ISBN: 978-3-95450-210-3 doi:10.18429/JACoW-FEL2019-TUP050

COMPARISON BETWEEN, AND VALIDATION AGAINST AN EXPERIMENT OF, A SLOWLY-VARYING ENVELOPE APPROXIMATION CODE AND A PARTICLE-IN-CELL SIMULATION CODE FOR FREE-ELECTRON LASERS

L.T. Campbell[1,3], H.P. Freund[4], J.R. Henderson[1,3], B.W.J. M^{c}Neil[1,2], P. Traczykowski[1,2,3] and P. J. M. van der Slot [5]
[1]SUPA, Department of Physics, University of Strathclyde, Glasgow, G4 0NG
[2]Cockcroft Institute, Warrington, WA4 4AD, UK
[3]ASTeC, STFC Daresbury Laboratory, Warrington, WA4 4AD, UK
[4]University of New Mexico, Albuquerque, New Mexico, 87131 United States of America
[5]Mesa+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Abstract

Free-electron lasers (FELs) operate at wavelengths down to hard x-rays, and are either seeded or start from noise. There is increasing interest in x-ray FELs that rely on Self-Amplified Spontaneous Emission (SASE), and this involves increasing simulation activity in the design, optimization, and characterization of these x-ray FELs. Most of the simulation codes in use rely on the Slowly-Varying Envelope Approximation (SVEA) in which Maxwell's equations are averaged over the fast time scale resulting in relatively small computational requirements. While the SVEA codes are generally successful, the predictions of these codes sometimes differ in various aspects of the FEL interaction. In contrast, Particle-in-Cell (PiC) simulation codes do not average Maxwell's equations and are considered to be a more complete model of the underlying physics. Unfortunately, they require much longer run times than SVEA codes and have not been validated by comparison with experiment as often as the SVEA codes. In order to remedy this, and to resolve issues that arise due to different predictions between the SVEA codes, we present a comparison between one SVEA code (MINERVA) and a PiC simulation code (PUFFIN) with the experimental measurements obtained at the SPARC SASE FEL experiment at ENEA Frascati. The results show good agreement between the two codes and between the codes and the experiment. Since the formulations of the two codes share no common elements, this validates both formulations and demonstrates the capability to model the FEL interaction from the start of the undulator through the undulator and into deep saturation.

INTRODUCTION

While free-electron lasers (FELs) have been intensively studied since the 1970s, new developments and concepts keep the field fresh. Intensive work is ongoing into new FEL-based light sources that probe ever shorter wavelengths with a variety of configurations. There presently exists a large variety of FELs ranging from long-wavelength oscillators using partial wave guiding to ultraviolet and hard x-ray FELs that are either seeded or starting from noise (SASE). As these new light sources come on-line, interest will grow in shorter pulses, new spectral ranges and higher photon fluxes. The increasing activity in the design and construction of FEL light sources is associated with increasing simulation activity to design, optimize, and characterize these FELs. Most of the FEL simulation codes in use at the present time can be categorized as either SVEA or PiC simulations. In the SVEA, the optical field is represented by a slowly-varying amplitude and phase in addition to a rapid sinusoidal oscillation. The field equations are then averaged over the rapid sinusoidal time scale and, thereby, reduced to equations describing the evolution of the slowly-varying amplitude and phase. Within the context of the SVEA, FEL simulation codes fall into two main categories where the particle trajectories are found by first averaging the trajectories over an undulator period (the so-called wiggler-averaged-orbit approximation), or by the direct integration of the Newton-Lorentz equations. There is a further distinction between the SVEA codes based upon the optical field representation, and codes have been written using either a grid-based field solver or a superposition of optical modes. Simulation codes using the wiggler-averaged-orbit analysis in conjunction with a grid-based field solver include (but are not limited to) GINGER [1], GENESIS [2], and FAST [3]. In contrast, SVEA codes that integrate the Newton-Lorentz equations in conjunction with a Gaussian mode superposition for the optical fields include MEDUSA [4] and MINERVA [5]. One common feature of all the SVEA codes, however, is the way in which time-dependence is treated. The fast time scale average results in a breakdown of the optical pulse into temporal slices each of which is a single wave period in duration. The optical slices slip ahead of the electron slices at the rate of one wavelength per undulator period. As a result, the SVEA codes integrate each electron and optical slice from $z \rightarrow z + \Delta z$ and then allow the optical slice to slip ahead of the electron slices. These codes have been extremely successful in modeling FELs; however, their predictions are not always identical for all aspects of the FEL interaction. In contrast, PiC codes do not average Maxwell's equations and are considered to represent a more fundamental model of the physics of FELs.

Content from this work may be used under the terms of the CC BY 3.0 licence (© 2019). Any distribution of this work must maintain attribution to the author(s), title of the work, publisher, and DOI

ISBN: 978-3-95450-210-3 doi:10.18429/JACoW-FEL2019-TUP050

Content from this work may be used under the terms of the CC BY 3.0 licence (© 2019). Any distribution of this work must maintain attribution to the author(s), title of the work, publisher, and DOI

A PiC code makes no average over the rapid sinusoidal oscillation and integrates the Newton-Lorentz equations for the particles. As a result, PiC codes require substantially more computational resources than SVEA codes and are not so commonly in use and have not been as extensively validated against experiments as have the SVEA codes. At the present time, the primary PiC code for FEL simulations is PUFFIN [6, 7]. In view of this, we undertake in this paper to present a comparison of one SVEA code (MINERVA) and a PiC code (PUFFIN) with experimental measurements. The properties/capabilities of these codes have been presented in the literature and will not be discussed here other than to emphasize that while MINERVA applies the SVEA it does not average the Newton-Lorentz equations over the undulator period. As such, both PUFFIN and MINERVA integrate the particle trajectories in the full magnetostatic and electromagnetic field representations. Other than this, the two codes share no common elements. In particular, the particle loading algorithms used to treat start-up from noise are different. MINERVA uses an adaptation of the algorithm described by Fawley [1] while PUFFIN uses an algorithm developed by McNeil et al. [8]. Our purpose in this paper is to compare the simulation results obtained by the two codes and to "validate" the codes by comparison with experimental measurements taken in a SASE FEL. To this end, comparisons between PUFFIN and MINERVA and between the two codes and experimental measurements at the "Sorgente Pulsata ed Amplificata di Radiazione Coerente" (SPARC) experiment which is a SASE FEL located at ENEA Frascati [9] are presented in following sections. The best estimate for the experimental parameters of SPARC are summarized in Table 1.

Table 1: Parameters of the SPARC FEL Experiment

Electron beam	
Energy	151.9 MeV
Bunch charge and duration	450 pC, 12.67 ps
ϵ_x, ϵ_y	2.5, 2.9 mm-mrad
RMS Energy spread	0.02%
σ_x, σ_y	132, 75 μm
α_x, α_y	0.938, -0.705
Undulators and quadrupoles	
Period and length	2.8 cm, 77 Periods
Amplitude and K_{rms}	7.8796 kG, 1.457
Gap Length	0.40 m
Quadrupole length	5.3 cm
Quadrupoles field gradient	0.9 kG/cm

A parabolic temporal bunch profile was used in MINERVA while PUFFIN employed a Gaussian temporal profile. The experiment employed six undulators for an overall length of about 15 meters, but this was too short to reach saturation given the bunch charge. In order to compare the codes in the saturated regime, we extended the undulator/FODO lattice to include 11 undulators. As a result, the experimental data is used to anchor the validation of the codes in the start-up and exponential growth regions, while the code results are compared for the initial start-up, exponential growth and deep saturation regimes. The quadrupole orientations were fixed and did not alternate. The electron beam was matched into the undulator/focusing lattice. The resonance occurred at a wavelength of 491.5 nm. The pulse energies were measured in the gaps after each undulator segments by opening the gap, thereby detuning the FEL interaction, in the further downstream undulators [9]. The simulated propagation of the beam through the undulator/quadrupole lattice is shown in Fig. 1, where we plot the beam envelope in x and y versus position as determined by PUFFIN. The MINERVA propagation results were similar. Observe that the beam is well-confined over the 28 meters of the extended lattice with an average beam size of approximately 115 μm.

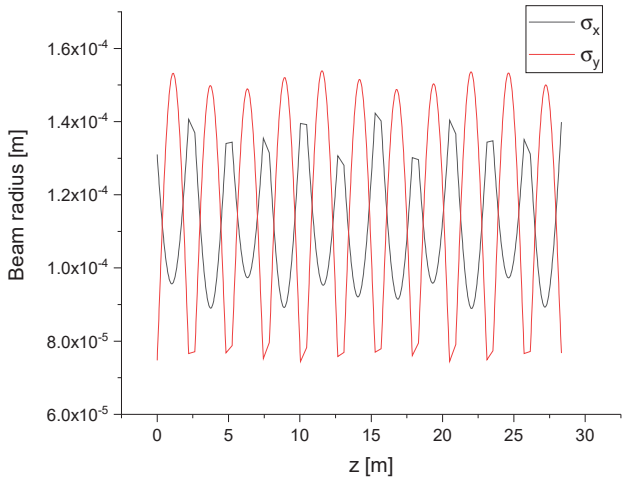

Figure 1: PUFFIN simulation propagation of the beam propagation through the undulator/quadrupole lattice.

A comparison of the evolution of the pulse energy as found in MINERVA and PUFFIN, and as measured in the experiment, is shown in Fig. 2 where the MINERVA simulation is indicated by the blue line and the PUFFIN simulation is indicated by the green line. The measured pulse energies for a sequence of shots are indicated by the red markers where the error bars indicate the standard deviation over a sequence of shots. Observe that the agreement between the two codes, and between the codes and the measured pulse energies, are excellent over the entire range of the experiment.

We remark that the exponential growth region starts in the second undulator and that the start-up region is encompassed in the first undulator segment. The experimental measurements indicate that the pulse energy after the first undulator falls into the range of about 8.4×10^{-12} through 1.74×10^{-11} J while MINERVA yields a pulse energy of 2.52×10^{-11} J and PUFFIN yields 4.02×10^{-11} J. The simulation results are in relatively close agreement with the experiment and

ISBN: 978-3-95450-210-3 doi:10.18429/JACoW-FEL2019-TUP050

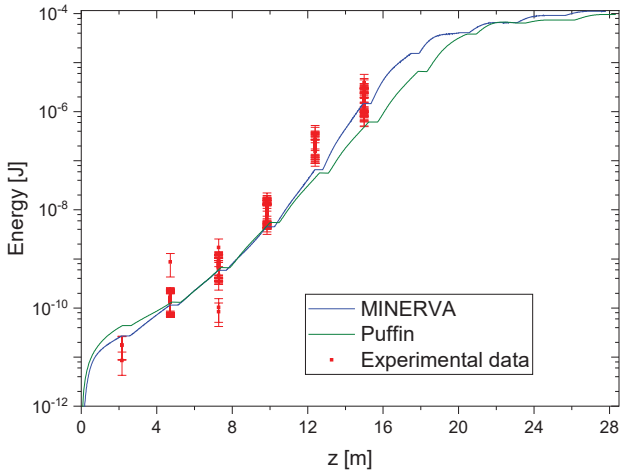

Figure 2: Comparison of simulation results with PUFFIN and MINERVA and the measured pulse energies versus distance through the undulator (data courtesy of L. Giannessi).

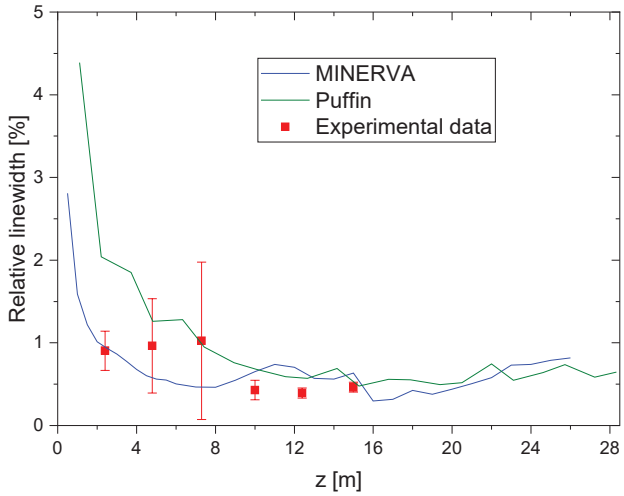

Figure 3: Comparison of the measured relative linewidth in red (data courtesy of L. Giannessi) with that found in the simulations (blue for MINERVA and green for PUFFIN).

with each other, although PUFFIN exhibits slightly higher start-up noise than MINERVA. This agreement is an important observation since the particle loading algorithms in the two codes share no commonality. Apart from differences that might derive from the parabolic versus Gaussian temporal profiles and the different particle loading algorithms, another source of the difference in the slightly higher start-up noise in PUFFIN is the fact that PUFFIN naturally includes a wider initial spectral range than MINERVA. The exponential growth region starts in the second undulator and the two codes are in excellent agreement with each other and with the experimental measurements out to the end of the sixth undulator. These results are in substantial agreement with the parameterization developed by Ming Xie [10]. Using a β-function of about 2 m, we find that the Pierce parameter $\rho \approx 2.88 \times 10^{-3}$ and that this parameterization predicts a gain length of 0.67 m, and a saturation distance of 18.1 m (including the additional 3.2 m represented by the gaps between the undulators). This is in reasonable agreement with the simulations which indicate that saturation occurs after between about 18-20 meters of undulator/FODO line. Finally, the predictions of the two codes in the saturation regime after about 20 m are also in remarkable agreement. After 28 m of undulator/FODO lattice PUFFIN predicts a pulse energy of 90 μJ while MINERVA predicts 111 μJ which constitutes a difference of about 18%.

The larger initial spectral linewidth excited in the start-up region exhibited by PUFFIN is shown more clearly in Fig. 3 which presents a comparison between the evolution of the relative linewidth as determined from PUFFIN and MINERVA and by measurement. It is clear that PUFFIN predicts a significantly wider initial spectrum than MINERVA. This is consistent with the wider bandwidth modelled by PUFFIN and the fact that, unlike MINERVA, it models the generation of the wider bandwidth coherent spontaneous emission. Exponential gain due to the resonant FEL interaction starts in the second undulator and this is expected to rapidly overcome any incoherent synchrotron radiation from the start-up region in the first undulator. In view of this, the PUFFIN results converge rapidly to that found by MINERVA and to the measured linewidths after the second undulator. Note, however, that the measured linewidth after the first undulator seems to be in better agreement with the MINERVA result, but this may be due to the bandwidth of the detector. Agreement between the simulations and the measured linewidth is within about 35% after 15 m. As shown in the figure, the predicted linewidths are in substantial agreement with the experimental measurements, and good agreement between the codes is found over the entire range of integration through the saturated regime.

SUMMARY AND CONCLUSION

In this paper, describe a comparison between simulation codes based on the SVEA formulation (MINERVA) and a PiC formulation (PUFFIN). The two codes have simulated the SPARC SASE FEL at ENEA Frascati. Good agreement has been found both between the two codes and between the codes and the experiment, thereby validating both formulations. This is significant because these two formulations have virtually no elements in common, and we can conclude from this that they both faithfully describe the physics underlying FELs. In particular, the agreement between the codes and the experimental measurements regarding the start-up regime in the SPARC FEL validates the different particle loading algorithms in both codes. One limitation of the SVEA models derives from the fast time scale average which means that these codes cannot treat ultra-short pulse production. This limitation is not present in PiC codes; hence, the validation of PUFFIN implies that it may be a useful model for future ultra-short.

Content from this work may be used under the terms of the CC BY 3.0 licence (© 2019). Any distribution of this work must maintain attribution to the author(s), title of the work, publisher, and DOI

ISBN: 978-3-95450-210-3 doi:10.18429/JACoW-FEL2019-TUP050

Content from this work may be used under the terms of the CC BY 3.0 licence (© 2019). Any distribution of this work must maintain attribution to the author(s), title of the work, publisher, and DOI

ACKNOWLEDGMENTS

The authors would like to thank: The Argonne Leadership Computing Facility - a DOE Office of Science User Facility supported under contract DE-AC02-06CH11357; The University of New Mexico Center for Advanced Research Computing, supported in part by the National Science Foundation, for providing high performance computing resources used for this work; Science and Technology Facilities Council (Agreement No. 4163192 Release #3); ARCHIE-WeSt HPC, EPSRC grant EP/K000586/1; John von Neumann Institute for Computing (NIC) on JUROPA at Jülich Supercomputing Centre (JSC), project HHH20. The authors acknowledge helpful discussions with L. Giannessi.

REFERENCES

[1] W. Fawley, "Algorithm for loading shot noise microbunching in multidimensional, free-electron laser simulation codes", *Phys. Rev. ST Accel. Beams* 5, 070701 (2002), doi.org/10.1103/PhysRevSTAB.5.070701

[2] S. Reiche, "GENESIS 1.3: a fully 3D time-dependent FEL simulation code", *Nucl. Instrum. Methods Phys. Res.* A 429, 243 (1999). doi:10.1016/S0168-9002(99)00114-X

[3] E.L. Saldin, E.A. Schneidmiller, and M. Yurkov, "FAST: a three-dimensional time-dependent FEL simulation code", *Nucl. Instrum. Methods Phys. Res.* A 429, 233 (1999). doi:10.1016/S0168-9002(99)00110-2

[4] H.P. Freund, S.G. Biedron, and S.V. Milton, "Nonlinear harmonic generation in free-electron lasers", *IEEE J. Quantum Electron* 26, 275 (2000). doi:10.1109/3.825873

[5] H.P. Freund, P.J.M. van der Slot, D. Grimminck, I. Setya, and P. Falgari, "Three-dimensional, time-dependent simulation of free-electron lasers with planar, helical, and elliptical undulators", *New J. Phys.* 19, 023020 (2017). 10.1088/1367-2630/aa59f1

[6] L.T. Campbell and B.W.J. McNeil, "Puffin: A three dimensional, unaveraged free electron laser simulation code", *Phys. Plasmas* 19, 093119 (2012). doi:10.1063/1.4752743

[7] L.T. Campbell, J.D.A. Smith, and P. Traczykowski, "An Updated Description of the FEL Simulation Code Puffin", in *Proc. 9th Int. Particle Accelerator Conf. (IPAC'18)*, Vancouver, Canada, Apr.-May 2018, pp. 4579–4582. doi:10.18429/JaCoW-IPAC2018-THPMK112

[8] B.W.J. McNeil, M.W. Poole, and G.R.M. Robb, "Unified model of electron beam shot noise and coherent spontaneous emission in the helical wiggler free electron laser", *Phys. Rev. ST Accel. Beams* 6, 070701 (2003), doi:10.1103/PhysRevSTAB.6.070701

[9] L. Giannessi *et al.*, "Self-amplified spontaneous emission for a single pass free-electron laser", *Phys. Rev. ST Accel. Beams* 14, 060712 (2011), doi:10.1103/PhysRevSTAB.14.060712

[10] M. Xie, "Design optimization for an x-ray free electron laser driven by the SLAC linac", *in Proc. IEEE 1995 Particle Accelerator Conference*, Vol. 183, IEEE Cat. No. 95CH35843 (1995).