

# THREE-DIMENSIONAL, TIME-DEPENDENT SIMULATION OF FREE-ELECTRON LASERS

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## Abstract

Simulation codes modeling the interaction of electrons with an optical field inside an undulator are an essential tool for understanding and designing free-electron lasers (FELs). A new code under development, named MINERVA, uses a modal expansion for the optical field. A Gaussian expansion is used for free-space propagation, and an expansion in waveguide modes for fully guided propagation, or a combination of the two for partial guiding at THz frequencies. MINERVA uses the full Newton-Lorentz force equation to track the particles through the optical and magnetic fields. We describe the main features of MINERVA, and show comparisons between simulations and experiments conducted using the LCLS.

## INTRODUCTION

Simulation codes modeling the interaction of electrons with an optical field inside an undulator are an essential tool for understanding and designing free-electron lasers (FELs). As there exists a large variety of FELs ranging from long-wavelength oscillators using partial wave guiding to single-pass soft and hard x-ray FELs that are either seeded or starting from noise (*i.e.*, Self-Amplified Spontaneous Emission or SASE), a simulation code should be capable of modeling this huge variety of FEL configurations. A new code under development, named MINERVA, is capable of modeling such a large variety of FELs. The code uses a modal expansion for the optical field including a Gaussian expansion for free-space propagation, or an expansion in waveguide modes for fully-guided propagation, or a combination of the two for partial guiding, which is typically used at THz frequencies. MINERVA uses the full Newton-Lorentz force equations to track the particles through the optical and magnetic fields. Here we describe the main features of MINERVA and compare simulations with experiments conducted using the LCLS at SLAC.

A variety of different free-electron laser (FEL) simulation codes have been developed over the past several decades such as GINGER [1], MEDUSA [2], TDA3D [3], and GENESIS [4], among others. These codes typically undergo continuous development over their usable lifetimes. As a result, the codes become increasingly complex as new capabilities are added or

older capabilities are deleted, and this tends to compromise their performance. It also renders it increasingly more difficult to make further modifications that might be needed. Because of this, we decided to develop a new code using a “clean-slate” approach having the properties and characteristics that we desired.

## SIMULATION PROPERTIES

The formulation used in MINERVA describes the particles and fields in three spatial dimensions and includes time dependence as well. Electron trajectories are integrated using the complete Newton-Lorentz force equations. No wiggler-averaged-orbit approximation is made. The magnetostatic fields can be specified by analytical functions for a variety of analytic undulator models (such a planar or helical representations), quadrupoles, and dipoles. These magnetic field elements can be placed in arbitrary sequences to specify a variety of different transport lines. As such, MINERVA can set up field configurations for single or multiple wiggler segments with quadrupoles either placed between the undulators or superimposed upon the undulators to create a FODO lattice. Dipole chicanes can also be placed between the undulators to model various optical klystron and/or high-gain harmonic generation (HG) configurations. A variety of undulator models is available, including: (1) either flat- or parabolic-pole-face planar undulators, (2) helical undulators, and (3) a representation of an APPLE-II undulator that can treat arbitrary elliptic polarizations. The fields can also be imported from a field map.

The electromagnetic field is described by a modal expansion. For free-space propagation, MINERVA uses Gaussian optical modes, while waveguide modes are used when the wavelength is comparable to the dimensions of the drift tube. As a result, MINERVA can treat both long and short wavelength FELs. A combination of the Gaussian and waveguide modes is also possible when there is partial guiding at, for example THz frequencies.

The electromagnetic field representations are also used in integrating the electron trajectories, so that harmonic motions and interactions are included in a self-consistent way. Further, the same integration engine is used within the undulator(s) as in the gaps, quadrupoles, and dipoles, so that the phase of the optical field relative to the electrons is determined self-consistently when propagating the particles and fields in the gaps between the undulators.

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Particle loading is done in a deterministic way using Gaussian quadrature that preserves a quiet start for both the fundamental and all harmonics. Shot noise is included using the usual Poisson statistics algorithm [5] so that MINERVA is capable of simulating SASE FELs; however, provision is made for enhanced shot-noise due to various levels of micro-bunching.

MINERVA has also been linked to the Optics Propagation Code (OPC) [6, 7] for the simulation of FEL oscillators or propagating an optical field beyond the end of the undulator line to a point of interest. We focus in this paper on the simulation of the LCLS SASE FEL so we will not discuss the coupling between MINERVA and OPC further, but this will appear in future papers.

MINERVA is written in Fortran 95 using dynamic memory allocation and supports parallelization using the Message Passing Interface. The memory allocated for a given simulation run is determined by the needs for a specific configuration. Since the field is described by a discrete set of wave modes characterized by distinct amplitudes, the description of the field requires relatively little memory. The principal demand on memory is, therefore, determined by the number of particles in the simulation but the amount of memory required is relatively modest for most cases studied to date.

Table 1: Parameters of the LCLS FEL Experiment

Electron Beam	
Energy	13.64 GeV
Bunch Charge	250 pC
Bunch Duration	83 fsec
Peak Current	3000 A (flat-top)
$x$ -Emittance	0.4 mm-mrad
$y$ -Emittance	0.4 mm-mrad
rms Energy Spread	0.01%
rms Size ( $x$ )	215 microns
$\alpha_x$	1.1
$\beta_x$	30.85 m
rms Size ( $y$ )	195 microns
$\alpha_y$	-0.82
$\beta_y$	25.38 m
Undulators	
Period	3.0 cm
Length	113 Periods
Amplitude (1 <sup>st</sup> segment)	12.4947 kG
$K_{rms}$ (1 <sup>st</sup> segment)	2.4748
Taper Slope	-0.0016 kG
Gap Length	0.48 m
Quadrupoles	
Length	7.4 cm
Field Gradient	4.054 kG/cm

### THE LCLS SASE FEL

The LCLS [8] is a SASE FEL user facility that became operational in 2009 and operates at a 1.5 Å wavelength. The fundamental operating parameters are listed in Table 3. It employs a 13.64 GeV/250 pC electron beam with a

flat-top temporal pulse shape of 83 fsec duration. The normalized emittance ( $x$  and  $y$ ) is 0.4 mm-mrad and the rms energy spread is 0.01%. The undulator line consisted of 33 segments with a period of 3.0 cm and a length of 113 periods including one period each in entry and exit tapers. A mild down-taper in field amplitude of -0.0016 kG/segment starting with the first segment (which has an amplitude of 12.4947 kG and  $K_{rms} = 2.4748$ ) and continuing from segment to segment of was used to compensate for energy loss due to Incoherent Synchrotron Radiation (ISR). This is referred to as a “gain taper”. The electron beam was matched into a FODO lattice consisting of 32 quadrupoles each having a field gradient of 4.054 kG/cm and a length of 7.4 cm. Each quadrupole was placed a distance of 3.96 cm downstream from the end of the preceding undulator segment. The Twiss parameters for this FODO lattice are also shown in Table 1.

The LCLS produces pulses of about 1.89 mJ at the end of the undulator line, and saturation is found after about 60 m. A comparison between the measured pulse energies (green circles) and the simulation (blue) is shown in Fig. 1. The data is courtesy of H.-D. Nuhn and P. Emma at SLAC, and the simulation results represent an average over an ensemble of runs performed with different noise seeds. As shown in the figure, the simulations are in good agreement with the measurements and with each other in the start-up and exponential growth regions. The simulation exhibits saturation where the exponential gain regime ends after 60 m at a pulse energy of 1.5 mJ. However, the pulse energy grows more slowly to about 1.92 mJ after 110 m, which is in good agreement with the measurements.

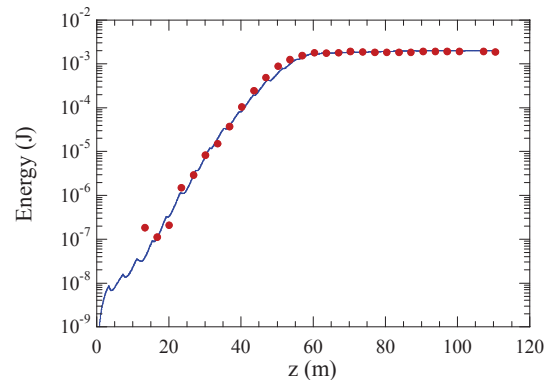


Figure 1: Comparison between experimental data (red circles) from the LCLS (data courtesy of P. Emma and H.-D. Nuhn) and simulation (blue).

Experiments have also been performed at the LCLS [9] to investigate enhancing the efficiency using a tapered undulator. This taper is referred to as the “saturation taper”. Saturation in an FEL occurs when the bulk of the electrons become trapped in the ponderomotive wave formed by the beating of the undulator and radiation fields. At that point the electrons have lost energy and dropped out of resonance with the wave. The tapered undulator has the effect of accelerating the electrons in

the axial direction and maintaining the resonance over an extended length [10]. Comparisons between tapered undulator amplifiers and simulation have demonstrated good agreement and high efficiencies [11]. Comparison between the use of tapered undulators in a seeded amplifier and an equivalent SASE FEL shows that while the efficiency enhancement is lower in the SASE FEL, substantial efficiency enhancements are possible [12].

The LCLS configured with a stronger taper for the last segments has demonstrated such enhancements in the efficiency [9]. This experiment employed an undulator in which the aforementioned mild linear down-taper is enhanced by the addition of a more rapid down-taper starting at the 14<sup>th</sup> undulator segment. The experimental taper profile is shown in Fig. 2 (data courtesy of D. Ratner).

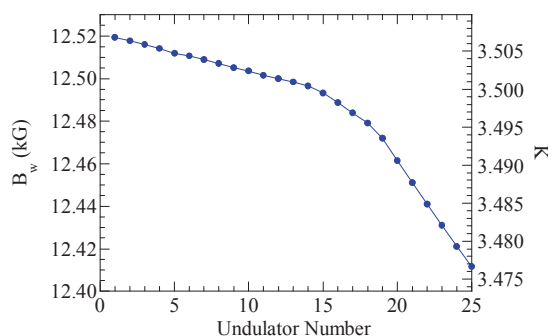


Figure 2: The experimentally applied saturation taper profile (courtesy of D. Ratner).

In comparison with the undulator and electron beam properties employed in the first lasing experiments, the tapered undulator experiment employed undulators tuned to somewhat different field strengths and an electron beam parameters that may have varied from the initial experiments. The pulse energies in the experiment were obtained by measuring the energy loss in the electron beam. Simulations were conducted over a parameter range including emittances of 0.40 mm-mrad – 0.45 mm-mrad and energy spreads of 0.010% – 0.015% that are thought to characterize the electron beam.

A comparison between the measured pulse energies and simulations over the parameter range that most closely agree with the experiment is shown in Fig. 3, where the experimental results are shown in red. Observe that the maximum pulse energy shown represents a substantial enhancement over that reported in the first lasing experiment. The simulation results represent averages over many noise seeds. As is evident from the figure, the simulations for the three choices are all very similar and are in good agreement with the measurements, indicating that the efficiency enhancement could be achieved for a variety of electron beam parameters.

### SUMMARY AND CONCLUSION

As shown in the paper, the current state of development of MINERVA yields good agreement for the experiments studied using the LCLS at SLAC. Consequently, we feel

that MINERVA can accurately, and with confidence, predict the performance of short wavelength FELs.

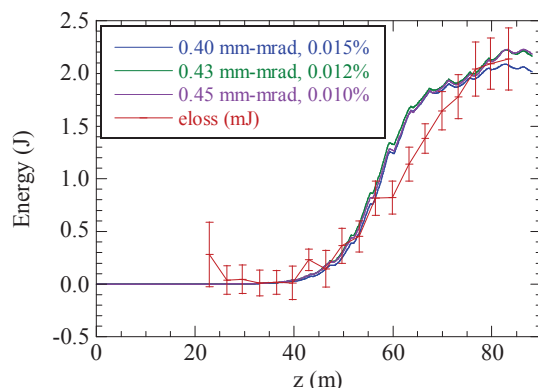


Figure 3: Comparison between the experimental data (red) and simulations for a variety of emittances and energy spreads (data courtesy of D. Ratner).

MINERVA is currently in beta-test and development will continue. At present, the inclusion of waveguide modes is under development that will permit the simulation of long wavelength THz FELs. In addition, several techniques necessary to import particles from beam generation and tracking codes and to export particles to these beam generation and tracking codes for start-to-end simulations are being developed including both statistical algorithms and the direct importation of particles on a one-to-one basis. These developments will be reported in future publications.

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