

## 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 (HGFG) 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 and makes the multi-parameter scanning be possible.

### 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 (HGFG) FEL. As the first HGFG 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 HGFG scheme.

The Quiet Start scheme, which reduces the number of macro particles largely in SASE simulation, uses only small number of distinguished phase  $\psi$  (usually 4). Each phase is filled with identical macro particle distribution of other 5 dimensions ( $\gamma$ ,  $x$ ,  $y$ ,  $p_x$ ,  $p_y$ ), 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 HGFG process.

In the article, we reconsider the existing quiet start method and find the condition that the modified quiet start method can be utilized when the modulator and dispersion sections exist. This method can reduce the macro particle number used in HGFG FEL simulation compared with the initialization with pseudo random generator or

Hammersley sequence in all 6 dimensions. 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 to reduce noise. One example is demonstrated to show the effectiveness of the method.

### ONE DIMENSION ANALYSIS

In the HGFG FEL scheme, the bunching factor after energy modulation and dispersion section can be calculated theoretically. 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,  $\gamma_c$  corresponds to the resonance energy,  $k_0$  and  $\omega_0$  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  $\sigma_\gamma$ ,

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

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

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

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  $(\gamma'', \theta'')$  is given by

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

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

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

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

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

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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  $(\gamma_0, \theta_0)$  to choose the macro-particles used in the simulation. Assuming the initially configuration is evenly distributed in phase variable  $\theta_0$ , and has Gaussian

distribution in energy spread  $\sigma_\gamma$  in  $\gamma_0$ . 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  $\theta_{0j}$ . In each  $\theta_{0j}$ , same configuration of energy  $\gamma_{0k}$ , totally  $N_k$  energy values, is assigned. Using this configuration, we need  $N_j \times N_k$  macro-particles for 1-D analysis.

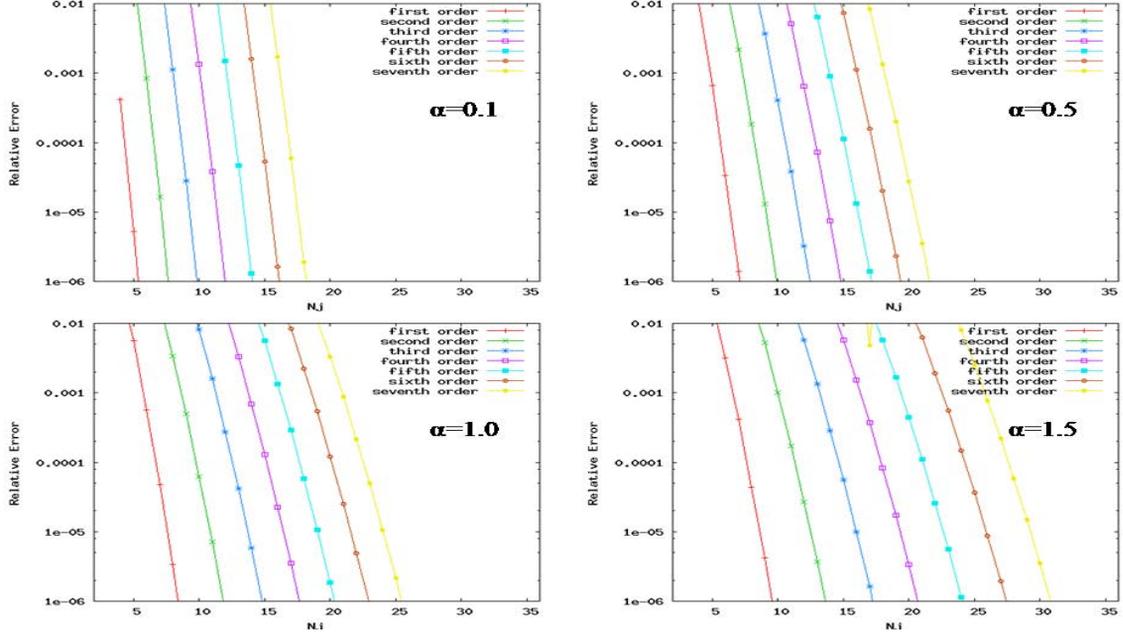


Figure 1: Bunching factor error as function of  $N_j$ .

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  $\theta_l$  as the final phase of  $l^{\text{th}}$  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.

$$\begin{aligned}
 b_m &= \langle e^{im\theta_l} \rangle = \sum_{l=1}^{N_j \times N_k} e^{im\theta_l} \\
 &= \frac{1}{N_j N_k} \sum_{j=1}^{N_j} \sum_{k=1}^{N_k} e^{im(\frac{d\theta}{d\gamma}(\gamma_{0k} + \Delta\gamma \sin(\theta_{0j})) + \theta_{0j})} \\
 &= \frac{1}{N_j N_k} \sum_{j=1}^{N_j} e^{im\theta_{0j} + im\alpha \sin(\theta_{0j})} \sum_{k=1}^{N_k} e^{im\frac{d\theta}{d\gamma}\gamma_{0k}}
 \end{aligned} \quad (6)$$

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  $\gamma_{0k}$ .

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.

$$\begin{aligned}
 &\frac{1}{N_j} \sum_{j=1}^{N_j} e^{im\theta_{0j} + im\alpha \sin(\theta_{0j})} \\
 &= \frac{1}{N_k} \sum_{j=1}^{N_j} \sum_{p=-\infty}^{+\infty} J_p(m\alpha) e^{\frac{i(p+m)2\pi j}{N_j}}
 \end{aligned} \quad (7)$$

After simple steps, the bunching factor gives

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

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).

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

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  $\alpha \sim 1$ . For example, if harmonic number is 3, other parameters are optimized 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. Two possible ways to generate these energy values are pseudo random generator (such as Mersenne Twister method) or Hammersley sequence mentioned earlier that manifest less noise.

Calculation result shows that the second sum in Eq.(8) yields high accuracy even use pseudo random generator when reasonable energy spread and dispersion strength is set. Usually, we have  $m \frac{d\theta}{dy} \sigma_y \leq 1$  to achieve large bunch factor. In Table 1, the relative RMS error of second sum is listed. The error of bunching factor due to initial energy spread is negligible if the total number of pseudo random sequence filled in each phase is larger than 200.

Table 1. relative RMS error of second sum

$N_k$	$m \frac{d\theta}{dy} \sigma_y = 0.1$	$m \frac{d\theta}{dy} \sigma_y = 0.5$	$m \frac{d\theta}{dy} \sigma_y = 1$
200	1.3e-6	8.3e-4	1.4e-2
300	1.1e-6	6.9e-4	1.2e-2
500	9.0e-7	5.3e-4	8.9e-3

### 3-D SIMULATION

In 3 dimension simulation, we use  $N_j$  distinguished phase, evenly distributed in  $[-\pi, \pi]$ , at macro particle initialization. In each phase,  $N_k$  set of other 5 dimensions ( $\gamma, x, y, p_x, p_y$ ) coordinate is filled using pseudo random number generator. One can also utilize Hammersley pseudo random sequence in coordinates other than phase to reduce initial noise and total macro particles needed.

Here, as an example, we simulate HGHG FEL in BNL DUV FEL from seed wavelength 800nm to radiation wave length 266nm. Main parameter used in simulation is shown in Table 2.

Table 2. Simulation parameter

Beam energy (in electron mass)	346.5
Energy spread	1e-4
Seed laser power (W)	25e6
Dispersion strength $d\theta/dy$	8.7
Modulator period (m)	0.08
Modulator length (m)	0.8
Radiator period (m)	0.039

As the harmonic number is 3,  $N_j$  is selected to be 16 for enough accuracy at optimized dispersion strength. For each phase value, we fill 256 macro particles using Hammersley pseudo random sequence, resulting 4096 total particles used in the simulation.

We use our method to generate initial distribution of above HGHG FEL process and import the initial distribution to Genesis 1.3.

Figure 2 shows the power of radiation as function of longitudinal coordinate with different number of total macro particles. We can see that the result converges as macro particle number increases. The same converging result, if all 6 dimensions is filled by pseudo random number, one needs more than 30K macro particles to get reliable results. 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).

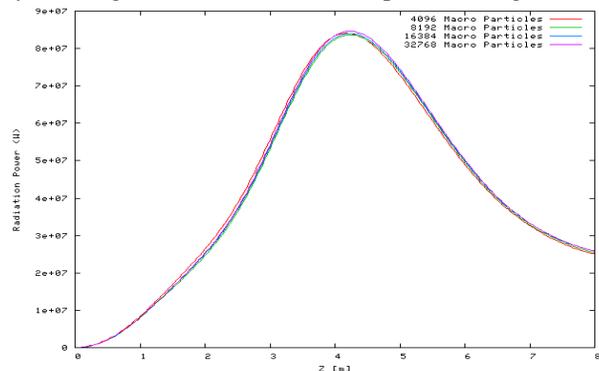


Figure 2: Radiation power vs. longitudinal coordinate.

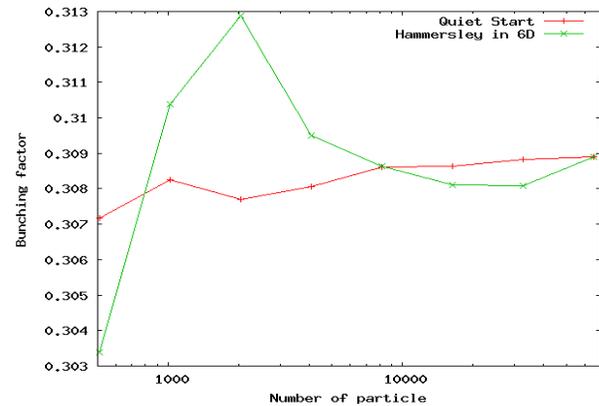


Figure 3: Comparison of Bunching factor before radiator.

### 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.

### REFERENCES

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