FEL SIMULATION USING THE LIE METHOD*

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Abstract

Advances in numerical methods for free-electron-laser (FEL) simulation under wiggler period averaging (WPA) are presented. First, WPA is generalized using perturbation Lie map method. The conventional WPA is identified as the leading order contribution. Next, a widely used shot-noise modeling method is improved along with a particle migration scheme across the numerical mesh. The artificial shot noise arising from particle migration is suppressed. The improved model also allows using arbitrary mesh size, slippage resolution, and integration step size. These advances will improve modeling of longitudinal beam profile evolution for fast FEL simulation.

INTRODUCTION

FEL design optimization often involve multiple times of numerical simulations with different system parameters. Such a study requires highly efficient simulation code. The WPA is the one of the best options. Indeed, most of the start-to-end design codes choose to incorporate the WPA FEL simulation code [1–5]. In this proceeding, we review the advances in numerical methods within the WPA framework presented in our previous work [6].

First, we generalize the WPA using the perturbation Lie map method. The conventional WPA is identified as the leading order contribution. The next order corrections we include are coupling between betatron and wiggling motion, transverse field gradient, and longitudinal field envelope variation.

Second, we present an improved shot-noise model within WPA framework. Unless particle migration across the numerical mesh is artificially suppressed, as in many old WPA codes [7], there can be large artificial shot noise due to the nature of the shot-noise modeling method [8]. We solve this problem by re-interpreting and combining the two widely used shot-noise modeling methods of Refs. [8] and [9]. The improved model can further benefit smoothness of numerical mesh through arbitrary weight and shape functions. Here, the weight function refers to the integral kernel used for particle deposition on numerical mesh points. The shape function refers to the shape of the field representation at numerical mesh points used for field interpolation from mesh points to particles’ coordinates. This, in turn, allows arbitrary mesh size, integration step size and slippage resolution. Especially, the arbitrary slippage resolution comes with many other benefits. It can naturally simulate correct slippage through non-resonant transport line other than wiggler and allows applying the operator split-composition method [10] on field solver for better accuracy. Last but the least, the particle loading method can naturally accept the particle data from upstream simulation enabling start-to-end simulation seamless.

GENERALIZATION OF WIGGLER PERIOD AVERAGING

In general, when a Hamiltonian can be decomposed into integrable part and a small parametric potential, one can build a perturbation map in order of the small parameters. In an undulator, if a map is constructed over a undulator period, the lowest order of the wiggling motion average out leaving the small coupling effects between the fast wiggling and slow betatron motion.

Magnus Series

We split the Hamiltonian into \( H = S + F(z) + V(z) \) where \( S \) is the wiggler period averaged Hamiltonian representing slow motion, \( V \) is the radiation field potential, \( F \) is the rest representing the fast wiggling motion. Accordingly, we factor the Lie map as the following [11]:

\[
\begin{align*}
\mathcal{H}(\lambda_u) &= S(\lambda_u) F(\lambda_u) V(\lambda_u), \\
S(\lambda_u) &= e^{\mathcal{G}_S(\lambda_u)}, \\
F(\lambda_u) &= e^{\mathcal{G}_F(\lambda_u)}, \\
V(\lambda_u) &= e^{\mathcal{G}_V(\lambda_u)},
\end{align*}
\]

where \( \lambda_u \) is the wiggler period. The generators can be written in terms of the Magnus’s series

\[
\mathcal{G}_F(z) = -\int_0^z dz_1 : F_1^{\text{int}} + \frac{1}{2!} \int_0^z dz_1 \int_0^{z_1} dz_2 : [2, 1] : + \frac{1}{3!} \int_0^z dz_1 \int_0^{z_1} dz_2 \int_0^{z_2} dz_3 : [3, 2, 1] : + [3, 2, 1] : \\
\mathcal{G}_V(z) = -\int_0^z dz : V^{\text{int}}(z) :,
\]

where the pair of colons is Dragt’s notation [11] of the Poisson bracket, i.e., \( : A : B = [A, B] \), and the numbers in the Poisson bracket is an abbreviation of \( i \equiv F_i^{\text{int}} \) with \( F_i^{\text{int}} = S(z_i) F(z_i) \). Since the raidaiton field strength is much weaker than external field strength only the 1st sequence is taken for \( \mathcal{G}_V \) [6].

Hamiltonian

Starting from the following Hamiltonian,

\[
H(x, p, c, \gamma; z) = -\sqrt{\gamma^2 - 1 - (p_x - a_x)^2 - (p_y - a_y)^2},
\]

where \( c t \) is the time multiplied by the speed of light and it’s canonical momentum pair is negative of the normalized

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energy $\gamma$. The normalized vector potential of the planar wiggler is assumed to be
\[
a_x = K \cosh(k_x x) \cos(k_y y) \cos(k_u z) + a_r,
\]
\[
a_y = K \frac{k_x}{k_y} \sinh(k_x x) \sin(k_y y) \cos(k_u z),
\]
where $k_u$ is the wiggler wave number, $k_x$ and $k_y$ are the natural focusing strength of the wiggler, $K$ is the normalized wiggler strength. We use the following ansatz for the vector potential $a_r$
\[
a_r = \Re \sum_{h \geq 1} K_h(x,t; z) e^{ihk_r(z-ct)},
\]
where, $K_h$ is the $h$-th harmonic field envelope, and $k_r$ is the fundamental wave number. The generating function,
\[
G_2(ct, \eta) = \left[k_r (z - ct) + k_u z\right] \eta
\]
transforms the Hamiltonian into
\[
H = (k_u + k_r) \eta - \sqrt{k_r^2 \eta^2 - 1} - (p_x - a_x)^2 - (p_y - a_y)^2,
\]
whose new conjugate variables are
\[
\theta = k_r (z - ct) + k_u z, \quad \eta = \gamma / k_r.
\]
Then, the split parts of the Hamiltonian are
\[
S = \frac{k_u}{k_x} + \frac{1}{2} \gamma \left[1 + p_x^2 + p_y^2 + \frac{K_x^2}{2} \left(1 + k_x^2 x^2 + k_y^2 y^2\right)\right] + O\left(\frac{q_3^3}{\gamma}, \frac{1}{\gamma^3}\right),
\]
\[
F = \frac{k_x}{4 \gamma} \cos(2k_u z) + \frac{K_x}{\gamma} p_x \cos(k_u z)
\]
\[
+ O\left(\frac{q_3^3}{\gamma}, \frac{1}{\gamma^3}\right),
\]
\[
V = -\Re \sum_h \left[\frac{K_x h}{\gamma} \cos(k_u z) + \frac{p_x}{\gamma} K_h e^{i h (q - k_u z)}\right]
\]
\[
+ O\left(\frac{K_h q_2^2}{\gamma}, \frac{K_h}{\gamma}, \frac{K_h^2}{\gamma^3}\right),
\]
where $q_3 \in \{k_x, p_x, k_y, p_y\}$ and
\[
K_x = K \left(1 + k_x^2 x^2 + k_y^2 y^2\right)
\]
is the effective wiggler strength.

### Lie Map Generators

The generator of the slow map is trivial:
\[
G_S(\lambda_u) = -\lambda_u : S:\n\]
Evaluating Eq. (3), the the fast map generator becomes
\[
G_F(\lambda_u) = -\lambda_u K^2 k_x^2 16k_y^2 \gamma^3.
\]
This corresponds to the coupling between slow betatron oscillation and fast wiggling oscillation. It is negligible in most cases as it scales as $\gamma^{-2}$ compared to the wiggling motion in Eq. (10). The smallness is due to the large frequency ratio between the betatron and wiggling oscillation. When strong quadrupole is present on top of the wiggler field, such coupling can be more relevant.

Before we evaluate Eq. (4), let us write the propagated field potential $V_{\text{int}} = SFV$ by
\[
V_{\text{int}} = -\left[\frac{K X}{\gamma} \cos(k_u z) + \frac{p_x}{\gamma} K_h e^{i h (q - k_u z)}\right],
\]
where the real value operator and the summation over $h$ is assumed for simplicity, and $K_{\text{int}} \equiv SF K_h$ and $\theta_{\text{int}} \equiv SF \theta$ are the propagated field envelope and FEL phase respectively. We neglected the propagation on terms in the square bracket of Eq. (15) assuming propagation on FEL phase and field envelope is more relevant.

In order to evaluate the integration in Eq. (4), we need to model the field envelope variation over the integration range. As the WPA presumes small field envelope variation over a wiggler period, we model as the following:
\[
K_h(z) = \Re_h + \frac{K x}{k_x \gamma} \sin(k_u z) \frac{\partial}{\partial x} \Re_h + z \partial_z \Re_h,
\]
where $\Re_h = \frac{1}{2} \int_0^z K_h \, dz$ is an averaged field envelope, $\partial_x \Re_h$ represent the first order longitudinal variation and the transverse gradient term is from the propagation by $F(z)$. On the other hand, the propagated FEL phase is
\[
\theta_{\text{int}} = \theta + \dot{\theta} z - \xi \sin(2k_u z) - \zeta \sin(k_u z),
\]
where
\[
\dot{\theta} = k_u - \frac{k_r}{2 \gamma^2} \left[1 + p_x^2 + p_y^2 + \frac{K_x^2}{2}\right],
\]
\[
\xi = \frac{k_r K^2}{8k_u \gamma^2},
\]
\[
\zeta = \frac{k_r K}{k_u \gamma^2} p_x.
\]
Note that $\dot{\theta} = 0$ exactly on resonance. The inclusion of it encompasses small off-resonant effects. Finally, the generator of the field potential map can be written by
\[
G_V = \lambda_u \Re \sum_h \frac{e^{ih \theta}}{\gamma}
\]
\[
\times \left[K_{\text{eff}} \int_0^h p_x \int_0^h + K \int_0^h \partial_z + \frac{K_{\text{eff}}^2}{k_u \gamma} \int_0^h \partial_x \Re_h\right],
\]
where the integration parameters are [6]:

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Here, the integration parameters are calculated to the first order of \( \dot{\theta}, \xi, \Delta_\xi \equiv \xi - \xi_{\text{R}} \) with \( \xi_{\text{R}} \equiv \frac{hK^2}{h\omega_q} \) and \( \gamma_R \) being the resonant energy. The first kind Bessel function of order \( i \) and argument \( h_\xi \) is abbreviated as \( J_i h_\xi \) and only integer \( i \) is allowed. Note that the integration parameter \( \int_{SC} \) coupled with the transverse gradient in Eq. (19) vanishes for odd harmonics but can be as large as the leading order terms for even harmonics.

**Effective Hamiltonian**

The factorized map Eq. (2) is not yet practically useful for numerical implementation since each factorized map is not solvable and the step size is fixed by one wiggler period. A trick is to concatenate the map using Baker-Campbel-Hausdorff (BCH) formula and define an effective Hamiltonian [11].

\[
H_{\text{eff}} = -\frac{1}{\lambda_u} (G_S + G_F + G_V) \quad (24)
\]

\[
-\frac{1}{2\lambda_u} (G_S \cdot G_F^* + G_F \cdot G_S^* + G_F \cdot G_V^* + G_V \cdot G_S^* + G_F^* \cdot G_V^* + G_V \cdot G_F^* + \cdots)
\]

Note that the effective Hamiltonian does not have explicit dependency on \( z \). Therefore, we can apply numerical methods like Runge-Kutta (RK) with arbitrary step size to solve the effective Hamiltonian. For example, a popular FEL simulation code GENESIS uses the 4th order RK method [7]. Figure 1 shows an order of magnitude improvement in accuracy of particle pusher compared to the conventional WPA. We used the GENESIS pusher to represent typical WPA. Since, we used converging small enough step sizes, the error from the exact solution originates from the differences of the effective equations of motion in use. However, such an accuracy improvement on particle pusher can easily become obscured by other sources of errors such as paraxial approximations of field solver, and numerical discretization.

**NUMERICAL SHOT NOISE MODELING**

**Review of 1D Model**

Here, we review two widely used 1D shot noise modeling methods in Ref. [8] and [9]. Figure 2 illustrates these two methods schematically. In both methods, the first step is to populate particles uniformly along the temporal coordinate with equal charge weight to remove artificial temporal shot-
where the number of particles is assumed to be twice of the maximum harmonic number to be modeled and $\xi_h$ is a random variable. Then, the bunching factor becomes

$$b_h = \frac{1}{N_e} \sum_{j=1}^{M} m_j e^{i h \theta_j} = 0.$$  \hspace{1cm} (25)

Here, index 0 denotes vanishing bunching factor, $N_e$ is the number of electrons, $M$ is the number of the simulated particles and $m_j = N_e/M$ is the electron number weight of the $j$-th particle. It vanishes as all the weights are equal, and the temporal coordinates $\theta_j = \theta_0 + j \Delta \theta$ are uniformly distributed with a equal distance $\Delta \theta = 2 \pi / M$.

The second step is to add proper perturbation on the temporal coordinates or charge weights so that, at least, the root-mean-square (RMS) bunching factor is that of physical shot-noise $\langle b_h^2 \rangle = 1/N_e$.

The perturbation on temporal coordinate of $j$-th particle is given by [8]

$$\delta \theta_j = \sum_{j'=1}^{M/2} \xi_{j'} e^{-i \theta_j'}, \hspace{1cm} (26)$$

where the number of particles is assumed to be twice of the maximum harmonic number to be modeled and $\xi_h$ is a random variable. Then, the bunching factor becomes

$$b_h = \frac{1}{N_e} \sum_{j=1}^{M} m_j e^{i h (\theta_j + \delta \theta_j)} = i h \xi_h.$$  \hspace{1cm} (27)

Therefore, we require $\langle \xi_h \xi_h' \rangle = 1/(h^2 N_e)$ so that

$$\langle b_h b_h' \rangle \approx h^2 \langle \xi_h \xi_h' \rangle \equiv \frac{1}{N_e}.$$  \hspace{1cm} (28)

On the other hand, when the charge weight perturbation [9] is applied, the RMS bunching factor becomes

$$\langle b_h b_h' \rangle = \frac{1}{N_e} \sum_{j=1}^{M} \sum_{k=1}^{M} \langle \tilde{m}_j \tilde{m}_k \rangle e^{i h (\theta_j - \theta_k)}$$

$$= \frac{1}{N_e} \sum_{j=1}^{M} \left( \langle \tilde{m}_j^2 \rangle - \langle \tilde{m}_j \rangle^2 \right) = \frac{1}{N_e} \hspace{1cm} (29)$$

where $\tilde{m}_j \equiv m_j + \delta m_j$ is the perturbed number weight with

$$\langle \tilde{m}_j \rangle = \langle \tilde{m}_j^2 \rangle - \langle \tilde{m}_j \rangle^2 = \frac{N_e}{M}.$$

Note that this is a property of the Poisson distribution [9].

**Review of 6D Extension**

One way to extend the 1D shot-noise method is the 6D volume division method. This is a natural extension of the 1D charge perturbation based on Poisson principle. Density function is represented by particles sitting at the center of each 6D volume division. As each volume does not overlap, all the particles are statistically independent. However, it requires a lot of particles as division over 6 dimension can be huge.

Another way is to mirror same 5D coordinates $x, y, p_x, p_y, \gamma$ among a set of particles called ‘beamlet’ [8] which models 1D shot-noise. Note that the member particles of a beamlet are not statistically independent as they share the same 5D phase-space coordinates. However, there can be large numerical shot-noise upon particles migration across the numerical mesh. This is because, the migration break the cancellation of bunching factor in Eq. (25).

Figure 3 illustrates these two 6D extension methods schematically.

**Particle Loading and Migration**

As the 6D volume division requires a lot of particles, we adopt the 5D mirroring strategy. Our idea is to interpret one beamlet as one statistically independent entity whose phase-space coordinate is given by the average over the member particles in it. This is based on the observation that the member particles are not statistically independent and the motion of the beamlets describe the macroscopic ($\gg \lambda_e$) dynamics while the motion of the individual member particles of the beamlet describe microscopic ($\lesssim \lambda_e$) dynamics.

This interpretation allows us to load particles naturally. First, the beamlet is loaded from a random generator or from external upstream tracking code. Then, each beamlet is divided into $M = 2 \lambda_{max}$ particles whose temporal coordinates and charge follows the 1D shot-noise model while the average coordinate is that of the beamlet. Here $\lambda_{max}$ is the maximum harmonic number to be modeled. This procedure is described in Fig. 4.

Since the beamlet is an independent entity, we migrate all the particles composing a beamlet when the beamlet migrate across the numerical mesh. This method grants us much smoother numerical discretization as the weight and shape functions are evaluated at the beamlet position regardless...
SLIPPAGE RESOLUTION

The beamlet migration enables us to use arbitrary slippage resolution through moving window. The typical implementation of slippage is to copy the field data from the previous temporal mesh point to the next temporal mesh point. This procedure as well as the moving window can be best understood by a pseudo code in Fig. 7. Note that the slippage resolution of the moving window is arbitrary while the slippage resolution of the copying data is one temporal mesh size. Furthermore, moving window with beamlet migration can naturally and correctly model the slippage through arbitrary length of non-resonant transport like drift. Figure 8 shows kinks on power gain curve due to rough slippage resolution for the copying data. The power difference is especially notable in the drift-quadrupole line.

SPLIT AND COMPOSITION METHOD IN FIELD SOLVER

The field solver can be split into two operation - diffusion and slippage. Let $F_{\perp}$ and $F_{\parallel}$ represent the diffusion and slippage operator respectively. Then, the following composition method of step size $\Delta z$

$$F_{\parallel} \left( \frac{\Delta z}{2} \right) F_{\perp} \left( \Delta z \right) F_{\parallel} \left( \frac{\Delta z}{2} \right)$$

is a second order method provided that $F_{\perp}$ and $F_{\parallel}$ are one-step method of order higher than two [10]. The arbitrary slippage resolution though moving window allow us to split $F_{\parallel}$ and build the 2nd order composition method. Figure 9 shows comparison of the power gain curve error using the 1st order the 2nd order method.

CONCLUSION

Several advances in numerical methods for FEL simulation under the WPA are presented. We generalized the WPA using the perturbation Lie map method. The perturbative correctional terms to WPA includes coupling between fast
wiggling and slow betatron motion, transverse field gradient, and longitudinal field variation. In addition, we improved the shot-noise modeling method. This allows us to combine advantages of two widely used shot-noise modeling methods in Refs. [8] and [9]. Such an improvement also leads us to develop a particle migration scheme suppressing artificial shot-noise upon migration. This enables much smoother numerical discretization and the temporal beam profile evolution modeling. All these methods are implemented in the parallel beam dynamics simulation framework IMPACT code suite [13].

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REFERENCE