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Generalized 3D beam dynamics model for industrial traveling wave linacs design and simulations

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A B S T R A C T

Beam dynamics simulations in traveling wave (TW) accelerating structures with significant beam loading is a challenging problem. Some codes are capable of calculating the TW electromagnetic fields, and some can track particles through such fields, but most cannot treat both self-consistently. A few commercial codes can model the physics correctly at the expense of many processor-hour computations to obtain converged self-consistent solutions. However, simple, accurate equations of motion for intensive beam dynamics in TW accelerating structure analysis have been previously obtained by Masunov and subsequently implemented in the Hellweg code, which was developed at the Moscow Engineering-Physics Institute. Hellweg is based on equations that allow fast simulations of beam dynamics while taking into account such effects as beam loading, space charge, and external magnetic fields. In this paper, we describe in detail some recent improvements to the Hellweg physics kernel. We have generalized the Masunov results into a 3D set of equations of motion, which include all spatial components of the radiofrequency (RF) and external magnetic fields. We have also improved the Lapostolle space charge model to the general 3D ellipsoid form for any dimensions' ratio, consideration for the particles outside the beam core, and the fields from the neighboring bunches that can exist in the real machine. These modifications allow approaching the Hellweg accuracy to the self-consistent commercial codes while keeping the simulation time short, which is essential during the linac design and optimization stage. The implementation of these new capabilities in Hellweg is carefully benchmarked against other codes and analytical calculations. The code is freely available with an open source license.

1. Introduction

Industrial accelerator applications include treatment of potable drinking water and wastewater, removal of pollutants from stack gasses, increased efficiency of material processing and replacement of radioactive sources in sterilization applications [1]. These applications involve exposing large mass streams to kGy-class radiation fields, which requires: high average electron beam power from 0.5 to 10 MW, wall plug efficiency of 50% or more, operation in harsh industrial settings and low capital and operating costs [2]. The most promising solution for high-current applications is to use traveling-wave RF structures with a modest accelerating gradient [3]. The pulsed current in such linacs can be as high as tens of amperes. Such high currents can cause some specific effects, which must be accurately considered in the design stage [4,5].

For example, acceleration of high current beam reduces power flow in the accelerating waveguide, accelerating field amplitude and by extension the output beam energy. For industrial accelerators, the beam power constitutes a considerable fraction of input RF power. Also, high currents require a proper consideration of space charge forces acting in the bunch, since they are comparable to the forces of the RF fields at low energy. Space charge may influence the stability of longitudinal (phase) or transverse (radial) dynamics. Next, the motion of grouped bunches along the waveguide can induce a reactive current component of the waveguide walls, changing the phase velocity of the electromagnetic wave, which in turn degrades the beam quality and acceleration efficiency. Finally, under certain conditions, electron bunches can excite asymmetric waves with a transverse on-axis component. Such waves deflect the beam away from the waveguide axis, which can lead to catastrophic beam loss.

Accurate treatment of beam loading is central to the design of high-power TW accelerators, and it is especially difficult to model in the meter-scale region where the electrons are nonrelativistic. Currently, there is no commercial software that provides fast, accurate calculations of beam loading in such linear TW accelerators. Some software packages are capable of calculating the TW electromagnetic fields, and some can track particles through such fields, but most cannot treat both self-consistently. For example, GPT [6] uses a simplified model of beam loading, relevant only to relativistic beams. Parmela [7,8] works with

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pre-calculated fields, but the beam-loaded amplitude and phase in each cell must be estimated by the user. RTMtrace [9] cannot simulate beam-loaded dynamics in the bunching section of a linac. Other codes require independent runs and many iterations to converge on a possible solution.

There are expensive[1] commercial codes like Magic 3D [10,11] and CST Particle Studio [12,13], which can model the physics correctly in a single GUI-driven workflow. However, the Courant criterion for numerical stability of finite-difference time domain (FDTD) solutions of Maxwell's equations [14] leads to disparate time scales, requiring an enormous number of time steps to obtain correct self-consistent solutions. An alternate technology should be developed that can avoid time-consuming transient electromagnetic (EM) simulations, while effectively and accurately coupling the traveling wave EM fields with beam dynamics to reach the accuracy compared with self-consistent solutions.

Meanwhile, a rather simple and convenient method for intensive beam dynamics in TW accelerating structures analysis has been proposed [15] and realized in the Hellweg code [16] that is used for the linac optimization, which is an intermediate step between analytical estimation of the linac parameters and accurate but extremely time-consuming[2] self-consistent simulations of the final linac design. Hellweg is based on equations that can accurately simulate beam dynamics while taking into account such effects as beam loading, space charge, and external magnetic fields. The reference data entered into this program allows automatic determination of the disk-loaded structure (DLS) with a known phase velocity and normalized electrical field strength, which enables the capability to synthesize the accelerating structure with desired beam parameters.

Hellweg code was developed in the late 2000s at RF Technology Laboratory of Moscow Engineering-Physics Institute directed by Prof. Nikolay Sobenin, and its capabilities were limited to the local needs of the laboratory for the development of industrial TW accelerators with energy modulation based on disk-loaded waveguide accelerating structures (DLS) [17,18]. For those applications, it was sufficient to consider two-dimensional beam dynamics model with the simplified ellipsoid-based space charge model developed by Lapostolle [19–21] and the fundamental accelerating mode in stationary regime.

Modern high-power accelerator applications, however, implement the non-axially-symmetric field profiles such as multipole magnetic fields or accelerating structures with a cyclic variation of azimuthal asymmetries [22,23], which requires the enhancement of the current reduced 2D equations of motion to 3D equations in general form. The space charge model must also be able to deal with 3D particle distributions and the particles outside the core of the bunch, which is important downstream of the linac, where the tails of the beam can be formed. To deal with this problem, we have improved the Lapostolle space charge model to the general 3D ellipsoid form for any dimensions' ratio, consideration of the space charge field for the particles outside the beam core, and the fields from the neighboring bunches that can exist in the real machine. In the following sections, we will describe the physics of each mentioned enhancement in details. First, we will describe the mathematical model and then follow up with the implementation of the code and benchmark with the test problems and actual industrial linac design.

2. Three-dimensional equations of motion

For the stationary regime, which settles when the accelerating waveguide is filled with RF power, the beam can be represented as a group of macro- or super-particles [24,25]. By solving the equations of motion for these macro-particles in EM fields, it is possible to obtain the phase and energy characteristics of the beam in general.

Now we will define the dimensionless variables to simplify the equations of the RF fields. From now on, we will proceed the derivations in cylindrical coordinates since cylindrical accelerating structures are the natural choice for the most accelerators.

$$\zeta = \frac{z}{\lambda} \tag{1a}$$

$$\eta = \frac{r}{\lambda} \tag{1b}$$

$$\alpha = \frac{r}{\lambda}\dot{\theta} = \eta\dot{\theta} \tag{1c}$$

$$\tau = \frac{ct}{\lambda} \tag{1d}$$

Here, λ is the wavelength of the accelerating RF field, and dot represents the differentiation with respect to dimensionless time τ. Now, the dimensionless velocity β can be defined as:

$$\vec{\beta} = \frac{\vec{v}}{c} = \frac{1}{c}\left(\frac{dr}{dt}, \frac{rd\theta}{dt}, \frac{dz}{dt}\right) = \left(\frac{d\eta}{d\tau}, \frac{\eta d\theta}{d\tau}, \frac{d\zeta}{d\tau}\right) = (\dot{\eta}, \eta\dot{\theta}, \dot{\zeta}) \tag{2a}$$

Using unit vectors $\overrightarrow{e_\eta}, \overrightarrow{e_\theta}$ and $\overrightarrow{e_\zeta}$, the expression for the vector $\vec{\beta}$ will have the following form:

$$\vec{\beta} = \dot{\eta}\overrightarrow{e_\eta} + \eta\dot{\theta}\overrightarrow{e_\theta} + \dot{\zeta}\overrightarrow{e_\zeta} \tag{2b}$$

Then the expression for the velocity change can be written as:

$$\dot{\vec{\beta}} = \ddot{\eta}\overrightarrow{e_\eta} + \dot{\eta}\dot{\overrightarrow{e_\eta}} + \left(\eta\ddot{\theta} + \dot{\eta}\dot{\theta}\right)\overrightarrow{e_\theta} + \eta\dot{\theta}\dot{\overrightarrow{e_\theta}} + \ddot{\zeta}\overrightarrow{e_\zeta} + \dot{\zeta}\dot{\overrightarrow{e_\zeta}} \tag{2c}$$

In cylindrical coordinates the unit vector derivatives are related as:

$$\dot{\overrightarrow{e_\eta}} = \dot{\theta}\overrightarrow{e_\theta} \tag{3a}$$

$$\dot{\overrightarrow{e_\theta}} = -\dot{\theta}\overrightarrow{e_\eta} \tag{3b}$$

$$\dot{\overrightarrow{e_\zeta}} = 0 \tag{3c}$$

Applying these simple relations to Eq. (2a), it is easy to get the expression for $\dot{\vec{\beta}}$:

$$\begin{aligned}\dot{\vec{\beta}} &= \ddot{\eta}\overrightarrow{e_\eta} + \dot{\eta}\dot{\theta}\overrightarrow{e_\theta} + \left(\eta\ddot{\theta} + \dot{\eta}\dot{\theta}\right)\overrightarrow{e_\theta} - \eta\dot{\theta}^2\overrightarrow{e_\eta} + \ddot{\zeta}\overrightarrow{e_\zeta} \\ &= \left(\ddot{\eta} - \eta\dot{\theta}^2\right)\overrightarrow{e_\eta} + \left(\eta\ddot{\theta} + 2\dot{\eta}\dot{\theta}\right)\overrightarrow{e_\theta} + \ddot{\zeta}\overrightarrow{e_\zeta}\end{aligned} \tag{2d}$$

At the same time, the general equation for the motion of relativistic charged particle in external electrical and magnetic fields can be written as:

$$\frac{d\vec{v}}{dt} = \frac{e}{m_0}\sqrt{1 - \frac{v^2}{c^2}}\left(\vec{E} + \frac{\vec{v} \times (\vec{B} + \overrightarrow{B_{ext}})}{c} - \frac{\vec{v}(\vec{v}\cdot\vec{E})}{c^2}\right) \tag{4}$$

Here $\vec{E}$, and $\vec{B}$ are the fields of the RF cavity and $\overrightarrow{B_{ext}}$ is the external magnetic field. Before equalizing the Eqs. (2b) to (4), we need to introduce the dimensionless parameters for electric and magnetic field components normalized to the electron rest energy W_0:

$$A = \frac{E\lambda}{W_o} \tag{5a}$$

$$H = c\frac{B\lambda}{W_o} \tag{5b}$$

Now,

$$\begin{aligned}\frac{d\vec{\beta}}{d\tau} &= \left(\ddot{\eta} - \eta\dot{\theta}^2\right)\overrightarrow{e_\eta} + \left(\left(\eta\dot{\theta}\right) + \dot{\eta}\dot{\theta}\right)\overrightarrow{e_\theta} + \ddot{\zeta}\overrightarrow{e_\zeta} \\ &= \frac{1}{\gamma}\left(\vec{A} + \vec{\beta}\times\left(\vec{H} + \overrightarrow{H_{ext}}\right) - \vec{\beta}\left(\vec{\beta}\cdot\vec{A}\right)\right) \\ &= \frac{1}{\gamma}\left(A_\eta\overrightarrow{e_\eta} + A_\theta\overrightarrow{e_\theta} + A_\zeta\overrightarrow{e_\zeta} + \begin{vmatrix}\overrightarrow{e_\eta} & \overrightarrow{e_\theta} & \overrightarrow{e_\zeta} \\ \beta_\eta & \beta_\theta & \beta_\zeta \\ H_\eta + H_\eta^{ext} & H_\theta + H_\theta^{ext} & H_\zeta + H_\zeta^{ext}\end{vmatrix}\right. \\ &\qquad \left. - \left(\beta_\eta\overrightarrow{e_\eta} + \beta_\theta\overrightarrow{e_\theta} + \beta_\zeta\overrightarrow{e_\zeta}\right)\cdot\left(\beta_\eta A_\eta + \beta_\theta A_\theta + \beta_\zeta A_\zeta\right)\right)\end{aligned} \tag{6}$$

[1] At the moment of the paper publication, the typical price started from tens of thousands of US dollars per license, depending on the license type and contents.

[2] The simulation time depends greatly on the complexity of the problem and the available hardware. Our experience at the moment of publication was ~8 h of simulation time to achieve stationary regime in the industrial linac. Refer to Section 5 for the details.

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