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START-TO-END SIMULATION OF FREE-ELECTRON LASERS

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Abstract

Start-to-end (S2E) modeling of free-electron lasers (FELs) normally requires the use of multiple codes to correctly capture the physics in each region of the machine. Codes such as PARMELA, IMPACT-T or MICHELLE, for instance, may be used to simulate the injector. From there the linac and transport line may be handled by codes such as DIMAD, ELEGANT or IMPACT-Z. Finally, at the FEL a wiggler interaction code such as GENESIS, GINGER, or MINERVA must be used. These codes may be optimized to work with a wide range in magnitude of macro-particle numbers (from 10^4-10^8 in different codes) and have different input formats. It is therefore necessary to have translator codes to provide a bridge between each section. It is essential that these translators be able to preserve the statistical properties of the bunch while raising or lowering the number of macro-particles used between codes. In this work we show a suite of such translators designed to facilitate S2E simulations of an FEL with a new wiggler code, MINERVA, and use these codes to provide benchmarking of MINERVA against other common wiggler simulation codes.

INTRODUCTION

The simulation of an FEL including the injector, linac, beam transport, and undulator requires modeling of the electron beam in a variety of regimes, all of which have differing dominant effects. To accurately perform these start-to-end simulations it is normally necessary to use of variety of codes, each of which is adapted to accurate simulation in a particular regime. It is therefore necessary to be able pass the beam distribution from one code onto another. Unfortunately, these codes often use a variety of conventions for representing the distribution and in the case of macro-particle based codes there is often great disparity in the number of macro-particles necessary for effective simulation. In this paper we describe a set of software tools built to provide translation between the particle tracking codes PARMELA [1], DIMAD [2], and ELEGANT [3] to the undulator simulation code MINERVA [4]. In particular we look at the use of an ELEGANT output to perform an FEL simulation in MINERVA.

MINERVA

MINERVA is a new FEL code under development capable of modeling a large range of FEL configurations, including seeded and self-amplified spontaneous emission (SASE) amplifiers and FEL oscillators (through interface with the optical propagation code OPC [5]). 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. 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.

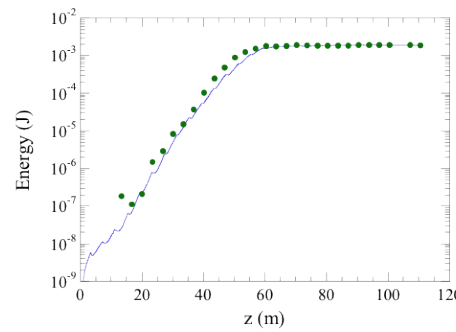

Figure 1: Comparison between experimental data for the LCLS (Green dots) and simulation in MINERVA (blue line).(LCLS data courtesy of P. Emma and H.-D. Nuhn.)

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 [6] so that MINERVA is capable of simulating SASE FELs; however, provision is made for enhanced shot-noise due to various levels of micro-bunching.

Shown in Fig. 1 is a comparison between measured and simulated pulse energies for the LCLS SASE FEL. The simulation results represent an average over an ensemble of runs performed with different noise seeds

ELEGANT

The code ELEGANT, ELEctron Generation And Tracking is a macro-particle code that can track particles in 6-D phase space using matrices, canonical-kick elements, numerically integrated elements, or a combination of techniques [3]. Of particular importance to linac-based FEL design, ELEGANT includes a 1-D coherent synchrotron radiation (CSR) model [7]. This allows for modeling the impact of CSR in the

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dipoles of bunch compression chicanes. ELEGANT also includes models for the interaction of CSR with the beam downstream of the dipole, which can be critical to fully capturing the impact of CSR in beam dynamics. In addition to CSR, ELEGANT can model a variety of other effects such as wakefields, intra-beam scattering, longitudinal space charge and includes a robust optimization package. There is, however, no full space charge model in ELEGANT so it cannot be used for tracking low energy beams.

The output files for ELEGANT utilize the so-called Self Describing Data Set (SDDS) format [8]. A wide variety of programs, the SDDS Toolkit, can then be used to modify, process, and analyze the data. This standardized output aids in making conversion of output distributions to other formats much easier.

TRANSLATOR

Ideally, it would be imagined that the translator would merely need to convert between units and file formats between any codes. Unfortunately, this is not the case when moving from an accelerator code to MINERVA. In the FEL interaction simulation the beam will be broken down into many slices in time, each a wavelength long. Each of these slices must contain enough particles for the FEL simulation to reach convergence. Due to computational constraints it is often necessary to space these slices several wavelengths apart. As an example consider the Linac Coherent Light Source (LCLS) [9]. With a wavelength of around 1.5 Å and bunch length of 74 ps this results in $1.5x10^5$ slices necessary. If every slice must have 8,000 macro-particles then there would be a total of 10^9 macro-particles for a simulation with contiguous slices. Another factor for the FEL codes is that they begin with a quiet-start distribution that would generate no amplification without some seed power. Some routine is then used to introduce jitter into the distribution that will create shot-noise that follows the correct Poisson statistics [10, 11]. Because of these two factors we do not port the macro-particle distribution directly into the FEL code. Rather the second-order moments of the beam and other statistical properties are extracted and passed to the FEL code instead. The procedure for doing this is described in the following section.

Translator Routine

Beam distribution files from ELEGANT consist of a header giving information about the contents of the file, a list of parameters with beam properties, and array data for the 6-D phase space coordinates of the particles. The translator, written in Fortran 95, begins by analyzing the contents of the header to find the structure of the file so it can pull all relevant parameters and the coordinate array. Allowance is made for unknown parameters as the file may have been modified by the SDDS Toolkit, though certain parameters are expected such as total bunch charge and central energy. Once the coordinate array has been read in it is converted to MINERVA's unit convention (see Table. 1).

Table 1: Coordinate Descriptions for ELEGANT and MINERVA. ELEGANT treats particles at t < 0 as the head while MINERVA follows the reverse convention.

Quantity	ELEGANT	MINERVA
x-position (x)	m	cm
x-momentum (x')	$\frac{p_x}{p_z}$	$\frac{p_x}{m_e c}$
y-position (y)	m	cm
y-momentum (y')	$\frac{p_x}{p_z}$	$\frac{p_x}{m_e c}$
t-position (t)	s	-s
Energy (E)	p_{total} $(m_e c)$	$\frac{p_z}{m_e c}$ and E_{total} (MeV)

The translator does not directly provide this coordinate data to MINERVA but rather will use it to extract statistical properties for the bunch. First the bunch is split into a specified number of equally-spaced, axial bins. Since each macro-particle in the bunch has the same charge weight extracting the statistical properties of each bin is straightforward. From this the charge, current, and energy of the bunch may be found. The relative energy spread is given by $\sigma_E = \sqrt{\langle (E - \langle E \rangle)^2 \rangle} / \langle E \rangle$ and the rms beam sizes by $\sigma_x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$ and $\sigma_y = \sqrt{\langle (y - \langle y \rangle)^2 \rangle}$ in x and y respectively. The emittances and Twiss parameters are calculated from equations (1) - (8).

$$\epsilon_x = \sqrt{\langle x - \langle x \rangle \rangle^2 \langle x' - \langle x' \rangle \rangle^2 - \langle (x - \langle x \rangle)(x' - \langle x' \rangle) \rangle^2} \quad (1)$$

$$\epsilon_y = \sqrt{\langle y - \langle y \rangle \rangle^2 \langle y' - \langle y' \rangle \rangle^2 - \langle (y - \langle y \rangle)(y' - \langle y' \rangle) \rangle^2} \quad (2)$$

$$\alpha_x = \frac{-\langle (x - \langle x \rangle)(x' - \langle x' \rangle) \rangle}{\epsilon_x} \quad (3)$$

$$\alpha_y = \frac{-\langle (y - \langle y \rangle)(y' - \langle y' \rangle) \rangle}{\epsilon_y} \quad (4)$$

$$\beta_x = \frac{\langle (x - \langle x \rangle)^2}{\epsilon_x} \quad (5)$$

$$\beta_y = \frac{\langle (y - \langle y \rangle)^2}{\epsilon_y} \quad (6)$$

$$\gamma_x = \frac{\langle (x' - \langle x' \rangle)^2}{\epsilon_x} \quad (7)$$

$$\gamma_y = \frac{\langle (y' - \langle y' \rangle)^2}{\epsilon_y} \quad (8)$$

This bin data is then passed on to MINERVA which uses the statistics to create its own distribution at run time. This method assumes that the beam may be well represented by the 2nd-order statistical properties. Obviously if this is not the case the bunch distribution passed to MINERVA may not be a fully accurate representation of the actual bunch.

RESULTS

Here we show comparison between output of a beam distribution created in ELEGANT and the distribution processed by the translator. The beamline is representative of a typical

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FEL design, consisting of an rf linac accelerating section, a higher-order mode linearization cavity, and a magnetic compression chicane. Quadrupoles are used throughout to provide appropriate focusing. The beam distribution in phase space and the transverse cross section as output from ELEGANT is show in Fig. 2. Some of the slice properties calculated from the translator and compared to calculations from ELEGANT are shown in Figs. 3 - 5.

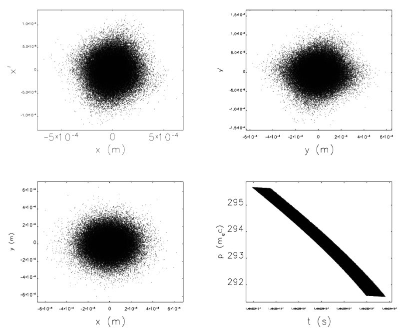

Figure 2: Beam distribution at entrance to the wiggler. Generated from ELEGANT.

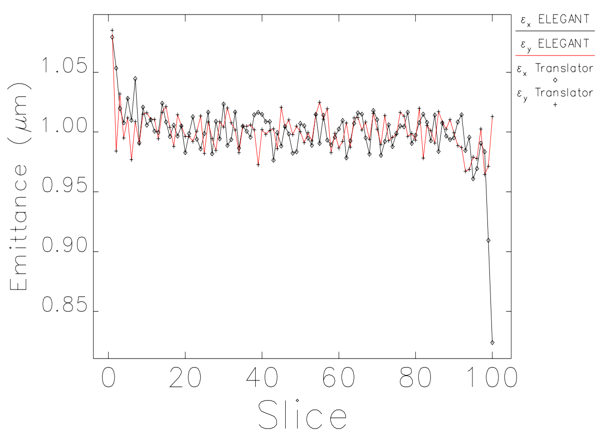

Figure 3: The x-emittance ϵ_x and y-emittance ϵ_y as calculated per slice by the translator and by ELEGANT.

CONCLUSION

We have demonstrated a translator program for converting beam outputs from Parmela, DIMAD, and ELEGANT to the FEL code MINERVA. An example of a bunch distribution from ELEGANT and converted to the MINERVA input format shows that all relevant statistic are correctly preserved in the translation. Use of this translator will aid in completing full start-to-end simulations of FELs using MINERVA code.

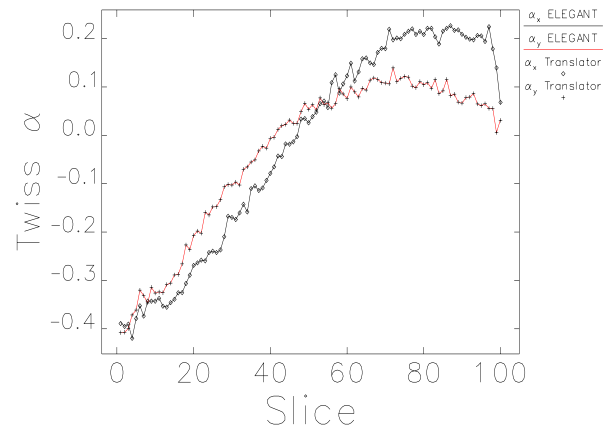

Figure 4: The Twiss α function in x and y as calculated per slice by the translator and by ELEGANT.

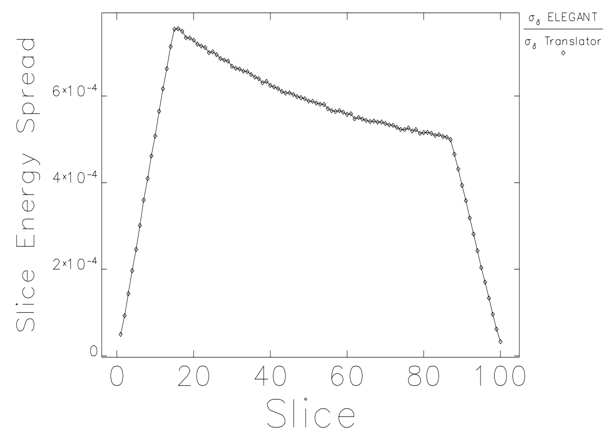

Figure 5: The the slice energy spread σ_δ as calculated per slice by the translator and by ELEGANT.

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