PRELIMINARY STUDY OF QUIET START METHOD IN HGHG FEL SIMULATION*

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Abstract

Quiet start scheme is broadly utilized in Self Amplified Spontaneous Radiation (SASE) FEL simulations, which is proven to be correct and efficient. Nevertheless, due to the energy modulation and the dispersion section, the High Gain Harmonic Generation (HGHG) FEL simulation will not be improved by the traditional quiet start method. A new approach is presented to largely decrease the number of macro-particles per slice that can be implemented in both time-independent and time-dependent simulation, accordingly expedites the high order harmonic cascade simulation or other small modulation HGHG cases.

INTRODUCTION

Great interest has been focused in single pass free electron laser (FEL) for many years for the capability of generating coherent radiation with high intensity and short pulse duration in short wavelength from deep ultraviolet (~100 nm) to hard x-ray (~0.1nm). The scheme, self amplified spontaneous radiation (SASE), has been carefully study in both theory and experiment. The simulation of SASE FEL process is achieved by using the quiet start method[1,2], which reduces the macro particle number and simulation time dramatically. However, SASE FEL is seeded by the shot noise of electron bunch, hence produce limited temporal coherence and large shot-to-shot intensity fluctuation.

An alternate approach for SASE FEL is the high gain harmonic generation (HGHG) FEL. As the first HGHG FEL experiment is accomplished successfully and overcome the limitation of SASE FEL [3], increasing projects were proposed to produce fully coherent VUV and soft X-ray radiations sources using cascade HGHG scheme. The Quiet Start scheme, which reduces the number of macro particles largely in SASE simulation, uses only small number of distinguished phase ψ (usually 4). Each phase is filled with identical macro particle distribution of other 5 dimensions (γ, x, y, px, py), which is generated by pseudo random number generator or Hammersley quasi-random sequence. However, the quiet start scheme does not lead to correct bunching factor in terms of HGHG process.

A quiet start method scheme for HGHG is introduced in [4]. In the article, we consider a more dedicate method to realize ‘Quiet Start’ initial particle loading in small modulation case when the modulator and dispersion sessions exist, in order to achieve correct bunching factor at the entrance of radiator. When energy modulation is small because of a weak seed laser, the beam energy spread is large or dispersion effect is large so that the beam is over bunched, the signal (bunching factor) generated by modulator and dispersion section will be small. Such small bunching factor will be overwhelmed by the noise of initial loading method such as Hammersley sequence, if the number of macro particles is not large enough. The quiet start loading method is to find a way to generate less noise with same number of macro particles compared with normal loading methods. To introduce our method on the small modulation HGHG FEL simulation, first we will derive the bunching factor errors produce by this quiet start scheme in 1-D case theoretically. Then 3-D scheme is carried out with utilizing Hammersley sequence on transverse dimensions to reduce noise. One example of small modulation HGHG scheme is demonstrated to show the effectiveness of the method in the last section.

ONE DIMENSION ANALYSIS

In the HGHG FEL scheme, the bunching factor after energy modulation and dispersion section can be calculated theoretically using a simplified one dimension model. Assuming that the phase space distribution is described by distribution written in variable \( γ = E/mc^2 - γ_c \), \( θ = (k_0 + k_w)z - ω_0 t \), where \( E \) is the energy of electron, \( mc^2 \) is electron mass, \( γ_c \) corresponds to the resonance energy, \( k_0 \) and \( ω_0 \) is the resonance wave number and resonance angular frequency, \( k_w \) is the undulator wave number.

The initial distribution function can be written as Eq. (1), with energy spread \( σ_γ \),

\[
f(\gamma_0, \theta_0) = \frac{1}{\sqrt{2\pi}σ_γ} \exp \left( -\frac{\gamma_0^2}{2σ_γ^2} \right) \tag{1}
\]

After the modulator, the electron bunch energy is modulated to \( (γ', \theta') \)

\[
γ' = γ_0 + Δγ \sin(θ_0) \\
θ' = θ_0
\tag{2}
\]

The energy modulation strength \( Δγ \) can be calculated from the modulator strength and seed laser power. The dispersion section gives rotation on the longitudinal phase space and change the energy modulation to density modulation. The new coordinate \((γ'', θ'')\) is given by

\[
γ'' = γ' = γ_0 + Δγ \sin(θ_0) \\
θ'' = \frac{dθ}{dγ} (γ_0 + Δγ \sin(θ_0)) + θ_0 \tag{3}
\]
Before the bunch enters the radiator, the distribution function is shown in Eq. (4). Here we change the notation \((y'', \theta'')\) to \((y + y_0, \theta)\) for simplicity.

\[
f(y, \theta) = \frac{1}{\sqrt{2\pi}\sigma_y} \exp \left( -\frac{(y - \Delta y \sin(\theta - \frac{d\theta}{dy} y))^2}{2\sigma_y^2} \right)
\]

(4)

The bunching factor after modulator and dispersion section can be calculated as

\[
b_m = J_m \left( m \frac{d\theta}{dy} \Delta y \right) \exp \left( -\left(m \frac{d\theta}{dy} \sigma_y\right)^2 / 2 \right)
\]

(5)

In HGHG simulation, the traditional quiet start method does not produce the desired bunching factor as derived in equation (5) using finite number macro-particles. To obtain the correct bunching factor after energy modulation and dispersion section, we must carefully consider two dimensional initial longitudinal phase space variables \((y_0, \theta_0)\) to choose the macro-particles used in the simulation. Assuming the initially configuration is evenly distributed in phase variable \(\theta\), and has Gaussian distribution with energy spread \(\sigma_y\) in \(y\). We choose the phase to be some equal-space discrete value \(\theta_0 j = 2\pi \times j / N_j\), where \(N_j\) is the total number of discrete value \(\theta_0 j\). In each \(\theta_0 j\), same configuration of energy \(y_0 k\), totally \(N_k\) energy values, is assigned. Using this configuration, we need \(N_j \times N_k\) macro-particles for 1-D analysis.

![Figure 1. Bunching factor error as function of \(N_j\)](image)

Now we can find the bunching factor of these \(N_j \times N_k\) particles before entering the radiator, using the Eq (3). Here we use \(\theta_l\) as the final phase of \(l^{th}\) particle after energy modulation and dispersion section, where \(l\) varies from 1 to \(N_j \times N_k\). Parameter \(\alpha = d\theta / dy \times \Delta y\) is introduced for simplicity.

\[
b_m = \langle e^{im\theta_l} \rangle = \frac{1}{N_j N_k} \sum_{j=1}^{N_j} \sum_{k=1}^{N_k} e^{im\theta_{0j}} \exp \left( -\left(m \frac{d\theta}{dy} \sigma_y\right)^2 / 2 \right)
\]

(6)

Now the two sums are decoupled and can be evaluated separately. The first sum only depends on \(N_j\); while the second relies on each \(y_0k\).

The first sum in Eq. (6) can be calculated easily using Jacobi-Anger expansion

\[
e^{ix \sin(\theta)} = \sum_{p=-\infty}^{\infty} J_p(x) e^{ip\theta}
\]

where \(J_p(x)\) is Bessel function of the first kind.
\[
\frac{1}{N_j} \sum_{j=1}^{N_j} e^{im\theta_{oj} + im\alpha sin \theta_{0j}} = \frac{1}{N_k} \sum_{j=1}^{N_k} J_p(m\alpha) e^{i(p+m)2\pi j/N_j}
\]

(7)

After simple steps, the bunching factor gives

\[
b_m = \sum_{t=-\infty}^{+\infty} J_{tN_j-m}(ma) \times \sum_{k=1}^{N_k} e^{im\theta t/\gamma k} \tag{8}
\]

Equation (8) shows the criteria of choosing \(N_j\). Quantitatively, we can define the bunching factor error \(E(m,\alpha)\) by comparing Eq. (8) and (5).

\[
E_1(m, \alpha) = \frac{\left| \sum_{t=-\infty}^{+\infty} J_{tN_j-m}(ma) - J_m(m\alpha) \right|}{J_m(m\alpha)} \tag{9}
\]

Figure 1 is the bunching error of the first sum with respect to \(N_j\), at different harmonic number \(m\) and parameter \(\alpha\). It shows that, as \(N_j\) increases, the error decrease dramatically. For large harmonic number \(m\), more discrete phase values are needed to maintain the same error value. Also, larger \(N_j\) is chosen as parameter \(\alpha\) increases. If the dispersion strength is optimized to yield maximum bunching factor, the parameter \(\alpha\) makes \(J_m(m\alpha)\) reach the maximum at around \(\alpha = 1\). For example, if harmonic number is 3, other parameters are optimize to achieve maximum bunching factor, \(N_{j}\) is selected to be no less than 16 to keep the error less than 1%. This also explains why quiet start for SASE FEL process (usually \(N_{j} = 4\)) does not yield correct result.

The accuracy of second sum in Eq. (8) depends on the distribution of \(N_k\) energy values deviated from ideal Gaussian distribution. Just follow the method which we treat the first sum, we use sequence \(a_k = (k - 1/2)/N, (k = 1 \cdots N_k)\) to represent uniform distribution in [0,1]. A transformation as (15) forms uniform Gaussian distribution.

\[
b_k = \sqrt{2\pi} erf^{-1}(-1 + 2a_k) \tag{10}
\]

One option is to simply choose \(N_k\) energy values as \(\gamma_k = \sigma_f b_k\). When \(N_k\) is approaching to infinity, the second sum will approaching right value expressed in second factor of equation (5). When \(N_k\) is not large enough, the error of second error is cannot be neglected. But in reality, we need to decrease \(N_k\) as small as possible to save computation time; meanwhile, the \(N_k\) energy values must produce the second sum with acceptable error.

In order to achieve the requirement listed above, we choose the \(N_k\) energy value as shown in (15).

\[
\gamma_k = \sigma_f b_k + c_k \tag{11}
\]

\(c_k\) is the small deviation from the number calculated in (10). The requirement can be listed in (15). All sums in (15) are added from 1 to \(N_k\).

\[
\sum_{k=1}^{N_k} c_k = 0 \quad \frac{1}{N_k} \sum_{k=1}^{N_k} \gamma_k^2 = \sigma_k \quad \frac{1}{N_k} \sum_{k=1}^{N_k} e^{im\theta t/\gamma k} = \exp\left(-\frac{(m \frac{d\theta}{dy})^2}{2}\right)
\]

With the restriction above, we can minimize the rms value of \(c_k\). By minimize the rms value, we expect all \(c_k\) values become zero when \(N_k\) approaches infinity.

Here we follow the procedure of Lagrangian multiplier to seek the minimum of \(\sum c_k^2\) with conditions in (15). First we define a new function in (15) after introducing new parameter \(\lambda_1, \lambda_2\) and \(\lambda_3\), where \(s_2\) is the right-hand side constant of last equation in (12).

\[
f(c_1, \cdots, c_{N_k}, \lambda_1, \lambda_2, \lambda_3) = \sum_{k=1}^{N_k} c_k^2 - \lambda_1 \sum_{k=1}^{N_k} c_k
\]

\[
- \lambda_2 \left( \sum_{k=1}^{N_k} \gamma_k^2 - \sigma_k \right) - \lambda_3 \left( \sum_{k=1}^{N_k} e^{im\theta t/\gamma k} - s_2 \right)
\]

Then we can write down \(N_k\) equations from the newly defined function as in (15). Combined with 3 equations in (12), we can solve these \(N_k + 3\) equations with \(N_k + 3\) variables \(c_1, \cdots, c_{N_k}, \lambda_1, \lambda_2, \lambda_3\). By accomplishing all the procedures we can get a deviated Gaussian distribution with correct bunching factor in the simplified 1D analytical model.

\[
\frac{\partial f(c_1, \cdots, c_{N_k}, \lambda_1, \lambda_2, \lambda_3)}{c_k} = 0, \quad (k = 1 \cdots N_k) \tag{14}
\]

**LIMITATION OF THE MODEL**

There are limitations of this simplified model. The first one comes from the fact that we ignore the dispersion in the modulator. When the modulator is long, the dispersion effect can’t be ignored, and equation (2) should be replaced by a set of coupled equations. Approximately, the dispersion of the modulator can be represented as (15), where \(N_k\) is the number of modulator period. We can include it in to the chicane dispersion and perform the Lagrangian multiplier procedure.

\[
\frac{d\theta}{dy}_{\text{modulator}} \equiv \frac{2\pi N_k}{\gamma_0} \tag{15}
\]

The second limitation is the Lagrangian multiplier process only generates sequence that leads to correct bunching factor at one specific position (the entrance of radiator). Along the undulator the dispersions at each
point are different; there will be errors when other points are calculated.

3-D SIMULATION

In one dimension model, we already had the \( N_j \times N_k \) multi-particles. To extend it to 3D case, we need to generate \( N_j \times N_k \times N_t \) sets for each one in \( N_j \times N_k \) multi-particles. Totally the number of particle in 3-D simulation is \( N_j \times N_k \times N_t \). For the transverse distributions we can use Hammersley pseudo random sequence to reduce fluctuation in transverse phase space distribution.

Here, as an example, we simulate the 2nd order HGHG scheme in soft X-ray regime. Main parameter used in simulation is shown in Table 1. In this example, the energy spread is larger than the energy modulation amplitude; the beam is slight over bunched after dispersion section. This leads the bunch factor at radiator entrance to be small (around 0.012).

![Figure 2. Comparison of Gain Length in Radiator](image1)

![Figure 3. Comparison of bunching factor before radiator](image2)

**CONCLUSION**

The quiet start scheme for HGHG FEL simulation is promising and easy scheme to save more macro particle. We generate the initial distribution of macro particles and import to an existing FEL simulation code. The total number of particle can be largely reduced by achieving precise bunching factor in radiator in small modulation case. But because we use some approximations in the analysis, there is systematic error in the result, which needs more study to correct.

**REFERENCES**