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SIMULATING SPACE CHARGE DOMINATED BEAM DYNAMICS USING FMM*

S. A. Schmid†, H. De Gersem, E. Gjonaj, TU Darmstadt, TEMF, Darmstadt, Germany
M. Dohlus, DESY, Hamburg, Germany

Abstract

In this contribution, we simulate the beam generation in the high brilliance photoinjector of the European XFEL developed at DESY-PITZ. The investigation addresses the influence of space charge on the emittance of bunches with up to 1.0 nC bunch charge. For the simulations, we implemented a mesh-less fast multipole method (FMM) in the 3D tracking code REPTIL. We present numerical convergence and performance studies as well as a validation with commonly used simulation tools ASTRA and KRACK3. Furthermore, we provide a machine parameter study to minimize the beam emittance in the injector.

INTRODUCTION

The photoinjector test facility at DESY-PITZ in Zeuthen (PITZ) develops the electron injector for the European XFEL. The photoinjector consists of a UV laser triggered Cs_2Te photocathode, a 1.6 cell L-band gun cavity, a focusing solenoid, and a 1.3 GHz booster module downstream of the gun [1]. Due to large charge density and saturation effects during photoemission, simulating the beam dynamics of the PITZ injector is a numerically cumbersome task. In order to resolve the space charge forces of bunches with a large number of macroparticles, we develop a simulation technique based on an adaptive FMM method. The FMM reduces the computational cost of the space charge calculation to linear scaling in the particle number N [2] and allows for high spatial resolution, in particular, in the region close to the photocathode. This method is implemented in the tracking code REPTIL. In the following, we present a numerical convergence and performance study of the code and validate the simulation results with ASTRA [3] and KRACK3 [4]. Furthermore, we provide a machine parameter optimization study with respect to the laser spot size on the photocathode.

THE FMM

For a detailed discussion of the FMM approach the reader may refer to [5]. We implemented an OpenMP parallelized FMM code which is optimized for particle tracking applications. The FMM solver uses an adaptive tree structure to classify the interaction between different subregions of the particle bunch. Figure 1 shows exemplary the tree structure for a relativistic particle bunch in the PITZ beam line. Three numerical parameters, n_0, l_0, and θ_0, control the trade-off between accuracy and speedup of the FMM approximation. The parameter n_0 controls the depth of the tree by defining the maximum number of particles in one leaf node. The admissibility parameter θ_0 categorizes the interaction between different subregions of the bunch into near- and far-field contributions. The smaller is θ_0 the larger is the proportion of near field contributions. For the far field approximation, we apply a spherical multipole expansion of maximum order l_0. The near-field contributions are computed as direct particle-to-particle interactions.

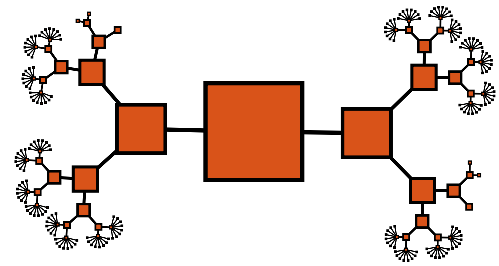

Figure 1: Tree structure of the FMM approach for a relativistic particle bunch in the PITZ beam line.

Figure 2 shows the trade-off between approximation error σ_{E_x} and speedup for the space charge field of a Gaussian bunch with 250 k macroparticles, 1 nC bunch charge, and 0.1 mm rms diameter. A direct particle-particle interaction approach provides the reference solution. The solid line shows the relative error as a function of θ_0 for $l_0 = 5$. In the region $\theta_0 > 0.3$, the truncation error of the multipole expansion dominates the total approximation error σ_{E_x}. For $\theta_0 < 0.2$, most of the interactions are computed by a near-field, particle-particle interaction approach rather than by the multipole expansion approximation. Therefore, the numerical efficiency of the method decreases significantly. In all cases, the error of the multipole approximation decreases exponentially with l_0 (dotted line).

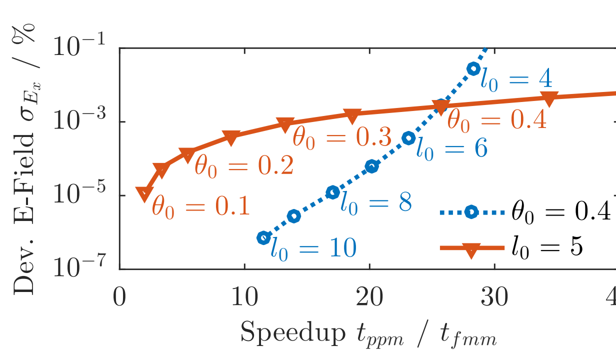

Figure 2: Approximation error and numerical speedup vs. admissibility parameter θ_0 and multipole order l_0.

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† schmid@temf.tu-darmstadt.de

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Figure 3 shows the deviation of the space charge field approximation in the xy-plane for three different FMM parameter sets (l_0, θ_0, n_0). The red-dashed circle indicates the 2σ extension of the Gaussian particle distribution. The box-pattern in plot a) originates from the adaptive refinement of the FMM tree structure. Regions of larger particle density, such as the center, result in smaller boxes allowing for a higher spacial resolution. Plot b) shows the error distribution for a smaller value of $\theta_0 = 0.2$. This results in an overall finer resolution of the FMM tree structure. Plot c) uses a higher order l_0 for the far field approximation. This does not influence the FMM tree structure and its spatial resolution. However, due to the better approximation of far-field interactions, the numerical error is reduced by two orders of magnitude.

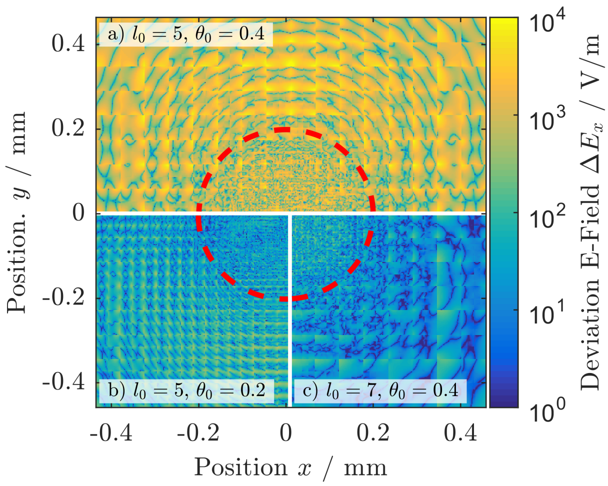

Figure 3: Numerical error in calculation of the space charge field for different FMM parameter sets.

PHOTOINJECTOR SIMULATIONS

The above simulation approach is implemented in the tracking code REPTIL. Using this code, beam dynamics simulations for a variety of operation parameters of the PITZ injector are performed. In a first step, in order to assess the numerical error in tracking simulations, the effect of numerical settings on accuracy is investigated. For this purpose, tracking simulations for the nominal PITZ bunch with a charge of 1.0 nC [1] are performed and the results are compared with a direct particle-particle interaction model. Restricted by the runtime of the particle-particle method (PPM) reference solution, the simulations use a comparably small macroparticle number of $N = 250$k. The transverse rms emittance

$$\varepsilon_x \equiv \sqrt{\langle x^2 \rangle \langle \dot{x}^2 \rangle - \langle x\dot{x} \rangle^2} \tag{1}$$

at $z_0 = 5.74$ m downstream of the photocathode is used to benchmark the quality of the FMM approximation. A scan of the FMM simulation error for different simulation parameters is depicted in Fig. 4. Using a maximum multipole order of $l_0 = 3$ and an admissibility parameter $\theta_0 = 0.5$, the deviation in $\varepsilon_x(z_0)$ becomes negligible. For this set of parameters, the FMM approach is 40 times faster than the PPM reference simulation. Due to different runtime scaling of the FMM approximation $\propto N$ and the PPM approach $\propto N^2$, this figure is expected to become even more significant for simulations using a larger number of macroparticles N.

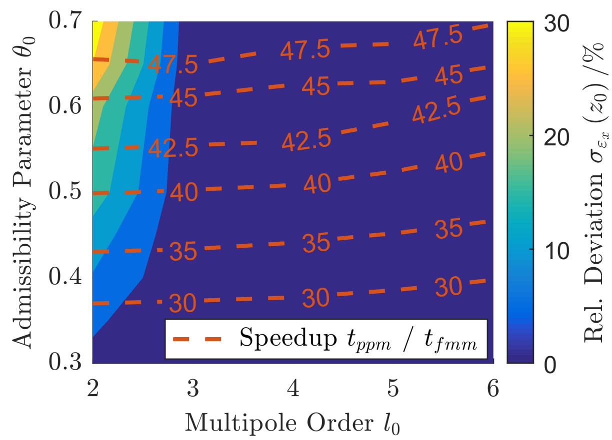

Figure 4: FMM parameter study for simulation of the nominal PITZ bunch. The density plot shows the relative deviation of the emittance ε_x. Contour lines indicate numerical speedup with respect to the PPM simulation approach.

Figure 5 compares the evolution of the transverse and longitudinal rms emittance of the FMM simulation and the PPM approach along the beam line. The FMM approach (dotted line) consistently reproduces the beam dynamics of the bunch. The deviation of the FMM approximation is less than 1 % over the full tracking distance. Hence, the FMM solver provides a computationally efficient, mesh-free alternative for space charge beam dynamics simulations.

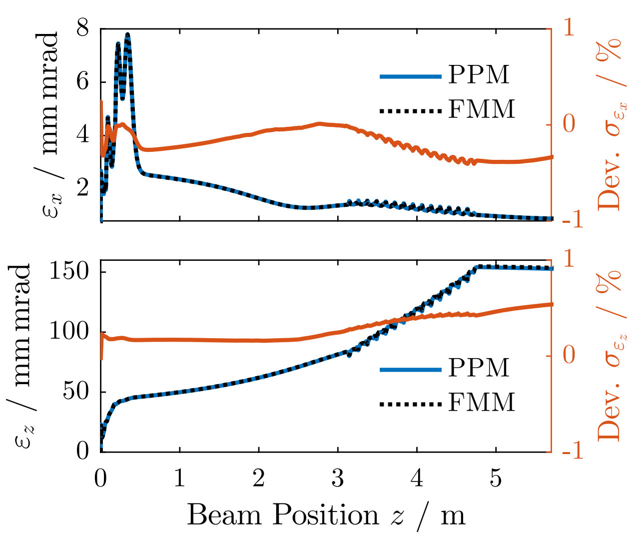

Figure 5: Comparison of transverse ε_x and longitudinal ε_z rms emittance evolution for FMM and PPM approach.

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Figure 6 compares the transverse phase-space at 5.7 m downstream of the photocathode for a rms laser spot size of $\delta x = 0.4$ mm. Simulations are performed for two bunch distributions with 500 k and 5 M macroparticles respectively. For comparison, phase-space pictures obtained with the codes ASTRA and KRACK3 are shown. As seen in the figure, a good agreement between the simulation codes is obtained. Furthermore, increasing the number of particles in the FMM simulation results in less particle noise. REPTIL, ASTRA and KRACK3 provide consistent simulation results with less than 3 % deviation in the transverse emittance ε_x.

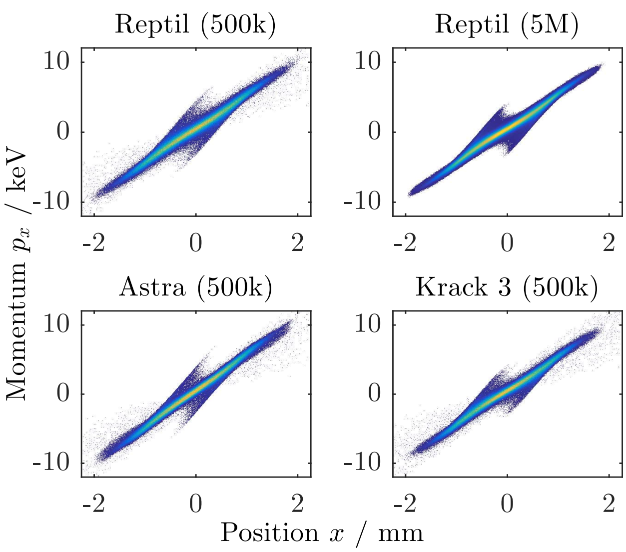

Figure 6: Comparison of the transverse phase-space at $z = 5.7$ m for REPTIL, ASTRA and KRACK3.

As a further application study, we investigate the dependency of the transverse emittance ε_x on the laser spot size on the photocathode. Figure 7 compares REPTIL, ASTRA, and KRACK3 simulations of the PITZ injector for 0.1 nC and 1.0 nC bunch charge. The photoemission process is modeled with a predefined particle distribution that is injected at the photocathode. All three codes agree nearly perfectly for all considered beam parameters as long as the beam current does not saturate. For both considered bunches, however, saturation occurs as the rms laser spot size is decreased as indicated in the figure. Due to the strong space charge fields, in this parameter region, it is impossible to extract the full bunch charge out of the cathode. For space charge limited (SCL) beam generation, the particle emission process at the photocathode influences strongly the beam dynamics and therefore the outcome of tracking simulations [6]. In the case of the PITZ injector, the results obtained for the beam dynamics in the current saturation region deviate substantially. This indicates, that the emission modeling under space charge limitation conditions needs to be reconsidered. In an upcoming simulation study, we plan to investigate the dynamics of space charge limited beam generation in more detail.

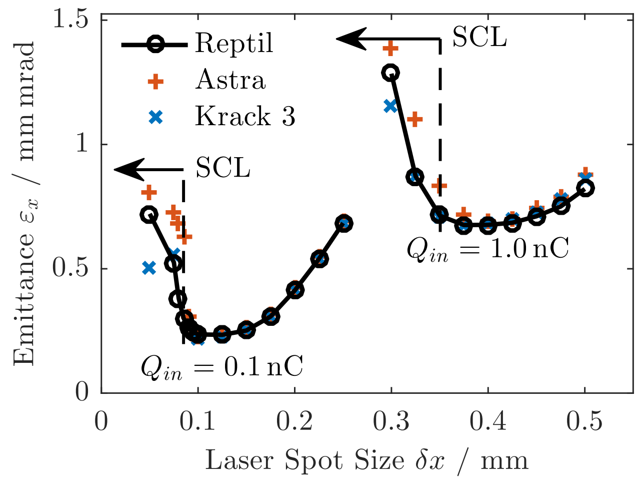

Figure 7: Parameter study for the photocathode laser spot size δx to minimize the transverse emittance ε_x of the PITZ injector.

CONCLUSION

In this contribution, we discuss numerical convergence and performance studies for the fast multipole method for tracking simulations. For an optimal choice of numerical parameters, the FMM approximation is 40 times faster than a direct particle-to-particle beam dynamics simulation model. The method is implemented in the tracking code REPTIL. The results of simulations for a variety of beam parameters of the PITZ injector are in very good agreement with ASTRA and KRACK3 simulations. Discrepancies are only observed in the current saturation region where photoemission is space charge limited. Further studies are needed for a better understanding of the beam dynamics in this operation region of the injector.

REFERENCES

[1] M. Krasilnikov *et al.*, "Experimentally minimized beam emittance from an L-band photoinjector", *Phys. Rev. Spec. Top. Accel Beams*, vol. 15, p. 100701, Oct. 2012. doi:10.1103/PhysRevSTAB.15.100701

[2] L. Greengard *et al.*, "A Fast Algorithm for Particle Simulations", *J. Comput. Phys.*, vol. 135, pp. 280-292, Aug.1997.

[3] K. Floettmann, "ASTRA: A space charge tracking algorithm", http://www.desy.de/~mpyflo/.

[4] M. Dohlus, "Krack 3", https://www.desy.de/~dohlus/Krack3/.

[5] J. Kurzak and B. M. Pettitt, "Fast multipole methods for particle dynamics", *Mol. Simul.*, vol. 32, pp. 775-790, Apr. 2006. doi:10.1080/08927020600991161

[6] Y. Chen *et al.*, "Modeling and simulation of RF photoinjectors for coherent light sources", *Nucl. Instrum. Methods Phys. Res., Sect. A*, vol. 889, pp. 129-137, May 2018. doi:10.1016/j.nima.2018.02.017