# **Simulation Issues for RF Photoinjectors**

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Abstract. Accurate simulation of radiofrequency photoinjector performance remains a challenge in predicting the performance of future linear colliders and next-generation light sources. Calculated performance consistently and significantly exceeds measured performance. This discrepancy can be traced to two principal sources: measurement uncertainty and unrealistic assumptions and approximations made in the numerical calculations. The dynamics involved make the calculation challenging: electrons are accelerated from rest to relativistic velocities in millimeters. Strong wakefield and space charge effects require that fields be accurately represented on very small distance scales over large volumes. These issues will be discussed, the results of detailed code-tocode comparisons for tracking and particle-in-cell codes will be shown, and recommendations for further tests and improvements will be made.

#### 1. Introduction

The RF photoinjector is an electron source that is widely used for particle accelerators and radiation sources. The ultimately performance of these devices is often directly linked to the beam quality produced by the electron source. Consequently, accurate simulation of photoinjector performance is an important part of designing and improving these devices.

Simulations have routinely predicted beam quality (in particular, the transverse emittance) that is significantly better than has been measured on real devices. There are two principal reasons for this: first, simulation codes make approximations of one kind or another and hence do not accurately reproduce the physics, and second, measurement uncertainty can be quite large for the figures-of-merit generally used to describe injector performance. It is the purpose of this paper to assess the importance of certain specific approximations made in a widely used tracking code, Parmela[1], and to discuss means for assuring that measurement and simulation are comparable.

Before proceeding with a discussion of the physics and simulation issues, it is worth commenting on the second source of the discrepancy, measurement uncertainty. Virtually all measures of beam quality from electron injectors depend on reducing a video image of the beam to statistical quantities. This image has added noise from dark current (field emission current not related to the photoemitted beam) and x-ray hits to the video system, resulting in bright pixels in the video image. Background image subtraction and despeckling algorithms generally are effective in dealing with these problems. However, the process of reducing the remaining beam profile to statistical quantities is generally

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either accomplished by computing RMS quantities directly or by least-squares-fitting a particular distribution (e.g. a Gaussian) to the measured profile. Both procedures make use of the squares of deviations—either from a mean or from the fitted curve—and are therefore quite sensitive to the outlying data points. This has led to a large collection of filtering techniques (thresholding, low pass filtering, and so on) to suppress the effects of outliers, through which a fair amount of subjectivity and variation can enter the measurements.

Two actions are recommended to aid in comparing experimental measurements to simulation, and in comparing data with other laboratories. First, the fitting procedures, including background subtraction, despeckling algorithms, baseline subtraction, filtering and fitting should be presented, in detail, together with the reduced data. Second, for comparison with simulation, the experimental measurement should be simulated in as much detail as is possible, and the simulated measurement compared against the actual measurement. Many simulation codes have canned algorithms for computing emittance, spot size, and so on, but these are often too idealized to be directly comparable. For example, if quadrupole scan emittance data is to be compared to simulation, beam propagation should be simulated at the same quad strengths used in the actual measurement and the simulated spot sizes compared with the actual data.

#### 2. Photoinjector Physics

The dynamics of rf photoinjectors pose a challenge to desktop-scale computer simulation for several reasons. The electron beam is produced essentially at rest by photoemission and accelerated in very strong electric fields ( $\sim 10^8$  V/m) to relativistic velocities in millimeters. Within this very short period of time, space charge forces rapidly expand the bunch by almost an order of magnitude in volume, resulting in rapid emittance growth in all dimensions. In addition, acceleration is so rapid that the image charges on the emission surface remain nearly fixed in position, viewed from the bunch reference frame, resulting in strong retarding forces on the emitted bunch. During this same period, the first emitted electrons are accelerated to a significant fraction of the speed of light before the last electrons are emitted giving rise to a time- and space-dependent focussing of the tail of the bunch from the induced magnetic field.

Rf photoinjectors produce short, dense bunches because the acceleration gradient is high enough that the electron bunch produced closely follows the spatial distribution of the laser pulse that produced it. The photoemission process is complicated by surface roughness effects and surface contaminants and is generally poorly understood and specific to each photoinjector cathode. Variations in emitted current density result in additional electrostatic potential energy being stored in the charge distribution than if the emission had been uniform, and this added energy generally results in increased emittance as the distribution evolves. Accurate determination of beam quality therefore depends on using measured current density functions for the cathode in question.

Alignment and harmonic content in the fields of the rf cavities and the external focussing system can also strongly impact performance. While simulating misalignment of components is routine, handling harmonic content requires 3D computations, is more troublesome, and is less frequently tackled.

## 3. Photoinjector Simulation

Numerous suitable codes exist for tracking and particle-in-cell simulation of rf photoinjectors. Parmela is the most widely used code for simulating rf guns, having been developed and extensively used at Los Alamos, and used in the design and analysis of the much-copied Brookhaven gun. It is presently used as the most detailed model for the LCLS gun[2], motivating this study. Published benchmarking of photoinjector codes is comparatively rare in the literature, and is a critical step to predicting performance.

Some of the more significant approximations made in Parmela include

- 1. Space charge forces are strictly electrostatic (test problem 1)
- 2. No wakefield effects are included except image charge effects on the cathode
- 3. Retardation effects are neglected (test problem 1)

In addition, common simulation practice often makes the following idealizations:

- 4. The microwave excitation in all cavities has the same amplitude
- 5. All injector components possess strictly axisymmetric, aligned fields (test problem 2)
- 6. Electron emission process is highly idealized (test problem 3)

In light of the strong velocity sheer present during emission, approximations (1) and (3) are invalid and were studied further. Approximation (1) has already received close attention in the context of electron beams in uniform motion[3] but not in the presence of large velocity sheer. Wakefield effects are also significant, but require detailed PIC modeling and will be studied and published in a subsequent paper. Field balance problems (4) have been studied and published elsewhere[4]. The approximation of rf cavity fields as axisymmetric (5) is also potentially significant and was studied. Nonuniform emission current density (6) has been studied with high spatial frequency checkerboard patterns[5] and measured laser profile data[6], and has been studied here from the vantage point of higher order mode content in the laser pulse.

Three test problems have been constructed to assess the impact of approximations (1), (3), (5), and (6). These problems are chosen to have parameters similar to the LCLS gun, but to be as abstracted and simple as possible, and in the case of test problem 1 to be amenable to fast, unambiguous calculation with very different simulation methods (e.g. tracking and PIC codes).

# 4. Test Problems with Results

### 4.1. Test problem 1: Electrostatic and Retardation-free approximations

The purpose of this problem is to test the electrostatic approximation of space charge forces and the influence of relativistic retardation effects during emission. This approximation is invalid in situations where the beam radiates (bends, strong quads), and at emission (where internal velocity sheer occurs, see Figure 1). This problem tests the latter circumstance.

Conceptually, the problem is similar to the emission process in the LCLS gun, but with rf effects suppressed by choosing a low working rf frequency. A bunched beam is emitted from a perfect conductor under a strong accelerating field and tracked until the mean velocity reaches  $\langle\beta\rangle=0.9$ . Radial RMS spot size, normalized emittance, bunch length, momentum spread, momentum/coordinate correlation function and  $\langle\beta\rangle$  are computed as a function of  $\langle z\rangle$ . Bunch space charge fields ( $E_z$ ,  $E_r$ ,  $B_\theta$ ) are plotted shortly after the entire bunch has been emitted.



**Figure 1.** Velocity sheer  $(\max(\beta_z)-\min(\beta_z))$  and mean bunch velocity  $<\beta_z>$  versus mean bunch position <z>.

The details of the problem are: an acceleration gradient of  $E_z=100$  MV/m (peak on cathode) is used, driven at 100 MHz. The electron bunch has a charge Q= 1nC, and is uniformly distributed in space and time in a 1 mm radius x 10 ps long cylinder. The beam is launched with 1 eV energy, strictly longitudinal, and is otherwise cold. (i.e. no transverse momentum, no energy spread) The beam is launched at the crest of the rf wave. No magnetostatic focussing fields are to be applied. Grid density and number of macroparticles should be chosen to achieve results that do not depend on the grid size or number of macroparticles.

Space charge fields are to be plotted at a single time ("snapshot fields") for the region around and within the bunch for PIC codes, and at the position of each macroparticle for tracking codes.  $E_r$ ,  $E_z$ , and  $B_\theta$  should be plotted as a function of z. Also, compute:  $\langle\beta\rangle$ ,  $\varepsilon_r$ ,  $\sigma_r$ ,  $\varepsilon_z$ ,  $\sigma_z$ ,  $\sigma_p$ , Corr(z,p), and  $\langle z \rangle$  every picosecond and record the 5D (or 6D) phase space when  $\langle\beta\rangle=0.9$ . Sums over the distribution are to be performed for all quantities taken at a single time ("snapshot" emittances), not a single z location. RMS definitions of all quantities are to be used:

$$\begin{split} \langle x \rangle &\equiv \sum_{i}^{N} q_{i} x_{i} / \sum_{i}^{N} q_{i} \\ \sigma_{r} &= \sqrt{\langle r^{2} \rangle - \langle r \rangle^{2}}, \mu_{r} = \langle r \rangle, \mu_{pr} = \langle p_{r} \rangle, p_{r} = \gamma \beta_{r} \\ \varepsilon_{r} &\equiv \sqrt{\langle (r - \mu_{r})^{2} \rangle \langle (p_{r} - \mu_{pr})^{2} \rangle - \langle (r - \mu_{r}) (p_{r} - \mu_{pr}) \rangle^{2}} \\ \sigma_{z} &= \sqrt{\langle z^{2} \rangle - \langle z \rangle^{2}}, \sigma_{p} = \sigma_{\gamma \beta_{z}} = \sqrt{\langle (\gamma \beta_{z})^{2} \rangle - \langle \gamma \beta_{z} \rangle^{2}} \\ Corr(z, p) &\equiv \langle z \gamma \beta_{z} \rangle / (\sigma_{z} \sigma_{p}) \end{split}$$

Results of this test problem are displayed in Figures 2 and 3 below. The Los Alamos version of Parmela (referred to here as "Parmela-lanl") and the UCLA version of

Parmela[6] (referred to here as "Parmela-ucla") are compared against Magic-2D[7] and Maxwell-T[8]. Space charge field strengths are displayed for Parmela-ucla and for Magic-2D in Figure 2. Particle tracking is completed for all four codes and is displayed in Figure 3.

There is good agreement of electric field strengths at the bunch extremities, but since Parmela uses the electrostatic approximation,  $B_{\theta}$  is zero everywhere, in stark contrast to the computed values shown from Magic-2D. Note that field plots from Magic-2D are plotted as functions of r and z, whereas fields from Parmela are plotted as functions of the macroparticle coordinates. The fields at the outer radius of the bunch compare reasonably well, with Magic-2D giving  $E_r \sim 6.3$  MV/m, and Parmela giving  $E_r \sim 5.9$  MV/m. The total space charge and image charge fields at the tail of the bunch also compare reasonable well, with Magic-2D giving  $E_z \sim 23.8$  MV/m, and Parmela  $E_z \sim 23$  MV/m. Magic-2D shows a maximum magnetic field of  $B_{\theta} \sim 0.015$ T, which gives the same approximate focusing force as a radial electric field of  $E_r \sim 3.4$  MV/m, and results in a sizable reduction in the effective radial space charge force when the bunch still has large velocity sheer.



**Figure 2**. Space charge and image charge fields for test problem 1, evaluated by Magic-2D (left) and Parmela-ucla (right). Upper left:  $E_z$ , middle left:  $E_r$ , lower left:  $B_\theta$ . Upper right:  $E_x(x)$ , lower right:  $E_z(z)$ .

Plots of the moments, spot sizes, and emittances are shown in figure 3 below. Agreement is surprising good amongst the four simulation codes, which use very different calculation methods. Still more surprising is that the transverse emittances are consistently better in the PIC code simulations, which include the time-and-space dependent effects of the sheer-induced magnetic field, and also correctly handle retardation effects with the cathode image charges. Agreement on the spot sizes, momentum spread, and momentum/phase correlation are all excellent.

It is reasonable to conclude from these results that omission of retardation effects and the velocity sheer fields in Parmela result in quite small errors in the spot size, bunch length and momentum spread, and to at most a  $\sim 20\%$  overestimation of the transverse emittances. It is likely that some of this discrepancy is traceable to the very different computation methods used and not to the physics approximations. Finally, it is noteworthy that the two Parmela variants agree well with each other, and the two PIC codes agree reasonably with each other, suggesting that the differences are indeed algorithmic in origin.



**Figure 3**. Transverse (left) and longitudinal (right) beam quantities. Upper left:  $<\beta>$ , middle left:  $\sigma_r$ , lower left:  $\varepsilon_r$ . Upper right:  $\sigma_z$ , middle right:  $\sigma_p$ , lower right: Corr(*z*,*p*).

#### 4.2. Test problem 2: Axisymmetric microwave field approximation

This second test problem is designed to address the importance of approximating the non-axisymmetric rf fields of the LCLS gun as axisymmetric. Efforts have been made to suppress the dipole asymmetry of the fields, leaving the quadrupole as the leading error term.

Conceptually, this test problem is quite specific to the geometry of the LCLS gun[2]. Beam is emitted and propagated through the 1.6 cell s-band LCLS gun, stopping at the exit of the gun, but using two different maps to represent the rf fields. The first map is strictly axisymmetric, generated by revolving a 2D map (generated by Superfish[9]) about the z-axis. The second map is fully 3D, generated from a fully 3D gun model computed with Mafia[10], including the laser ports, and the power couplers, each of which induce quadrupole field structure.

Specifically, the gun gradient will be taken to be  $E_z=100$  MV/m, the frequency frf=2856 MHz, and the geometry will be that of the LCLS gun. Solenoid focusing is to be used with a peak on-axis field strength of 2.7 kG. The electron bunch will be 1mm radius by 10ps length, uniformly distributed, but should have zero charge, to suppress space charge effects. The beam is to be launched with only a longitudinal velocity corresponding to 1 eV kinetic energy. The grid density and macroparticle number should be chosen to give results independent of either. Care must be exercised that the two field maps are equivalent in resolution and spatial extent.

Compute and plot the "difference fields", defined as the difference of the 3D and 2D maps on a component-by-component basis:  $\Delta E_x = E_x(3D) - E_x(2D), \dots, \Delta B_z = B_z(3D) - B_z(2D)$ . Compute  $\varepsilon_r$ ,  $\sigma_r$ , at the exit of the gun and compare.



**Figure 4**. Difference fields  $\Delta E_z$  (top) and  $\Delta B_z$  (bottom).

Computation of the beam transverse emittance (defined in test problem 1 above) with the 2D and 3D maps is summarized in Table 1. For nominal LCLS beam parameters, there is no statistically significant emittance increase for the 3D field map case (N=10000, observed increase is 0.8%). As a check of this negative result, the initial beam size was increased five-fold and the simulations run again. The much larger beam size significantly increases the rf-induced emittance growth. This case yielded a 10% increase in the emittance due to the added multipole errors, and is also displayed in Table 1.

The conclusion is that the rf cavity asymmetries induced by the input power coupler and laser ports do not significantly impact the emittance.

	Exit Spot Size		Exit Emittance		Exit Energy [m <sub>e</sub> c <sup>2</sup> ]	
	2D	3D	2D	3D	2D	3D
R=1mm	0.849 mm	0.878 mm	0.387 π μ	0.390 π μ	10.75	11.06
R=5mm	3.626 mm	3.589 mm	3.319 π μ	3.689 π μ	10.85	11.01

Table 1: Transverse emittance and spot size at gun exit for the 2D vs 3D comparison.

4.3. Test problem 3: Uniform current emission approximation

The purpose of this test problem is to test sensitivity of beam transverse emittance to variations in the emitted current density. Variations arise from several factors: laser nonuniformity, cathode roughness leading to variations in Shottky enhancement, and cathode contamination leading to variations in quantum efficiency.

Conceptually this specific problem addresses nonuniformities of the laser, as would be caused by higher-order modes being generated in the laser by, scattering, variations in amplifier gain with position, optics damage, and so on. Electron beam distributions are derived by standard rejection techniques to have Gauss-Laguerre form[11].

Parmela-lanl will be used for this case as it has an advanced 3D mesh-based space charge calculation method. The gradient will be  $E_Z=120$  MV/m, frequency frf=2856 MHz, and geometry that of the LCLS gun[2]. Solenoid focusing is to be used with a peak on-axis fields strength of 2.7 kG. The bunch charge will be Q= 1nC, and distributed approximately uniformly in time with a 10 ps length and 0.7 ps risetime, but with transverse distributions specified by the Gauss-Laguerre eigenfunctions with waist parameter wo=0.6\*sqrt(2) mm and a distribution cutoff of r=1.2 mm. The laser striking the cathode is presumed to be focussed on the cathode, so the phase front radius of curvature R= $\infty$ , and the Guoy phase angle  $\phi_0=0$ . Launch energy: 1 eV, strictly longitudinal, with 0.4  $\pi \mu$  thermal emittance added. The number of macroparticles, and mesh density should be chosen as required to achieve results that do not depend on either. Propagate the beam to the exit of the gun, and compute the transverse emittance at this location (using the definitions given in test problem 1).



**Figure 5**. Transverse charge distributions at the cathode (left) and at the exit of the gun (right).

Transverse beam profiles both at launch and at the gun exit are shown in Figure 5 below. Washout of the initial distributions has clearly begun, and the action of the solenoid focussing are visible as a rotation of the distribution about the axis.

Transverse emittances for the lowest four Gauss-Laguerre modes are summarized in Table 2 below. The cases computed here correspond to excitation of single laser modes, which gives some indication of what types of distortion (azimuthal, low spatial frequency) are most damaging to the beam quality. In reality a large collection of these modes combine to make the actual laser profile used to illuminate the cathode, and realistic simulations will require examining more realistic combinations of these modes, which will be the subject of future work.

	0
Laser Mode	Exit Emittance
Radially uniform distribution	2.84 π μ
TEM <sub>00</sub> (Gaussian)	4.37 π μ
TEM <sub>01</sub> (azimuthal modulation only)	8.42 π μ
TEM <sub>10</sub> (radial modulation only)	4.87 π μ
TEM <sub>11</sub> (both radial and azimuthal modulation)	5.98 π μ

Table 2. Transverse emittance at exit of gun for lowest four Gauss-Laguerre modes.

# 6. Conclusions

These three test problems address four of the approximations commonly made in simulating rf photoinjector performance. The electrostatic and retardation-free approximations are most dramatically violated shortly after emission, but as test problem 1 shows, the time during which these effect apply is so short that their inclusion has little impact on beam quality. The approximation of the rf fields as strictly axisymmetric is also reasonable for the symmetrized case of the LCLS gun. Accurate modelling of injector performance, however, depends directly on the fidelity with which the electron distribution is initially produced. Detailed measurements of emission current density over the active area of the cathode is essential data that has to be incorporated into injector simulation before accurate results can be expected.

During the course of these studies, several difficulties arose from the very different nature of the simulation codes used, and from the challenge of getting exactly comparable results from these codes.

Benchmarking codes and conducting fully integrated multi-code simulations are and will remain essential tasks for making reliable simulations of rf photoinjectors and for estimating the overall performance of systems which use rf photoinjectors. We therefore offer these recommendations with the hope of making both processes more efficient and reliable:

*Recommendation 1.* Adopt the Self-Describing Data Sets (SDDS)[12] format for all input and output files whose primary user is another program. Often-edited input files, such as beamline descriptions or run control files, or output files intended solely for human consumption, should remain in easily understood formats that need not be standardized. Interchange between users of different simulation codes, either for comparison purposes or for continuing a complex multi-step simulation process, will be greatly facilitated by the adoption of a standard format.

*Recommendation 2.* Devise abstracted, minimal test problems which reveal quantitatively the importance of the various approximations made in the simulations, and *publish these problems and their results with sufficient detail to be exactly replicated.* Three such problems are presented here.

Studies of wakefield effects will address the importance of one of the last remaining approximations made to the physics, and will be conducted for the LCLS gun in the near future. Other issues, specifically numerical in origin, also deserve attention such as the integrity of field maps and the symplecticity and convergence of the integrator.

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