

BENCHMARK OF RF PHOTOINJECTOR AND DIPOLE USING ASTRA, GPT, AND OPAL*

N. R. Neveu^{†1}, L. K. Spentzouris, Illinois Institute of Technology, Chicago, USA

J. G. Power,¹ Argonne National Laboratory, Argonne, USA

P. Piot², Fermi National Accelerator Laboratory, Batavia, USA

²Department of Physics and Northern Illinois Center for Accelerator & Detector Development, Northern Illinois University, DeKalb, USA

C. Metzger-Kraus, Helmholtz-Zentrum Berlin, Berlin, Germany

S. J. Russell, Los Alamos National Laboratory, Los Alamos, USA

A. Adelman, Paul Scherrer Institut, Villigen, Switzerland

G. Ha, POSTECH, Pohang, South Korea

Abstract

With the rapid improvement in computing resources and codes in recent years, accelerator facilities can now achieve and rely on accurate beam dynamics simulations. These simulations include single particle effects (e.g. particle tracking in a magnetic field) as well as collective effects such as space charge (SC), and coherent synchrotron radiation (CSR). Using portions of the Argonne Wakefield Accelerator (AWA) as the benchmark model, we simulated beam dynamics with three particle tracking codes. The AWA rf photoinjector was benchmarked, primarily to study SC, in ASTRA, GPT, and OPAL-T using a 1 nC beam. A 20° dipole magnet was used to benchmark CSR effects in GPT and OPAL-T by bending a 1nC beam at energies between 2 MeV and 100 MeV. In this paper we present the results, and discuss the similarities and differences between the codes.

INTRODUCTION

The AWA group has used several beam codes in the past including: T-STEP/PARMELA [1], ASTRA [2], and GPT [3]. In order to take advantage of computing resources offered by Argonne National Laboratory (ANL), an effort was made to investigate OPAL [4], an open source and parallel code that comes in two flavours; OPAL-CYL and OPAL-T. The latter was installed on the Blues cluster at the Laboratory Computing Resource Center (LCRC) provided by ANL [5]. Since no members of AWA had experience with OPAL-T, this benchmark was done to compare results to GPT and ASTRA.

There are three main collective effects of interest to the AWA: SC, CSR, and wakefields. The AWA facility houses a 70 MeV RF photoinjector [6] with a large dynamic range: 20 pC to 100 nC. In many cases, the beam is SC dominated. In the AWA's Emittance Exchange (EEX) beamline [7], CSR has a large effect on the beam as it passes through the dipoles, and wakefields are present in the two beam acceleration (TBA) beam line [8]. ASTRA, GPT, and OPAL-T are capable of simulating 3D SC, and wakefield effects. The latter two codes also include a CSR model, making them a good fit for the AWA.

* Work supported by DE-SC0015479 and DE-AC02-06CH11357

[†]nneveu@hawk.iit.edu

CODE COMPARISON

ASTRA, GPT, and OPAL-T are capable of modelling RF photoinjectors, linacs, and XFEL beamlines (excluding undulators). There are also several differences between the codes, some of which are listed in a short comparison of code features done in Table 1.

Table 1: Features of ASTRA, GPT, and OPAL-T

Feature	GPT	OPAL-T	ASTRA
Runs on Windows	Yes	No	Yes
Runs on Mac	Yes	Yes	Yes
Runs on Linux	Yes	Yes	Yes
Open Source	No	Yes	No
Parallel	Yes	Yes	No#
Autophase	No	Yes	Yes
Adaptive Time Step	Yes	No	No
3D SC Algorithm	Yes	Yes	Yes
1D CSR Algorithm	Yes*	Yes	No
Wakefield Algorithm	Yes*	Yes	Yes

*In-house modules added to the AWA version of GPT

#A parallel version is available from DESY

Although, CSR and wakefield algorithms do not come in the standard installation of GPT, users can install modules as needed. A CSR routine was written by the authors of [9] and ported to the windows version of GPT for use at the AWA. A wakefield module was also written. It is based on the model in ELEGANT [10].

SIMULATION OF THE GUN

The SC algorithms were probed using the AWA photoinjector, a 1.5 cell copper standing-wave cavity at 1.3 GHz, with bucking, focusing, and matching solenoids. The rf gun and solenoid fields seen by the beam are shown in Fig. 1. Note, in the remainder of this paper, the word gun is used in place of photoinjector.

The simulation parameters were chosen to approximately generate the canonical “1 μm at 1 nC” case. The initial beam parameters were based on gun operations at PITZ [11], due to the similarities between the PITZ and AWA rf guns. The PITZ parameters came close to achieving the 1 μm target without any optimization. A coarse 1D minimization of the emittance was done to

determine the value of the laser radius used in this benchmark. The resulting minimum emittance was $1.16 \mu\text{m}$.

A genetic and multi-objective optimizer was not used in any of the codes. A multi-objective genetic optimizer may have been able to achieve a lower minimum emittance by varying the laser radius and matching solenoid simultaneously. OPAL developers plan to implement an optimizer in their next release [12]. GPT comes packaged with a built in optimizer, and all three codes can be used with external optimizers.

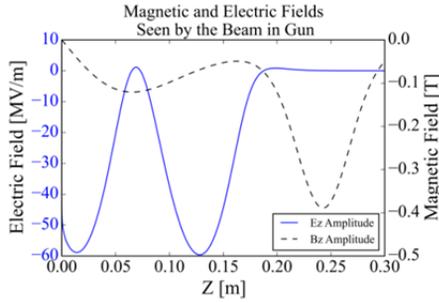


Figure 1: Magnet and electric fields in the gun.

The initial bunch distribution parameters as well as the on-axis gun gradient (E_z) and magnetic field (B_z) used in the benchmark are listed in Table 2. The rf gun and solenoid field maps were generated with the SUPERFISH/POISSON codes [13]. The gradient was chosen to match typical operations at PITZ [11] and the AWA. Note that the codes use various methods to model the rf and magnetic fields, SC, and image charge.

Table 2: Input Parameters

Parameter	Value
Charge	1 nC
Laser Radius	0.75 mm
Rise and Fall Time	6 ps
Flattop FWHM	20 ps
Phase	On Crest (Max Energy)
Kinetic Energy at Cathode	0.55 eV
Gradient on Cathode	60 MV/m
Buck and Focusing	-0.12 Tesla
Matching	-0.389 Tesla

The ASTRA simulations used the axial E field of the gun and solenoids, and then expanded the fields to find the transverse components using the paraxial approximation (e.g. $E_r = -\frac{r}{2} \frac{dE_z}{dz}$). The simulations used a 2D cylindrical-symmetric SC algorithm with a uniform particle-deposition mesh; see ASTRA user manual pg. 8 [2]. The radial and longitudinal number of cells composing the mesh were taken to $N_r = 32$ and $N_z = 64$ respectively with 100k particles. The image charge close to the cathode was accounted for until the bunch reached 9.7-cm from the cathode surface.

GPT read in the 2D electric and magnetic field files, and used a square 3D adaptive SC mesh of $N_x = N_y = N_z = 46$ with 100k particles, see spacecharge3Dmesh option in GPT manual pg. 132 [3]. To calculate image

charge, GPT uses a Dirichlet boundary condition at the cathode ($z=0$). The calculation is turned off when the distance between the beam and cathode is longer than the mesh box.

OPAL-T also read in the field maps, and used a block structured equidistant SC mesh, see OPAL manual pg. 27 for SC calculation [4]. Several square mesh sizes were run, the results plotted in Fig. 2 and 3 correspond to a mesh of $N_x = N_y = N_z = 46$ with 1 million particles. The image charge calculation uses a shifted integrated Green function [14].

In general, the simulation results are in reasonable agreement and within expectations based on previous benchmarks [15]. See Figs. 2 and 3 for beam envelopes in the gun and drift. The apparent disagreement of emittance between ASTRA and the other two codes in the gun is because the former removes the angular momentum induced by the solenoid, while the later two codes do not. After the beam exits the solenoid, the emittance results are in good agreement, as shown in Fig. 3.

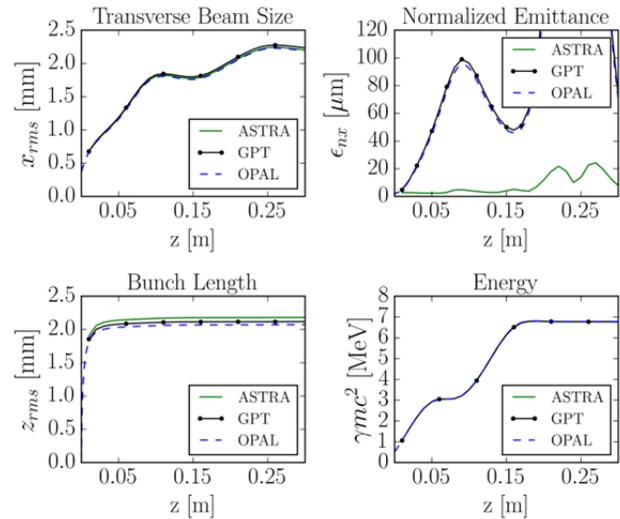


Figure 2: Beam envelopes in the gun.

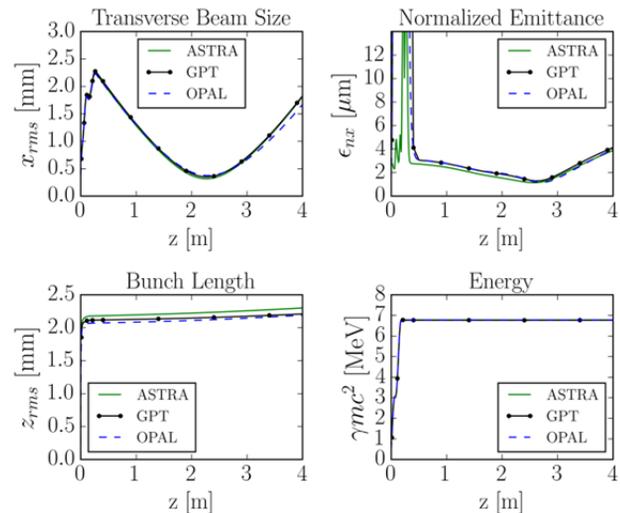


Figure 3: Beam envelopes in drift.

DIPOLE SIMULATIONS

Simulations of a hard edge dipole were done in GPT and OPAL-T in order to probe CSR. Short mono-energetic Gaussian bunches with zero initial emittance were sent through the dipole. Beam and dipole parameters are shown in Table 3.

The CSR routine used in OPAL-T is based on the routine used in ELEGANT [8], which is known to assume the beam is ultra-relativistic. The CSR routine in GPT does not use the ultra-relativistic approximation ($\beta=1$) and as a result, works at all energies [9]. Therefore, we expected the routines to match well at high energy and diverge at lower energy. Results of the CSR simulations are shown in Fig. 4. As expected, the results between GPT and OPAL-T disagree at low energies.

Table 3: Parameters for CSR Simulations

Parameter	Value
X & Y RMS	1.0 mm
Z RMS	0.3 mm
Dipole Length	0.3 m
Bending Angle	20°
Energy:	2 MeV to 100 MeV

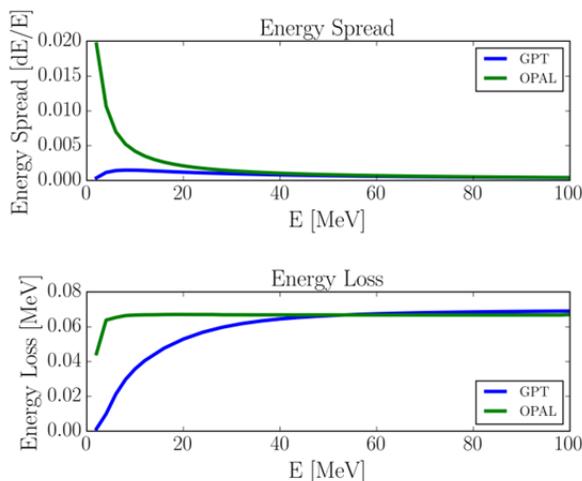


Figure 4: Energy spread and loss due to CSR.

OPAL CONVERGENCE STUDIES

Convergence runs were done for three parameters: time step, SC mesh size, and number of particles. Each case was tested in the gun using the same field maps and baseline settings that were used to compare SC in OPAL-T, ASTRA, and GPT. All OPAL-T simulations were run on 16 cores, taking advantage of parallel calculations.

The number of particles was varied from 20k to 3.2 million. The longitudinal parameters (energy, bunch length) showed no variation, but there were slight deviations in the transverse emittance and beam size. The same results were observed when the time step was varied from 0.1 to 10 ps. The grid size was changed from 32, 44, 46, and 64 cubed; again the results lacked any major discrepancies. In all cases, no appreciable differences were observed in the energy, emittance, beam size, or bunch length. In most cases, if unreasonable parameters were

chosen, OPAL-T would not complete the run (crash or hang up).

CONCLUSION

Based on the experience gained during this benchmark, all three codes are capable of accurate simulations. With respect to resources at the AWA, GPT and ASTRA are better suited for use on windows, and OPAL-T is better suited to Linux and parallel systems.

ACKNOWLEDGMENT

We gratefully acknowledge the computing resources provided on Blues, a high-performance computing cluster operated by the LCRC at Argonne National Laboratory.

This work was funded by the Department of Energy under the grant no. DE-SC0015479, and by the Office of Science Graduate Student Research (SCGSR) program, which is under contract number DE-SC0014664. The work by the AWA group is funded through the U.S. Department of Energy Office of Science under Contract No. DE-AC02-06CH11357.

REFERENCES

- [1] L. M. Young, "PARMELA," Los Alamos National Laboratory report LA-UR-96-1835 (Revised April 22, 2003).
- [2] *ASTRA Manual*, April 2014, http://www.desy.de/~mpyflo/Astra_manual/Astra-Manual_V3.1.1.pdf
- [3] GPT, <http://www.pulsar.nl/gpt/>
- [4] A. Adelman and A. Gsell (PSI), T. Kaman (UZH), C. Metzger-Kraus (HZB), Y. Ineichen (IBM), S. J. Russell (LANL), C. Wang and J. Yang (CIAE), S. Sheehy and C. Rogers (RAL), D. Winklehner (MIT), "The OPAL (Object Oriented Parallel Accelerator Library) Framework", Paul Scherrer Institut, Rep. PSI-PR-08-02, 2008-2016.
- [5] LCRC, <https://www.lcrc.anl.gov>
- [6] M. Conde *et al.*, in *Proc. of NAPAC'16*, paper TUA21002.
- [7] G. Ha *et al.*, in *Proc. of IPAC'16*, pp. 1065-67.
- [8] M. Conde *et al.*, in *Proc. of IPAC'15*, pp. 2472-24.
- [9] I. V. Bazarov and T. Miyajima, in *Proc. of EPAC'08*, pp. 118-120.
- [10] *User's Manual for ELEGANT*, http://www.aps.anl.gov/Accelerator_Systems_Division/Accelerator_Operations_Physics/manuals/elegant_latest/elegant.pdf
- [11] F. Stephan *et al.*, "Detailed characterization of electron sources yielding first demonstration of European X-ray Free-Electron Laser beam quality," *Phys. Rev. ST Accel. Beams*, vol. 13, p. 020704, Feb. 2010.
- [12] A. Adelman, private communication, Sept. 2016.
- [13] *Reference Manual for the POISSON/SUPERFISH Group of Codes*, Los Alamos Accelerator Code Group, Los Alamos National Laboratory document LA-UR-87-126, Jan. 1987.
- [14] J. Qiang, S. Lidia, R. D. Ryne and C. Limborg-Deprey, "Three-dimensional quasistatic model for high brightness beam dynamics simulation," *Phys. Rev. ST Accel. Beams*, vol. 9, p. 044204, April 2006.
- [15] C. Limborg *et al.*, in *Proc. of PAC'03*, pp. 3548-3550.