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 limit 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, p_x, p_y), 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 $\gamma = E/mc^2 - \gamma_c$, $\theta = (k_0 + k_w)z - \omega_0 t$, 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,

$$f(\gamma_0, \theta_0) = \frac{1}{\sqrt{2\pi}\sigma_\gamma} \exp\left(-\frac{\gamma_0^2}{2\sigma_\gamma^2}\right) \tag{1}$$

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

$$\begin{aligned} \gamma' &= \gamma_0 + \Delta\gamma \sin(\theta_0) \\ \theta' &= \theta_0 \end{aligned} \tag{2}$$

The energy modulation strength $\Delta\gamma$ 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

$$\begin{aligned} \gamma'' &= \gamma' = \gamma_0 + \Delta\gamma \sin(\theta_0) \\ \theta'' &= \frac{d\theta}{d\gamma}(\gamma_0 + \Delta\gamma \sin(\theta_0)) + \theta_0 \end{aligned} \tag{3}$$

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Before the bunch enters the radiator, the distribution function is shown in Eq.(4). Here we change the notation (γ'', θ'') to $(\gamma+\gamma_0, \theta)$ for simplicity.

$$f(\gamma,\theta) = \frac{1}{\sqrt{2\pi}\sigma_\gamma}\exp\left(-\frac{\left(\gamma-\Delta\gamma\sin\left(\theta-\frac{d\theta}{d\gamma}\gamma\right)\right)^2}{2\sigma_\gamma^2}\right) \qquad (4)$$

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

$$b_m = J_m\left(m\frac{d\theta}{d\gamma}\Delta\gamma\right)\exp\left(-(m\frac{d\theta}{d\gamma}\sigma_\gamma)^2/2\right) \qquad (5)$$

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 (γ_0, θ_0) to choose the macro-particles used in the simulation. Assuming the initially configuration is evenly distributed in phase variable θ, and has Gaussian distribution with energy spread σ_γ in γ. We choose the phase to be some equal-space discrete value $\theta_{0j} = 2\pi \times j/N_j$, where N_j is the total number of discrete value θ_{0j}. In each θ_{0j}, same configuration of energy γ_{0k}, totally N_k energy values, is assigned. Using this configuration, we need $N_j \times N_k$ macro-particles for 1-D analysis.

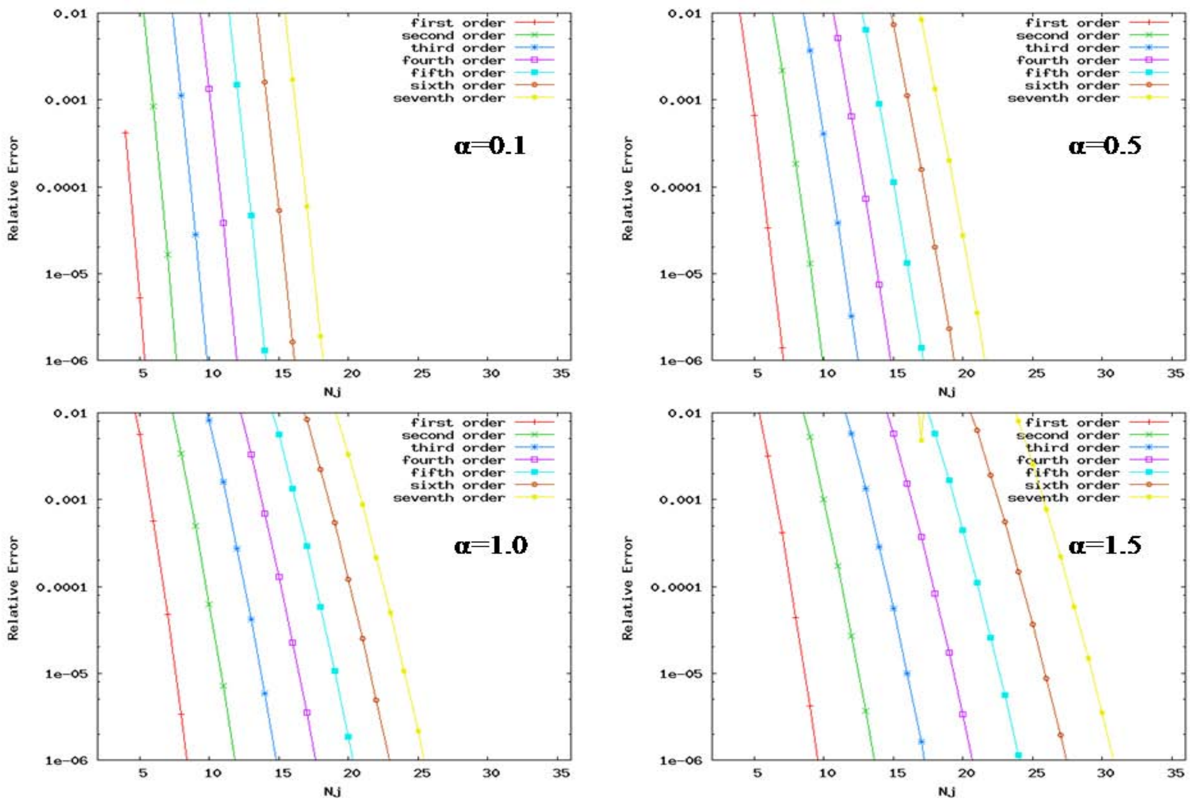

Figure 1. Bunching factor error as function of $\boldsymbol{N_j}$

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 θ_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 $\alpha = d\theta/d\gamma \times \Delta\gamma$ is introduced for simplicity.

$$b_m = \langle e^{im\theta_l}\rangle = \sum_{l=1}^{N_j\times N_k} e^{im\theta_l} \qquad (6)$$

$$= \frac{1}{N_j N_k}\sum_{j=1}^{N_j}\sum_{k=1}^{N_k} e^{im(\frac{d\theta}{d\gamma}(\gamma_{0k}+\Delta\gamma\sin(\theta_{0j}))+\theta_{0j})}$$

$$= \frac{1}{N_j N_k}\sum_{j=1}^{N_j} e^{im\theta_{oj}+im\alpha\sin(\theta_{0j})}\sum_{k=1}^{N_k} e^{im\frac{d\theta}{d\gamma}\gamma_{0k}}$$

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 γ_{ok}.

The first sum in Eq. (6) can be calculated easily using Jacobi-Anger expansion $e^{iz\sin(\theta)} = \sum_{p=-\infty}^{+\infty} J_p(z)e^{ip\theta}$, where $J_p(z)$ is Bessel function of the first kind.

$$\frac{1}{N_j}\sum_{j=1}^{N_j} e^{im\theta_{oj}+im\alpha sin\,(\theta_{0j})} = \frac{1}{N_k}\sum_{j=1}^{N_j}\sum_{p=-\infty}^{+\infty} J_p(m\alpha)\, e^{\frac{i(p+m)2\pi j}{N_j}} \tag{7}$$

After simple steps, the bunching factor gives

$$b_m = \sum_{t=-\infty}^{+\infty} J_{tN_j-m}(m\alpha) \times \sum_{k=1}^{N_k} e^{im\frac{d\theta}{d\gamma}\gamma_{0k}} \tag{8}$$

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

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

Figure 1 is the bunching error of the first sum with respect to N_j, at different harmonic number m and parameter α. 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 α increases. If the dispersion strength is optimized to yield maximum bunching factor, the parameter α makes $J_m(ma)$ reach the maximum at around $\alpha\sim 1$. 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.

$$b_k = \sqrt{2}Erf^{-1}(-1+2a_k) \tag{10}$$

One option is to simply choose N_k energy values as $\gamma_k = \sigma_\gamma b_k$. 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).

$$\gamma_k = \sigma_\gamma b_k + c_k \tag{11}$$

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.

$$\begin{gathered}\sum c_k = 0\\ \frac{1}{N_k}\sum \gamma_k^2 = \sigma_k\\ \frac{1}{N_k}\sum e^{im\frac{d\theta}{d\gamma}\gamma_k} = \exp\left(-(m\frac{d\theta}{d\gamma}\sigma_\gamma)^2/2\right)\end{gathered} \tag{12}$$

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 approches 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 λ_1, λ_2 and λ_3, where s_2 is the right-hand side constant of last equation in (12) .

$$\begin{aligned} f(c_1,\cdots,c_{N_k},\lambda_1,\lambda_2,\lambda_3) &= \sum_{k=1}^{N_k} c_k^2 - \lambda_1\sum_{k=1}^{N_k} c_k \\ &- \lambda_2\left(\sum_{k=1}^{N_k}\gamma_k^2 - \sigma_k\right) \\ &- \lambda_3(\sum_{k=1}^{N_k} e^{im\frac{d\theta}{d\gamma}\gamma_k} - s_2)\end{aligned} \tag{13}$$

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 1-D analytical model.

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

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_u is the number of modulator period. We can include it in to the chicane dispersion and perform the Lagrangian multiplier procedure.

$$\left.\frac{d\theta}{d\gamma}\right|_{modulator} \cong \frac{2\pi N_u}{\gamma_0} \tag{15}$$

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_t different transverse distribution (x, y, p_x, p_y) 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).

Table 1: Simulation parameter

Beam energy (in electron mass)	8806
Energy spread	6e-4
Seed laser power (W)	1.0e8
Dispersion strength $d\theta/d\gamma$	0.171
Modulator period (m)	0.06
Modulator length (m)	4
Radiator period (m)	0.05

As the harmonic number is 2, N_j is selected to be 16 for enough accuracy at given dispersion strength according to Figure 1. For each phase value (θ, γ), we fill N_t sets of transverse Gaussian distribution using Hammersley pseudo random sequence. Now the left variance is N_k, the number of gamma values. And the total number of macro particles is $N_t \times N_k \times 16$. N_k needs to relatively large because small number of N_k will lead to large error at the dispersion other than the optimized point. N_t also need a large number because the energy modulation varies at different transverse location. Table 2 shows the choice of each dimension

Table 2: Number of particle in each dimension

N_k	32, 64
N_j	16
N_t	100, 200, 300, 400, 500

We use our method to generate initial distribution of above HGHG FEL process and import the initial distribution to Genesis 1.3. As comparison, we also use the loading method of Genesis, which uses Hammersley sequence for all 6 dimensions.

Figure 2 shows gain length in Radiator as function of different number of total macro particles. We can see that the result converges as macro particle number increases (both N_t and N_k increases). When N_k is small, the gain length calculation shows a small offset because the gain length depends on the energy distribution.

We can also compare this quiet start scheme with the 6-D coordinate generated by Hammersley sequence. Using quiet start scheme we can achieve accurate bunching factor before entering radiator by utilizing small amount of macro-particles (Figure 3) The systematic error caused by limitation stated in last section is small compare with the signal (<1%).

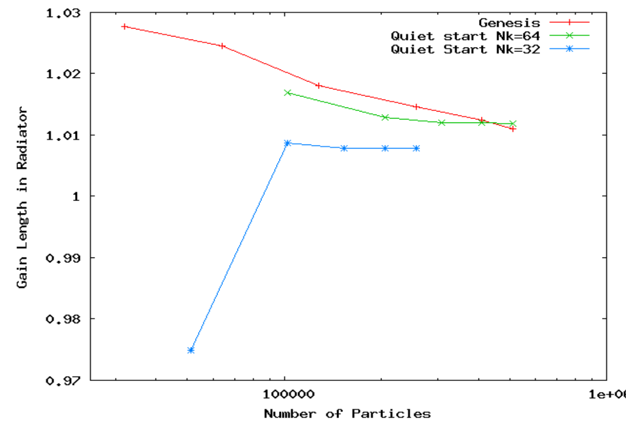

Figure 2. Comparison of Gain Length in Radiator

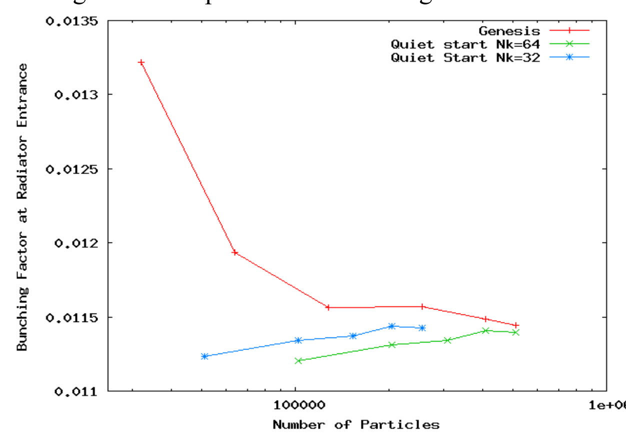

Figure 3. Comparison of bunching factor before radiator

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.

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