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FEL CODE COMPARISON FOR THE PRODUCTION OF HARMONICS VIA HARMONIC LASING*

G. Marcus†, W. M. Fawley, SLAC, Menlo Park, CA, USA
E. A. Schneidmiller, M. V. Yurkov, DESY, Hamburg, Germany
S. Reiche, PSI, Villach, Switzerland

Abstract

Harmonic lasing offers an attractive option to significantly extend the photon energy range of FEL beamlines. Here, the fundamental FEL radiation is suppressed by various combinations of phase shifters, attenuators, and detuned undulators while the radiation at a desired harmonic is allowed to grow linearly. The support of numerical simulations is extensively used in evaluating the performance of this scheme. This paper compares the results of harmonic growth in the harmonic lasing scheme using three FEL codes: FAST, GENESIS, and GINGER.

INTRODUCTION

Numerical simulation has been a critical tool both in the design and the commissioning of short wavelength free-electron lasers based upon the principle of self-amplified spontaneous emission (SASE) such as FLASH and the LCLS. In part due to the complex physics such as the varying exponential growth rates as a function of wavelength, the effective startup noise, and radiation-electron beam slippage effects that help develop longitudinal coherence, accurate numerical modelling for SASE configurations can be more challenging than that required for more simple time-steady FEL amplifiers. Over the past three decades, numerous simulation codes have been developed for FEL modelling purposes, ranging from 1D, time-steady approximations to fully 3D, time-dependent approaches. Some code-to-code benchmarking has been done for high gain FEL's. The study by Biedron *et al.* [1] in the very late 1990's compared results from five different codes for the linear growth rates and saturated power for a time-steady test case based upon parameters corresponding to the Argonne LEUTL FEL. A decade later Giannessi *et al.* [2] compared fundamental and harmonic power vs. z profiles for both single frequency and time-dependent, externally-seeded test cases, finding good agreement between the 1D PERSEO code and the 3D GENESIS and MEDUSA codes. However, apart from a comparison of SASE startup in the GENESIS and GINGER codes with theoretical predictions [3], there appear to be few if any code comparison studies in the literature for full SASE cases.

Here we give the results of a small SASE benchmarking study where we have concentrated upon cases with parameters related to the operating LCLS-1 FEL at SLAC and to the upcoming, soft x-ray LCLS-2 machine. The codes used were FAST, GENESIS, and GINGER, each of which has been used extensively to model SASE-based FELs and each of which has sufficient dimensionality to examine the development of longitudinal and transverse coherence at both the fundamental FEL resonant wavelength and higher odd harmonics. Because of the recent interest in trying to reach higher output photon energies via use of harmonic emission (see, *e.g.*, [4, 5]), we also wanted to look reasonably carefully at the gain and saturation of the third harmonic in "lasing mode", *i.e.*, in situations where the fundamental is suppressed allowing the third harmonic to grow to much higher saturated powers than would be true otherwise. The remainder of this paper is arranged as follows. In §II, we give brief descriptions of each of the three codes concentrating on the features most relevant to SASE and harmonic emission. In §III we present the results of two LCLS-related cases: a) 6-keV fundamental and 18-keV third harmonic emission for a continuous (*i.e.*, non-segmented) LCLS-1 undulator initiated by shot noise b) 1.67-keV fundamental and 5-keV third harmonic emission for a hypothetical, segmented LCLS-II undulator with break sections in which there are special phase shifters tuned to suppress the fundamental via phase shifts of 2/3 and 4/3 wavelengths. We conclude in §IV with a short discussion of our findings.

CODE DESCRIPTIONS

In this section we describe some basic characteristics of the three codes used for this study. They share many common features including a 3D particle mover, an eikonal (*i.e.*, slowly varying envelope approximation) field solver and wiggle-period averaging for calculating the coupling between the radiation and the beam electrons. Each code works in the time domain (*i.e.* spectral decomposition is done only via post-processing) and also subdivides the electron beam into "slices" whose longitudinal centers are spaced uniformly.

FAST

FAST is the generic name for a set of codes developed for analysis of the FEL amplification process in the framework of 1-D and 3-D models using different techniques as described in [6–9]. Analytical techniques implemented in these codes allows analysis of beam radiation modes via an eigenvalue equation and the amplification process during the exponential growth stage (initial-value problem). The simulation codes can simulate the FEL process with both steady-state and time-dependent models and can also treat odd harmonic emission in planar undulator geometries [10]. The three-dimensional version of FAST [11] takes into ac-

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† gmarcus@slac.stanford.edu

count all important physical effects: diffraction, slippage effects, space charge, and emittance and energy spread in the electron beam. The field solver uses retarded potentials and expands the radiation via azimuthal modes. FAST has been thoroughly tested in the high gain exponential regime using analytical results for the beam radiation modes (complex eigenvalues and eigenfunctions) [6–8]. It has also been tested from shot noise start-up through the linear stage of amplification against three-dimensional analytical results for the initial-value problem [9]. Start-up from electron beam shot noise can be simulated either by an artificial macroparticle ensemble [12, 13] or by tracing the *actual* number of electrons in the beam [14], initially randomly distributed in the full 6D phase space. All the FAST results presented in this paper are calculated with actual number of electrons.

GENESIS

GENESIS [15] is a time-dependent 3D FEL simulation program where the radiation field and macroparticle source terms are discretized on a Cartesian mesh. As with FAST and GINGER, shot noise can be simulated by standard methods [12, 13]; since the latest GENESIS version runs on reasonably large computer clusters, in some situations the code can model the actual number of beam electrons, thus *a priori* providing the correct shot noise at any frequency. Harmonic emission has been implemented by using the effective coupling factors [16] for odd and even harmonics. The user can choose either to model the self-consistent interaction of the higher harmonics of the radiation field with the electron beam (*i.e.*, true lasing) or, alternatively, to calculate the so-called non-linear emission associated with the strong harmonic bunching factor that occurs as the fundamental approaches saturation.

GINGER

GINGER [17] differs from the previous two codes in that the standard field solver model employs 2D cylindrical axisymmetry. Thus any gain, energy spread and saturation effects due to modes with higher order azimuthal number will be neglected. The radial grid follows a mathematical *sinh* function giving a nearly constant spacing near the axis and exponentially-expanding spacing much farther out, thus permitting quite distant boundaries with reasonable numbers of grid cells (e.g., $nr = 128$). Recently, the GINGER field solver has been extended to handle true harmonic lasing (*i.e.*, not only the nonlinear harmonic emission that was discussed in [18]). The z-advance control algorithm is such that arbitrary length drift spaces are properly modelled (including vacuum field propagation); their length is not required to be an integer of the nominal z-step size.

BENCHMARK CASES

We looked at two cases that would test numerically various SASE physics at both the fundamental and third harmonic radiation wavelengths such as the effective input noise signal, the growth rate in the linear regime, and the saturation level. We now discuss each of them in turn.

Table 1: Test Case e-Beam and Undulator Parameters

parameter	unit	LCLS-1	LCLS-2
Current	kA	3.0	1.0
Emittance	mm-mrad	0.40	0.40
Energy	GeV	11.62	4.0
σ_E	keV	1400	500
$< \beta_{x,y} >$	m	26.0	12.0
λ_u	mm	30.0	26.0

LCLS-I Continuous Undulator

For our first study we chose a case that nominally corresponds to the LCLS-1 FEL at SLAC operating at a 6-keV fundamental. For purposes of simplification, we considered a continuous, unsegmented undulator, *i.e.*, one without any break sections. The electron beam and undulator parameters are shown in the third column of Table 1. For this and the other cases, energy loss and increased incoherent energy spread due to broadband spontaneous emission was artificially suppressed. Artificial harmonic focusing was applied resulting in a 26-m beta function, a value comparable to the average value due to the quadrupole focusing in the actual LCLS. Due to the low normalised emittance and high current, there is strong gain at the fundamental and power saturation occurs by $z \approx 45$ m. As shown in Fig. 1, each code shows a saturation level of about 30 GW. The initial noise levels depend upon the dimensionality of the field solver with GINGER and FAST with enforced axisymmetry showing good agreement as would be expected. The GENESIS results are nearly identical to those of FAST run that included up to $m = \pm 2$ azimuthal mode number. As pointed out in [3], the magnitude of the startup spontaneous emission is a function of the transverse gridding with finer spacing including more transverse modes and thus more power.

The results for the situation with third harmonic lasing only (fundamental emission artificially suppressed) are quite similar. Examining Fig. 2 one sees that GINGER saturates at a few percent higher power level and GENESIS slightly differs from FAST with $|m| \leq 2$ in the linear gain region from 25 to 55 m. But overall, the three independent codes agree strikingly well in both the effective noise level and final saturation power. We also found that the final saturation power in FAST is essentially independent of the maximum allowable azimuthal mode number, at least through $m = \pm 3$.

LCLS-II Optimized Third Harmonic Lasing with Phase Shifters

Our second benchmarking case corresponds to LCLS-2 operating in the soft x-ray regime. Compared with LCLS-1, the hypothetical LCLS-2 design has much lower current and energy but significantly stronger focusing. Here the

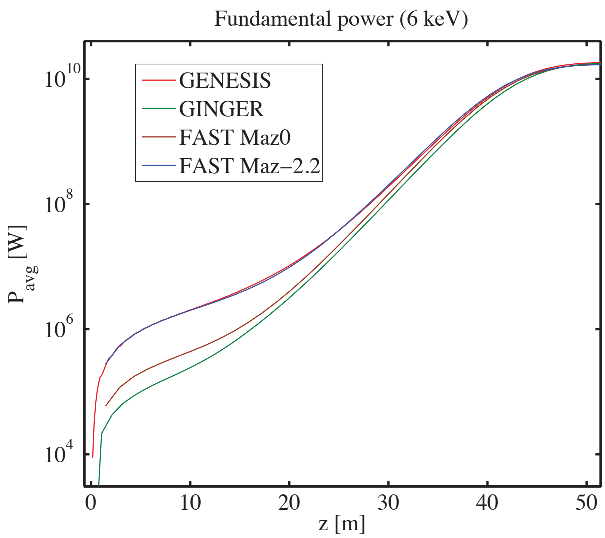

Figure 1: Growth of fundamental vs. z for LCLS-1 parameters. One FAST run corresponds to axisymmetry ("Maz0") while the other includes azimuthal modes in the interval $m = \pm 2$ ("Maz-2.2").

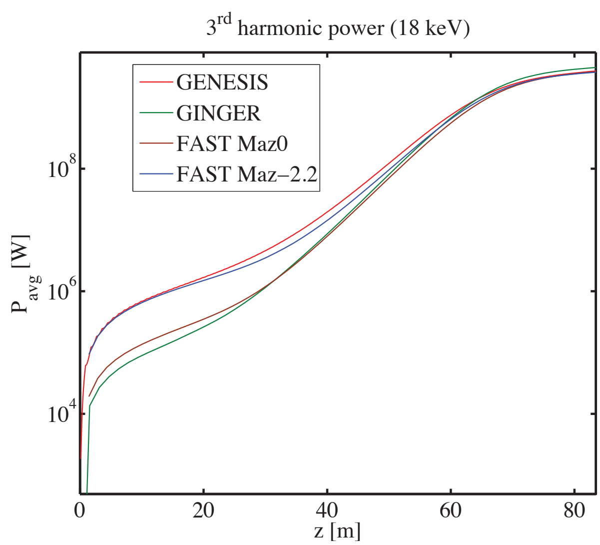

Figure 2: Growth of third harmonic vs. z for LCLS-1 parameters with the fundamental emission completely artificially suppressed.

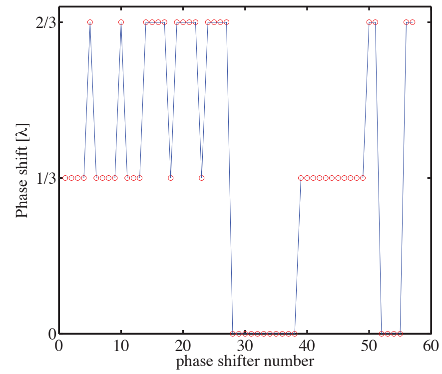

Figure 3: Graphical representation of phase shifter values (normalised to the radiation wavelength) versus break section position in the LCLS-II benchmark case. A positive value corresponds to an incremental *increase* of the electron beam's delay (and a decrease in ponderomotive phase) relative to what would give exact phase resonance with the electromagnetic field.

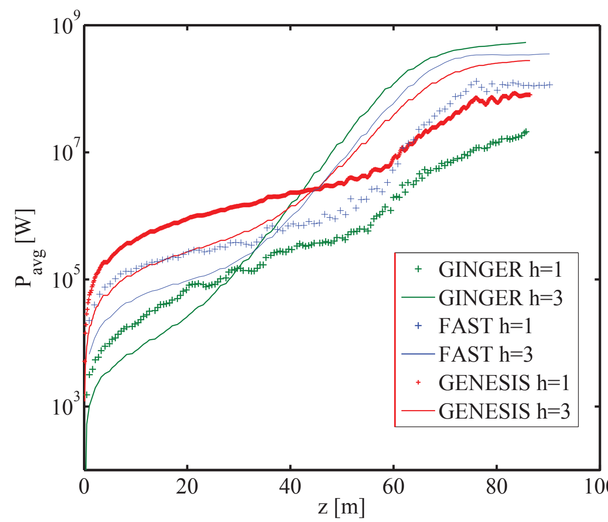

Figure 4: Growth of fundamental (1.67 keV; symbols and thick line) and third harmonic (5 keV; thin lines) vs. z for a hypothetical LCLS-II case in which phase shifters suppress growth at the fundamental.

26−mm period, planar-polarised, variable-gap undulator is segmented with a periodicity of two short break sections ($L = 0.13$ m) and one long break ($L = 0.78$ m) with the active undulator segments having lengths of 1.17 m. For focussing, the dominant term in the GENESIS run was provided by a FODO quadrupole lattice while FAST and GINGER adopted an artificial, continuous in z harmonic component.

Since LCLS-II will have wavelength tunability via a changing K, the break sections will have active phase shifters in order to keep the electron beam and radiation in phase. This capability gives the option of following suggestions by McNeil *et al.* [19] and Schneidmiller and Yurkov [5] to purposefully use combinations of $\Delta\Phi = 2\pi/3$ and $\Delta\Phi = 4\pi/3$ phase shifters to suppress the lasing of the fundamental while not affecting that of the third harmonic. In principle this scheme allows the harmonic to reach saturation without its gain being depressed by incoherent energy spread associated with growth in the fundamental power. We followed the general prescription of Ref. [5] for picking phase shifter values as a function of break position. Figure 3 shows the particular values chosen (but note that we plot the increase in electron beam delay, not $\Delta\Phi$ which has the opposite sign).

Our simulation results, as displayed in Fig. 4, show the variable phase shifter disruption succeeds quite well in suppressing the SASE growth of the fundamental at 1.67 keV

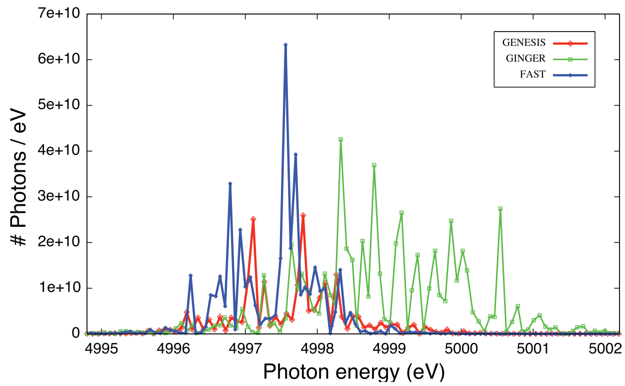

Figure 5: Output spectrum in 5 keV region for the hypothetical LCLS-II of the previous two figures. The spectral intensity corresponds to a pulse length of 54 fs. The difference in the mean wavelength between the GINGER run and the other codes is due to a slightly different K.

with barely any growth beyond the normal spontaneous component up to $z = 60$ m. In the next twenty meters there does appear to be some coherent exponential gain but by this point the third harmonic at 5 keV photon energy has saturated at a value of ~ 500 MW average power, nearly an order of magnitude greater than is true for the fundamental. The integrated output spectra from a single SASE run, as shown in Fig. 5, show an inverse normalized RMS bandwidth of about 5000.

While the code agreement is reasonably good with respect to the third harmonic power vs. z, FAST and especially GINGER show greater saturated power than does GENESIS . At present we do not fully understand the reasons for the discrepancy. Tests with FAST appear to rule out a dependence of the saturated output power on the number of included azimuthal modes. Both GENESIS and GINGER show some dependence of $P(z)$ on the macroparticle number per slice; the final power in GINGER at $z = 86$ m drops by 20% for a 4× increase in particle number to 65K per slice. For GENESIS simulation of the LCLS-I case, the effective noise power in the fastest growing mode can change 2× for a 8× increase in macroparticle number although the asymptotic power is virtually unchanged.

DISCUSSION

In this study we have examined the predictions of three standard multi-dimensional FEL simulation codes, FAST , GENESIS , and GINGER , regarding SASE growth of the fundamental and third harmonic for two cases related to LCLS parameters. We have found for an LCLS-1 like case the independent growth and saturation of the fundamental and third harmonic power are nearly identical in the three codes once the exponentially growing modes dominate the spontaneous background. The fully 3D codes GENESIS and FAST agree best in the "spontaneous regime" before the fastest growing modes dominate when the latter is limited to azimuthal modes with $|m| \leq 2$. GINGER and FAST also agree in this regime when the latter is run with azimuthal symmetry, *i.e.*, only the $m = 0$ mode.

A second test case involving a segmented, LCLS-II like undulator with phase shifters shows that following the prescription of Ref. [5] introducing shifts of $\Delta\Phi = 2\pi/3$,$4\pi/3$ successfully suppresses the fundamental growth so that the third harmonic at 5 keV reaches saturation at levels of 500 MW. While the code agreement is generally good, there are differences in the saturation regime that at present are not fully understood. The differences suggest that numerical modelling of higher harmonics is likely more sensitive to choices of shot noise algorithms, gridding, and macroparticle number.

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