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COMPARING FEL CODES FOR ADVANCED CONFIGURATIONS

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Abstract

Various FEL codes employ different approximations and strategies to model the FEL radiation generation process. Many codes perform averaging procedures over various length scales in order to simplify the underlying dynamics. As FELs are developed in more advanced configurations beyond simple SASE, the assumptions of some codes may be called into question. We compare the unaveraged code Puffin to averaged FEL codes including a new version of GENESIS in a variety of situations. In particular, we study a harmonic lasing setup, a High-Gain Harmonic Generation (HGHG) configuration modeled after the FERMI setup, and a potential Echo-Enabled Harmonic Generation (EEHG) configuration also at FERMI. We find the codes are in good agreement, although small discrepancies do exist.

INTRODUCTION

Numerical simulation is an important tool in assessing the performance of any X-ray FEL. While there has been significant work benchmarking numerical codes to SASE studies [1,2], comparatively little has been done on other operation modes. In this study, we consider advanced schemes designed to extend the maximum attainable photon energy (harmonic lasing [3]) and improve the temporal coherence (beam-based seeding [4]).

The first harmonic lasing of a self-seeded X-ray FEL has recently been achieved [5], and there is considerable interest in employing this technique to XFELs. In these harmonic lasing setups, the fundamental radiation is disrupted while the higher harmonic emission is allowed to grow unfettered.

We also consider both the High-Gain Harmonic Generation (HGHG) [6,7] and Echo-Enabled Harmonic Generation (EEHG) [8,9] seeding schemes. This type of seeding potentially allows the full longitudinal coherence of conventional lasers to be transferred to an X-ray FEL.

Previous work has compared the harmonic generation capabilities of some codes for a seeded beam [10]. This was extended by work which compared the results of FAST, GENESIS, and GINGER in the cases of both artificial and phase-shifted harmonic lasing [11] starting from noise. We extend this result by adding additional simulation results from the un-averaged code PUFFIN. We then provide benchmarks for FERMI inspired HGHG [12] and EEHG configurations between both PUFFIN and GENESIS.

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CODE DESCRIPTIONS

The FEL simulation codes used in this study are PUFFIN [13] and GENESIS [14]. While for the harmonic lasing studies results from the codes FAST and GINGER are presented, no new simulations are performed with these codes and a description of these previous results is found in [11]. Although PUFFIN and GENESIS are both high gain FEL simulation codes, they contain some important differences so we briefly describe each in turn.

GENESIS

GENESIS is a time-dependent, 3D FEL simulation code in which both the radiation field and electron macroparticles are distributed on a Carteisan mesh. GENESIS averages over the motion of an individual undulator period, and therefore computes harmonic emission by employing an effective coupling factor [15]. Furthermore, GENESIS employs the so-called Slowly Varying Envelope Approximation (SVEA) [16] which allows one to average the radiation envelope over a radiation wavelength. While these approximations offer a large computational speedup, advanced FEL configurations may violate one or more of them.

Recent updates to GENESIS, referred to here as GENESIS V4, have made it possible to model each individual electron [17]. These so-called one4one simulations (one electron is one macroparticle) have noise statistics that are automatically correct at any wavelength. This allows for the electron beam to be re-sliced at any harmonic where the dynamics between current spikes, which result from HGHG or EEHG processes, can be modeled consistently. The HGHG and EEHG simulations shown below use this new version while the harmonic lasing simulations from 2014 use the nominal Fortran version.

PUFFIN

In contrast to GENESIS, PUFFIN does not employ the SVEA or average the electron motion. The electric field is instead discretized on a sub-wavelength scale with frequency resolution limited only by the Nyquist frequency. Similarly, the detailed electron motion resolution is limited only by the number of integration steps performed per undulator period. The cost of this is an orders of magnitude increase in computational complexity and memory requirements. While the physics captured is ostensibly more accurate as a result, one would like to benchmark the two codes in only a few

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Table 1: Electron beam and undulator parameters for the various benchmarking cases.

	LCLS-I	LCLS-II	HGHG	EEHG
$E[GeV]$	11.62	4	1.24	2
$\sigma_E[keV]$	1400	500	150	1000
$\epsilon_n[\mu m]$	0.4	0.4	2	1
$I_{\text{peak}}[kA]$	3	1	0.3	0.65
$\lambda_u[cm]$	3	2.6	5.5	3
K	3.5	2.23	3.45	2.28
$\langle\beta\rangle[m]$	26	12	10	25

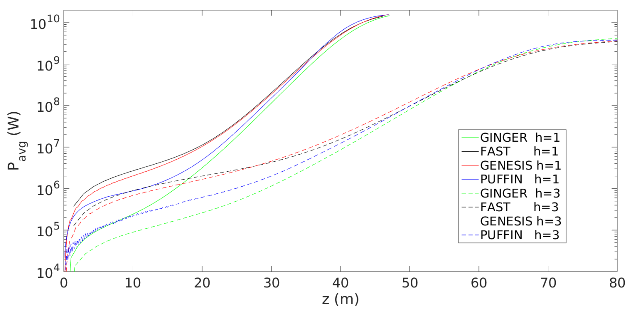

Figure 1: Growth of the fundamental (6 keV) and third harmonic (18 keV) radiation versus z for the LCLS-I like setup. The dashed curves are a separate simulation in which the fundamental is artificially suppressed.

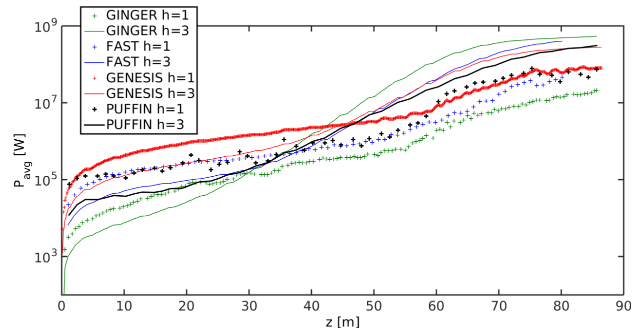

Figure 2: The power in the first and third harmonics versus z in the LCLS-II realistic harmonic lasing setup for various codes.

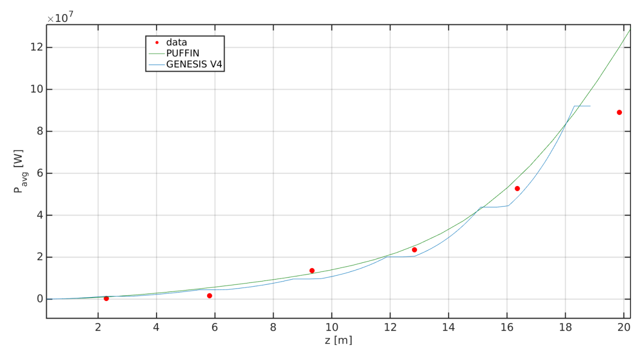

Figure 3: The average power versus z for the FERMI HGHG setup from PUFFIN, GENESIS, and measured data.

representative cases and leave the heavy design work to the more computationally efficient GENESIS.

HARMONIC LASING BENCHMARKS

To begin, we extend the harmonic lasing benchmarks of Marcus et. al. [11] with new PUFFIN simulations. The first case is an LCLS-I like setup operating at a 6 keV fundamental radiation energy. The resulting beam parameters are listed in table 1 and the power curves for each simulation are shown in Fig. 1.

After establishing the SASE benchmark, an artificial harmonic lasing setup is studied. The averaged codes (FAST, GENESIS, and GINGER) artificially suppress the fundamental radiation by toggling its interaction off in the code. PUFFIN, however, applies a high-pass filter which allows only the 3rd harmonic to pass. The power curves for these simulations are shown as the dashed curves in Fig. 1.

The disagreement in the startup section is due to the various competing modes in the SASE process and the limit of any given code to resolve them. Since there is not significant FEL interaction with these modes, this mild disagreement does not affect the amplified fundamental.

A similar comparison can be made using a realistic harmonic lasing scheme. In this study, the FEL is now LCLS-II like (parameters in table 1) and accommodates various phase shifters and break sections along its length. The phase shifters are generally tuned to a third-multiple of the fundamental wavelength, i.e. $\lambda/3$ or $2\lambda/3$ to disrupt the gain in the fundamental while leaving the third harmonic unperturbed [18]. The power curves for this LCLS-II case are shown in Fig. 2.

While all codes are in general agreement, differences begin to emerge in this more realistic harmonic lasing scenario. As the physics of harmonic lasing are not the focus here, we merely remark that the averaged codes appear to be sufficient for modeling the harmonic lasing.

HIGH-GAIN HARMONIC GENERATION

We now turn towards benchmarking various beam-based seeding schemes, the simplest of which is the HGHG setup. The particular setup we consider is similar to the FERMI FEL operating in single-stage HGHG mode with 266 nm seed laser, with the parameters shown in table 1.

The HGHG settings for these simulations have scaled parameters $A = 6$ and B optimized for bunching at the eighth harmonic. The resultant gain curves for PUFFIN simulations, GENESIS V4, and the experimental data from FERMI are shown in Fig. 3. The PUFFIN simulation did not include breaks in the undulator lattice, so the distance along the undulator is scaled to approximately compensate. Good agreement in the gain curve is obtained between the simulations and experimental data. The spectrum at the end of the undulator line is also shown in Fig. 4. One clearly identifies the various harmonics produced by the HGHG

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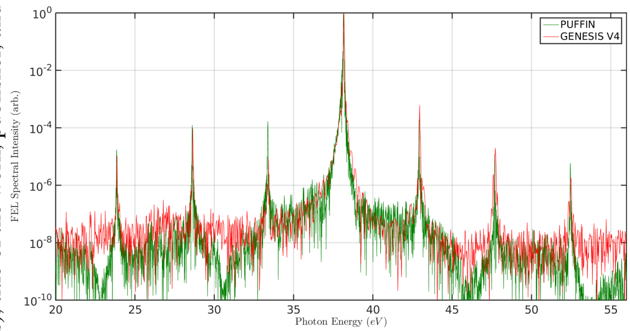

Figure 4: The FEL spectral intensity at the final undulator for the GENESIS and PUFFIN simulations for the FERMI HGHG setup.

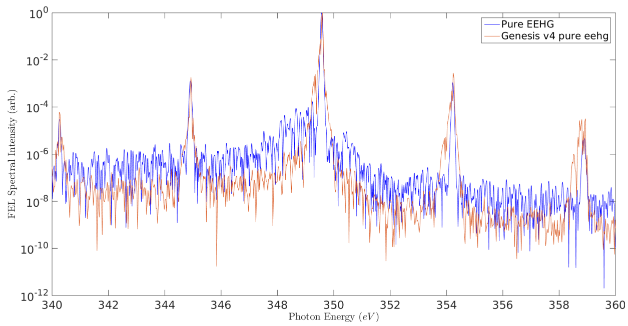

Figure 5: The saturated EEHG spectrum with both PUFFIN and GENESIS.

process, of which only the primary is significantly amplified by the FEL.

ECHO-ENABLED HARMONIC GENERATION

We turn now to the more complicated phase space manipulation of EEHG [8]. The FEL imagined in these simulations is also a rough approximation to the FERMI FEL, with slightly altered parameters as listed in table 1. As this is only a benchmark, the employed parameters differ from those quoted in FERMI's studies of potential EEHG experiments [19].

The Echo configuration is provided by two 266 nm lasers, each of which modulates the beam as perfect sinusoid by 3 MeV ($A_{1,2} = 3$). The chicanes are optimized for bunching at 3.5 nm with $B_1 = 25.95$ and $B_2 = 0.353$.

First, we compare the results in GENESIS vs PUFFIN for the case of a perfect electron beam, i.e. one with no microbunching structure; the final spectra are shown in Fig. 5. The agreement in both the central harmonic peak and the side-band harmonics is excellent between the two codes.

Energy modulations due to the microbunching instability [20] can be amplified and produce unwanted sidebands in the bunching spectrum. We compare the codes for this EEHG setup in response to a single energy modulation mode.

This modulation is applied prior to the EEHG manipulations, and is of the form $p \longrightarrow p + A_0 \sin(k_\mu z + \phi)$, for amplitude A_0, wavenumber k_μ and arbitrary phase ϕ, where

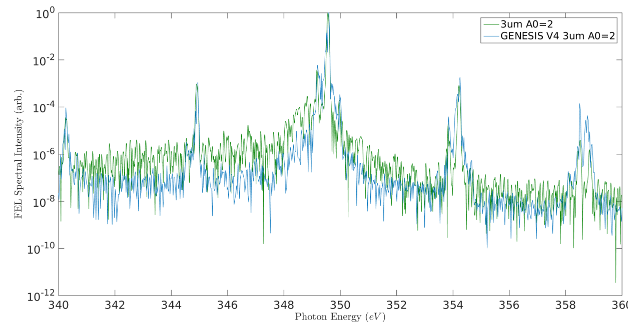

Figure 6: The saturated EEHG spectrum with an included $A_0 = 2$, 3um modulation. The extra modulation creates additional sideband structures around each of the EEHG harmonic peaks.

$p = \Delta E/\sigma_E$ is the energy deviation scaled to the slice energy spread. We select a modulation with amplitude $A_0 = 2$ and $\lambda_\mu = 2\pi/k_\mu = 3$ um, which is a fairly representative mode for the instability in the LCLS [21]. The resulting FEL spectra at saturation are shown in Fig. 6. The effect of this extra energy modulation is to introduce a sideband to the main EEHG peaks, which in this case is slightly redshifted from the main peaks. The agreement between the codes on the amplitude and location of these sidebands is excellent. This confirms that GENESIS V4 is a sufficient tool for simulating EEHG beams even with high harmonic energy structure.

DISCUSSION

We have extended the previous work benchmarking against harmonic lasing to include the non-averaged code PUFFIN. While all codes are in good agreement in the artificial harmonic lasing setup, the phase-shifting induced harmonic lasing does show some disagreement. It is possible that this disagreement stems from choices in transverse gridding or how shot noise is handled, as these were not controlled for. Even a detailed study, however, of Fig. 2 could not reveal which codes are averaged and which are not, so we conclude that averaged codes are sufficiently accurate to model this harmonic lasing setup.

For the seeded cases considered, the agreement between GENESIS and PUFFIN was in general excellent. For relatively small ($\Delta E/E$) energy modulations, it seems that GENESIS is a sufficient tool for modeling both HGHG and EEHG beams. It remains possible that in more extreme settings, such as those with very large energy modulations, the assumptions of GENESIS could cause inaccurate results. Future work should continue to push this boundary and discover exactly which configurations require a more complete simulation model.

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