Q_{j}(2 + \varepsilon Q_{j})}{1 + |\bar{\rho}_{1j}|^2} \right) \]

In deriving the equations the only approximations made are the neglect of space charge and the paraxial approximation. There are no restrictions on the electron energy allowing large changes to be modelled.

In the scaled variables used here, the normalised beam emittance is given by

\[
\epsilon_\text{m} = \sqrt{\gamma_r \sigma_\text{x} \sigma_\text{p}.} \quad (13)
\]

For an electron beam matched to a focussing channel the radius of the electron beam envelope is given by

\[
r_b = \left( \frac{\epsilon_\text{m} \beta}{\gamma_r} \right)^{1/2} \quad . \quad (14)
\]

The electrons experience a natural focussing force due to the magnetic field of the heligical wig [4] resulting in a beta-function of \( \beta = \gamma_r / a_w k_\text{w} \). This restoring force is approximated by the final linear term in (8) and may be simply modified in magnitude to approximate other, e.g. FODO, focussing channels.

The scaled Rayleigh range (in units of \( \bar{z} \)) can be shown to be \( \bar{z}_R = \sigma_{\text{e}}^2 / 2\rho \), where \( \sigma_{\text{e}} \) is the radius of the beam in scaled units of \( \bar{x}, \bar{y} \).

It can be shown that the above equations satisfy energy conservation, written in the form:

\[
\int_{\text{all space}} |A|^2 d\bar{x} d\bar{y} d\bar{z}_2 + \frac{1}{\gamma_r \rho} \sum_{k=1}^{N_p} \chi_k \gamma_k = 0 \quad (15)
\]

where \( \gamma_k = \sqrt{\frac{(1 + |\bar{\rho}_{1k}|^2)(1 + \varepsilon Q_k)^2}{\varepsilon Q_k(1 + \varepsilon Q_k + 2)}} \)

which may be used as a check in the numerical solution.

In the relativistic Compton limit \( \epsilon, \rho \ll 1 \) the above equations can be shown to reduce to those of [1].

**NUMERICAL SOLUTION**

The field evolution of the scaled equations (7)-(12) are solved by applying a modified parallel Fourier split-step method [5] in conjunction with a finite element method [6]. This allows the effects of coherent spontaneous emission (CSE), self-amplified spontaneous emission (SASE) and diffraction to be modelled numerically. The parallel code was developed using the Numerical Algorithms Group (NAG) parallel routines to control the parallel processing. The Fourier split-step method involves solving the wave equation in two steps. The first step considers the field diffracting in the transverse direction and propagating in the \( \bar{z} \) direction freely without the electron source term:

\[
- i\rho \left( \frac{\partial^2 A}{\partial \bar{x}^2} + \frac{\partial^2 A}{\partial \bar{y}^2} \right) + \frac{\partial A}{\partial \bar{z}} + 2i\rho \frac{\partial^2 A}{\partial \bar{z} \partial \bar{z}_2} = 0. \quad (16)
\]

This equation can be solved by taking the Fourier transforms in \( \bar{x}, \bar{y} \) and \( \bar{z}_2 \) resulting in an ordinary differential equation in the Fourier transformed field \( \hat{A} \), with the following analytic solution:

\[
\hat{A}(\bar{z} + \Delta \bar{z}) = \hat{A}(\bar{z}) \exp \left[ -i\rho k_\text{z}^2 \frac{\Delta \bar{z}}{(1 - 2\rho k_\text{z}^2)} \right], \quad (17)
\]

where the transverse Fourier transform variable pairs are given by \( (\bar{x}, k_\text{x}), (\bar{y}, k_\text{y}), (\bar{z}_2, k_\text{z}_2) \) and \( k_\text{x}^2 = k_\text{x}^2 + k_\text{y}^2 \). The inverse numerical Fourier transform is then applied and the solution \( A(\bar{x}, \bar{y}, \bar{z}_2, \bar{z} + \Delta \bar{z}) \) is then used as the initial field for the second part of the split-step method where the diffraction terms are neglected and the source term acts alone:

\[
\frac{\rho A}{\rho \frac{\partial A}{\partial \bar{z}_2}} = \gamma_r \frac{1}{a_w \bar{n}_p} \sum_{j=1}^{N} \bar{\rho}_{1j}(\varepsilon Q_{j} + 2)^{1/2} \frac{1}{(1 + |\bar{\rho}_{1j}|^2)^{1/2}} \delta(\bar{r} - \bar{r}_j)e^{i\bar{z}_2} \quad (18)
\]

The finite element method is then used to solve the wave equations (18) and (8)-(12) along with a fourth order Runge-Kutta method for electron variables to give the final solution.

Before applying the finite element method to the wave equation, the summation over the real electrons has to be changed to a summation over a group of macroparticles, each of which represents many real electrons. This reduces the computational memory load and operation:

\[
\frac{1}{\bar{n}_p} \sum_{k=1}^{N_p} \chi_k \gamma_k = \frac{1}{\bar{n}_p} \sum_{k=1}^{N} N_k (\cdots)_k \quad (19)
\]

where subscripts \( j \) and \( k \) indicate evaluation at the particle position, \( N_p \) is the total number of macroparticles and \( N_k \) is the charge weight of the macroparticle in units of the electron charge.

The Galerkin method of the finite elements is used. The field is described by a set of 8-node hexahedral elements.
with linear basis functions $\Lambda_m(\bar{x}, \bar{y}, \bar{z}_2)$ and nodal values $a_m(\bar{z})$:

$$A(\bar{x}, \bar{y}, \bar{z}_2) = \sum_m a_m(\bar{z})\Lambda_m(\bar{x}, \bar{y}, \bar{z}_2).$$

where $m$ is the global node index of the 3D system. Note that $\Lambda_m(\bar{x}, \bar{y}, \bar{z}_2) \equiv 0$ ouwith the elements to which it belongs. The wave equation then reduces to a matrix equation for the nodal points:

$$K\frac{\partial a_m(\bar{z})}{\partial \bar{z}} = \sum_{p=1}^{N_p} \frac{\bar{x}_k p_{\perp k}(\bar{z}_k \Lambda \bar{z}_k + 2))^{1/2}}{V_e} \times$$

where $K$ is the stiffness matrix constructed from the elemental equations [6]. $\bar{x}$ is a macroparticle weighting function and $V_e$ is the scaled volume of an element of the system, $V_e = \Delta\bar{x}\Delta\bar{y}\Delta\bar{z}_2$.

**A SIMULATION IN THE 1D LIMIT**

To test the 3D model a comparison with the 1D results of [1,2] was made. In these one-dimensional models the wave equation was integrated analytically over the common electron/radiation transverse area before numerical solutions were obtained.

Here, one element is used in the transverse plane approximating the radiation field to a plane wave and allowing integration over the transverse area and comparison with the 1D results. The electron beam radius was set greater than the electron orbital radius ensuring the electron beam does not move significantly in the transverse plane of the element. A gaussian distribution for the electrons in the transverse plane was used with a range of six times the standard deviation. The results of [1] Fig. 2 showing self-amplified coherent spontaneous emission (SACSE) for a top-hat pulse current are reproduced in Fig. 1. (Note that there is a scale reversal as [1] plots the power as a function of $z_1$ while here it is plotted as a function of $z_2$.) The coherent spontaneous emission, including the effects of shot noise, from both square and gaussian shaped pulses of [2] were also reproduced. In Fig. 2 the top hat case of [2] Fig. 4 is plotted. Good agreement between the 1D models of [1,2] and the 1D limit of the 3D model of this paper are observed.

**A SIMULATION IN 3D**

An example of the code operating in 3D is now presented. The parameters used are not intended to model any specific system, but rather to demonstrate the functioning of the code and its associated post-processing and plotting routines. A relatively simple system was chosen with a short electron pulse so that coherent spontaneous effects can be observed and large computational effort is not required.
Electron beam parameters

| Parameter                | Value          |
|-------------------------|----------------|
| Energy \(E\)            | 250 MeV        |
| Bunch Charge \(Q\)      | 100 pC         |
| Peak Intensity \(I_{pk}\) | \(\sim 9394\) A |
| Distribution in \(\bar{x}, \bar{y}\) | Gaussian |
| Sigma in \(\bar{x}, \bar{y}\) | \(\sim 0.228\) |
| Distribution in \(\bar{z}_2\) | Top-hat |
| Length of pulse in \(\bar{z}_2\) | 1.5 |
| Emittance and energy spread | 0 |

Undulator parameters

| Parameter                | Value          |
|-------------------------|----------------|
| Undulator Type          | Helical        |
| Pierce parameter \(\rho\) | \(\sim 1.5e-2\) |
| Wiggler deflection \(a_w\) parameter | 1.5 |
| Propagation distance \(\bar{z}\) | 5.00 |

Radiation parameters

| Parameter                | Value          |
|-------------------------|----------------|
| Initial seed field over pulse \(A_0\) | 0.01 |
| Seed distribution in \(\bar{x}, \bar{y}\) | Gaussian |
| Sigma in \(\bar{x}, \bar{y}\) | \(\sim 0.228\) |
| Rayleigh length \(\bar{z}_R\) | 1.74 |
| Distribution of seed in \(\bar{z}_2\) | Top-hat |
| Length of seed in \(\bar{z}_2\) | 1.5 |

Table 1: 3D parameters

CONCLUSION

A new parallel code has been developed which models the FEL amplifier by solving a system of scaled equations describing the FEL interaction in three spatial and the time dimension. The aim has been to introduce as few approximations into the model as possible, the main assumptions being the neglect of space charge and any backward propagating radiation fields. This allows the effects of coherent spontaneous emission, diffraction and full electron transport throughout the region of integration to be modelled. Furthermore, the sub-wavelength discretisation of the model allows a significantly wider range of radiation frequencies to be modelled than is possible with most other codes that use a minimum discretisation interval of a radiation wavelength. A 1D limit of the computational model was identified and simulation results in this limit show agreement with previous 1D numerical and analytical models. A further example simulation has been presented which demonstrates the code operating successfully using an electron pulse in three dimensions. Further optimisation of the code is ongoing. While the code is undoubtedly slower to operate than other 3D averaged codes, the extended physics that it can model may be expected to yield interesting new phenomena in FEL physics.

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