ELECTRON BEAM DYNAMICS SIMULATIONS FOR THE LOW EMITTANCE GUN

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We report on theoretical simulation performed for the development of a high brightness, field emitter based electron gun suitable for an Angstrom wavelength free electron laser[1]. First simulations have been done with available codes in 2½ and 3D for basic gun configurations showing the global and local (due to the granularity of the emitter array) effects on the emittance dilution. They indicate no stumbling blocks for the overall project. Design work has started on a test setup consisting of a 100 keV electron gun with solenoidal focusing and a diagnostics module. Experiments on the performance of field emitter arrays will be evaluated and compared to theoretical simulation codes. Beam parameters as well as electrical results for the gun itself are presented. For advanced simulations of field emitter based guns allowing to resolve individual emitters and to capture the influence of mechanical imperfections, a massive parallel code for 3D particle-in-cell simulations is in development. The electromagnetic field solver is fully functional and the particle tracker has been completed in its basic structures.

INTRODUCTION

The principal behind a free electron laser (FEL) is such that the field radiated by a beam passing a periodic transverse field and giving the beam a corresponding transverse motion is strong enough to act back on the charge distribution inside the beam, modulating it and so that a coherent self stimulated emission takes place.

Requirements are a certain minimum beam current and, equally important, a sufficiently parallel and ordered electron distribution, such that no phase cancellation can take place by oscillations at opposite phases.

Using the normalized rms emittance ϵ_t as a measure for the phase space occupied by the beam, we get the following upper limit for it as a function of particle energy and the generated photon wavelength (in the laboratory frame, not the particle rest frame):

$$\frac{\epsilon_t}{\gamma} \leq \frac{\lambda_{ph}}{4\pi}$$

where λ_{ph} is the radiation wave length and $\gamma = E/m_0c^2$ the normalized electron energy. For a compact and cost effective design of a FEL with a beam energy of 5 GeV and wavelengths in the order of 1 A (A photon beam able to resolve individual atoms), this would require normalized emittances below 10^{-7} m rad, a factor of ten better than current designs.

Directly after emission, the transverse emittance is more or less proportional to the product of the transverse momentum spread and the diameter of the emitting surface (assuming no correlation between these two), so with a momentum spread corresponding to an electron temperature of 300 K or 25 meV, the cathode diameter is limited to a few hundred microns for the given emittance.

Assuming peak currents in the order of 50 A, space charge forces can not be neglected in the simulation even for accelerating gradients of several hundred MV/m. A further complication in the analysis comes from the use of field emitter arrays as electron sources. Here we can not expect a smooth, slowly varying distribution of the current density, the beam consists of thousands of thread like beamlets arranged in a two dimensional array with a pitch of an order of a micron.

High precision results for this kind of problem need a fully consistent treatment of the underlying physics equations. Solving the problem via the Vlasov equations, treating the dynamics with density distributions in the six dimensional phase space, would be inefficient, even if it were possible with today's supercomputers. So we are using as the principal (but not exclusive) method the particle-in-cell (PIC) method. Particle dynamics is represented as equations of motion for a large (up to 10^7, 10^8) number of macroparticles, Maxwell's equations are solved in the time domain on a discrete grid and the coupling between both is done by representing the particle motion as excitation currents on the grid and calculating particle forces from the field values on the grid. As can be seen, the method solves only sets of linear equations and avoids e.g. nonphysical diffusion effects inherent in other methods.

The principal goals of current theoretical work on the electron dynamics inside the electron source are the following:

- With the available commercial PIC code (MAFIA TS2 and TS3 [2]) and assuming smooth current distribution, we are in the process of exploring the parameter space for the gun designs as e.g. minimum accelerator gradients for various peak currents. Within the limits given by the computer codes, first very preliminary simulations of the effect of the granularity of the transverse current density on the beam parameters are performed.

- Using MAFIA TS2 and Parmela[3] (a tracking code using approximations), establish strategies to limit and/or compensate for global emittance diluting effects like space charge forces and nonlinear field distributions by e.g. adapted geometric gun designs or linear/nonlinear magnetic focussing. In order to calibrate theoretical models and evaluate the strategies, work is focussed on a test stand consisting of a relatively low energy ($\leq$ 100 keV) DC gun with an advanced diagnostics setup.

- In order to capture the effects of the beam granularity (due to the individual field emitters) and to allow a full scale, high precision 3D computer simulation of the complete structure, a project for the development of a massive parallel PIC code has been launched. Apart from the simulation of ideal structures, also the analysis of mechanical tolerances, stochastic variations in the field emitter efficiencies and other imperfections and deficiencies will give an important feedback for the hardware development.

Simulation of high brightness beams

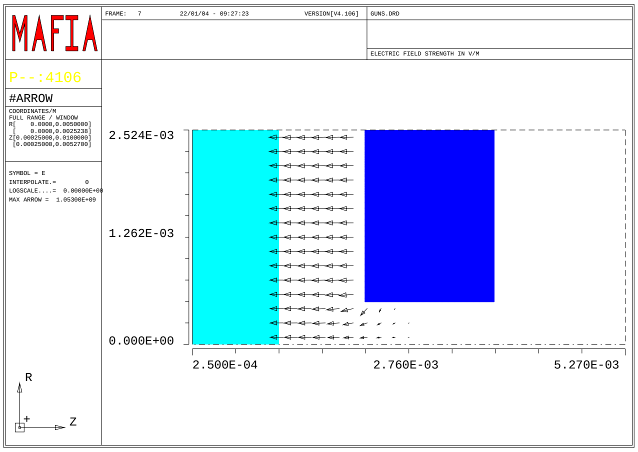

Fig. 1: Basic gun geometry shown with accelerating field of 1 MV over the 1 mm gap.

Estimates of the performance of a high brightness gun were performed using the simple geometry in figure 1. It is a basic design of a DC type diode gun assuming rotational symmetry in the structure as well as in the emitted transverse current density, so that a 2½D solver like MAFIA TS2 can be used for the simulation. In accordance to the introductory remarks, a cathode radius of 0.25 mm is assumed emitting a rectangular pulse of 10 A with a pulse length of 1 ps.

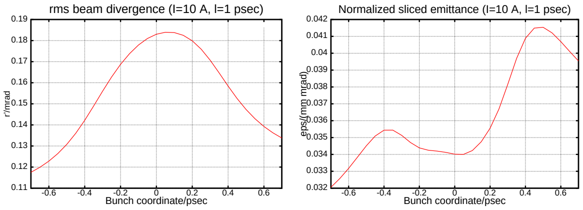

Fig. 2: rms beam divergence and sliced emittance along the beam axis for a rms slice length of 100 fs.

The PIC simulation gives an overall rms emittance of $4.2 \cdot 10^{-8}$ m with the emittance being defined as

$$\epsilon_t = \gamma \sqrt{< r^2 >< r'^2 > - < r \cdot r' >^2}.$$

For FEL applications, the interesting parameter is the emittance within a small transverse slice of the bunch, where the interaction between the electrons is taking place. In order to compute the sliced values for the emittance and other values, we weighted the averages with a shifted Gaussian and set e.g.

$$r^2_{rms,t_0} =< r^2 >_{z_0} = \frac{1}{A} \sum r_i^2 e^{-\frac{t_i - z_0/c_0}{2\sigma^2}}$$

where A is a suitable constant for normalizing the weight function and $t_i = z_i/c_0$ is the position of the individual macroparticle inside the bunch. As a compromise between numerical noise and possible resolution, an rms slice length of $\sigma = 100$ fs was chosen - in principle, the interaction length is still smaller than 1 fs. The beam divergence inside the bunch, as shown in the first graph of figure 2, follows quite well the expected pattern. The space charge forces are most pronounced in the middle of the bunch, thus the strongest divergence can be seen there.

For the sliced emittance, space charge forces do not per se constitute a problem. For an infinitely long bunch with a perfect constant charge distribution, these forces are linear and thus do not contribute to any emittance dilution. It is only nonlinearities at the extremities of the bunch or due to variations in the charge density, yielding a deterioration. This is clearly seen in the second graph of figure 2, where the sliced emittance peaks near the head and the tail of the bunch at ± 0.5 ps. An interesting option to be explored is the compensation of these nonlinear space charge forces via nonlinear focusing.

A special effect for field emitter array (FEA) cathodes arises from the fact that the emitted current density is not smoothly distributed over the cathode. A large number of thread like beamlets lead to a kind of granularity in the distribution and correspondingly also to very localized nonlinearities of space charge forces, which can not be compensated by conventional methods. A precise theoretical simulation is only possible after completion of the parallel PIC solver described below, but a first coarse 3D simulation is described in the following.

As a gun, the most primitive configuration of two metallic plates with a constant electric field of 1 GV/m was assumed. Emission was modeled from 316 point like emitters arranged as an array with a pitch of 20 μm on the circular emission area of 500 μm diameter. For the case shown, we used a Gaussian longitudinal profile of 1 ps rms and a peak current of 100 A. The three dimensional calculation grid had 1.6 million cells (about 10 million unknowns) sufficient to capture the interaction between beamlets, but not showing the simultaneous intra beamlet effects.

When comparing results with those of the 2½D computation shown before, it should be kept in mind that the longitudinal density distribution is now Gaussian, compared with a rectangular pulse before. Nonetheless, the basic effects of space charge on the beam are similar, as can be seen in figure 3. Beam divergence and correspondingly the beam radius are highest in the central slices of the bunch. This can also be seen in the second graph showing the macroparticle positions in the transverse plane. In the absence

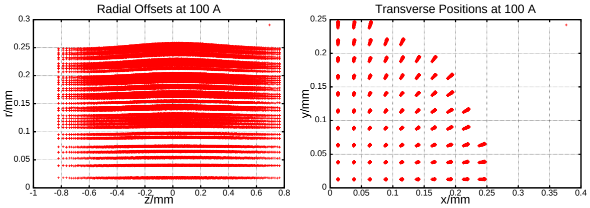

Fig. 3: Radial offsets of macroparticles versus longitudinal position and particle positions projected into the transverse (x-y) plane.

of space charge, the scatter plot would simply correspond to the distribution of the emitter array - the self field gives radial excursions of the beamlets.

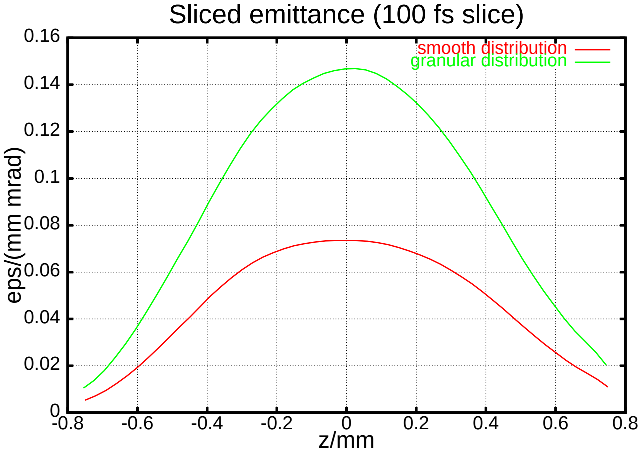

Fig. 4: Sliced emittance for granular bunch with 316 beamlets compared to equivalent smooth current distribution.

The interesting case is to compare these results with those simulations using an equivalent beam with the same longitudinal distribution and peak current, but with a smooth constant transverse current distribution. The global rms emittances do not differ much with 0.36 versus 0.375 mm mrad for the smooth versus the granular distribution, but the effect becomes more pronounced when looking at the sliced emittances as plotted in figure 4. Where a smooth distribution gives a peak value of around 75 nm rad, these approximately double for the granular one. The peak current of 100 A used for the results here seems to be some kind of a threshold. As one lowers the peak current to e.g. 40 A the difference become negligible compared to the global emittance blow up (peak sliced emittance of approx. 50 nm rad for both distributions.).

As a first approximate view at the dynamics of high brightness electron beams, we can conclude the following. There seem to be no principal roadblocks in a way toward a high brightness electron gun with sliced emittances below 10^{-7} m rad. Future theoretical computations will have to explore the two main areas.

Current results assume simultaneously very high current densities (up to 50 kA/cm^2) and high accelerating gradients (1 GV/m). For a parametrized study of bunch compression schemes (eventually allowing for lower beam currents), parameter sets for current and field gradient will be generated for more realistic geometries.

As the parallel PIC model described below becomes functional, more realistic models for a field emitter based electron gun will be simulated. The effects of a larger number of emitters as well as the influence of inhomogeneity of individual emitters concerning the amplitude, position and transverse momentum of the emitted beam will be explored.

100 keV TEST STAND

In order to characterize the electron beam generated by pulsing an FEA cathode in vacuum under high voltage and to study emittance minimization by space charge compensation it was decided to build a 100 keV gun test stand. First components have already been ordered and the estimated start of construction will be in March 2004. The test stand will consist of a HV power supply deck, removable in-vacuum electrodes, solenoid magnets, drift line and diagnostic module.

The specification of the cathode mount, anode structure and diagnostic equipment requires precise knowledge of the beam dynamics within a beam already “stiffened” by relativistic effects on one hand, but not yet highly relativistic ($\gamma = 1.196$ and $\beta = 0.548$ at 100 keV) on the other. Key parameters of interest (see Table 1) are beam spot size σ_r, divergence $\langle r\prime\rangle$, normalized transverse emittance $\beta\gamma\epsilon_t$, bunch length σ_z and momentum spread σ_p/p.

	$z = 40$ mm	$z = 340$ mm
σ_r	0.72 mm	6.0 mm
$\langle r\prime\rangle$	16 mrad	18 mrad
$\beta\gamma\epsilon_t$	1.8·10^{-7} m·rad	3.1·10^{-7} m·rad
σ_z	3.4 mm	3.7 mm
σ_p/p	0.1%	0.2%

Tab. 1: MAFIA results for key parameters of the gun test stand (100 keV DC accelerating field). It was assumed that the active emitter area had a radius of $r_{fea} =$ 100 μm and the anode iris radius was $r_{iris} =$ 500 μm. Longitudinally, the pulse was expected to be Gaussian ($\sigma_z =$ 20 ps) with a cut-off at ±3·σ_z. The pulse charge was $\simeq -5$ pC, resulting in a peak current of $\widehat{I} =$ 100 mA. The results given here were calculated for the exit of the gun ($z =$ 40 mm) and the end of the drift ($z =$ 340 mm).

A first attempt at tracking particles within such a structure was done with the PARMELA code. The code is capable of tracking small ensembles of macro-particles (N≃500) along the beam line in rather short time. Therefore it proved to be useful for first quick parameter studies. However, the constraints on the initial parameters are too strong (for example allowing only uniform or Gaussian structure of the pulse). Additionally, exact modeling of the gun was not possible and the code wasn't suitable for DC acceleration without RF.

Due to these inadequacies it was decided to use the MAFIA code. This code allows DC acceleration of various initial temporal distributions in arbitrary cylindrically symmetric electrode structures. Large ensembles of up to $4 \cdot 10^5$ macro-particles have been tracked, whereby run time quickly exceeds a couple of hours when the underlying mesh size is chosen small enough to resolve all details of the chosen gun geometry. The current gun geometry (see Figure 5) has been optimized for low emittance, high current and lowest peak field strength.

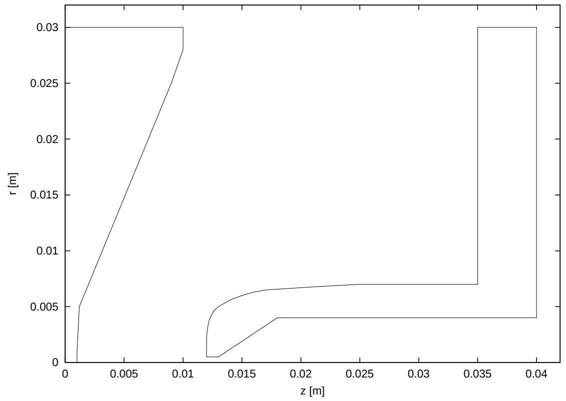

Fig. 5: The geometry for the current design of the cathode mount (left) and anode structure (right) of the test stand gun.

The final gap size between the copper electrodes has been determined by observing the maximum resulting field strength for a given position of the anode iris. The chosen working point (anode iris at z = 12 mm) yields a peak field strength of 20 MV/m which should be feasible (see Figure 6) with the available vacuum conditions and polishing techniques.

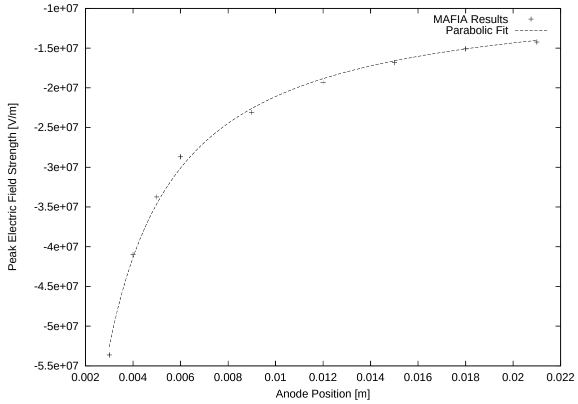

Fig. 6: Resulting peak electric field strength vs. anode position for cathode potential -100 keV and grounded anode. The position of the cathode is z = 1 mm.

The next step will be to incorporate a solenoid into the MAFIA input model. Its influence on the beam and its efficiency to fight the emittance blow-up due to space charge forces will be investigated in order to find an optimum working point.

PARALLEL 3D MAXWELL PIC COMPUTER SIMULATION

A parallel high-performance 3D Maxwell time-domain field solver with PIC particle tracking has been implemented from scratch in C++ using the POOMA II[4] framework for parallel computing on the Linux platform. Sophisticated C++ expression templates techniques deliver Fortran performance combined with high-level programming and development comfort. Electromagnetic static field solvers are currently being added to the simulation.

In the following, we present some details on the implemented program parts. A status report is given.

3D Maxwell field solver

The parallel 3D Maxwell time-domain field solver is based on the Finite Integration Method (like MAFIA) on a non-uniform rectilinear grid. A dual grid is introduced and Maxwell's equations are exactly discretized by storing integrated electric quantities on the normal grid lines and integrated magnetic quantities on the dual grid lines.

Transformations between integrated fields and flux densities are carried out at every calculation step by applying constant material operators. For the first time, approximations come into play as material properties get averaged onto discrete grid points by optimizing the electromagnetic energy density. Anisotropic ϵ and μ constants and perfect electric/magnetic materials stored in triangulated grid cells are supported as well as open, electric and magnetic boundary conditions. Several dipole excitation models have been implemented for testing.

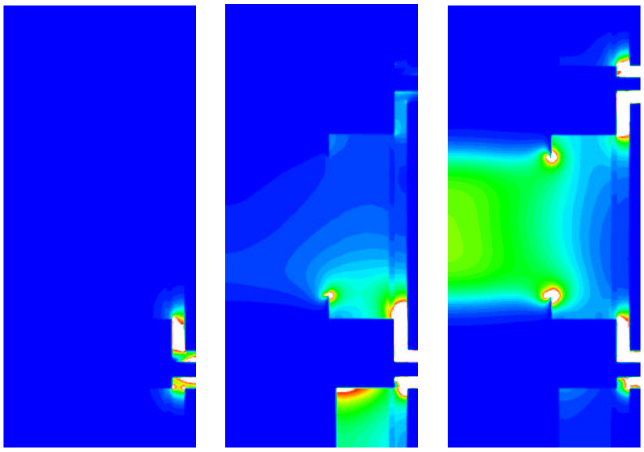

Fig. 7: *Sequence showing simulated electromagnetic energy density flow into kicker element.*

The simulation code renders identical results to MAFIA

T3 and is able to import MAFIA data files containing grid geometry, material properties and other parameters.

Parallelization of the resulting sets of linear equations is accomplished by domain partitioning and allows full 3D simulations of problems with up to 10^9 grid points on a modern Beowulf cluster.

PIC simulation

Tracking of electron macroparticles in electromagnetic fields is done by integrating the classical relativistic equations of motion. Coupling between particles and fields is accomplished by using first-order interpolation. Charge and current densities are assigned from the particles to the grid and resulting field forces back to the particles. Efficient parallelization is accomplished by distributing the particles according to the neighbouring field components to allow fast local interpolation. We are currently testing, optimizing and extending the PIC code, e.g. by adding elaborate emitter models.

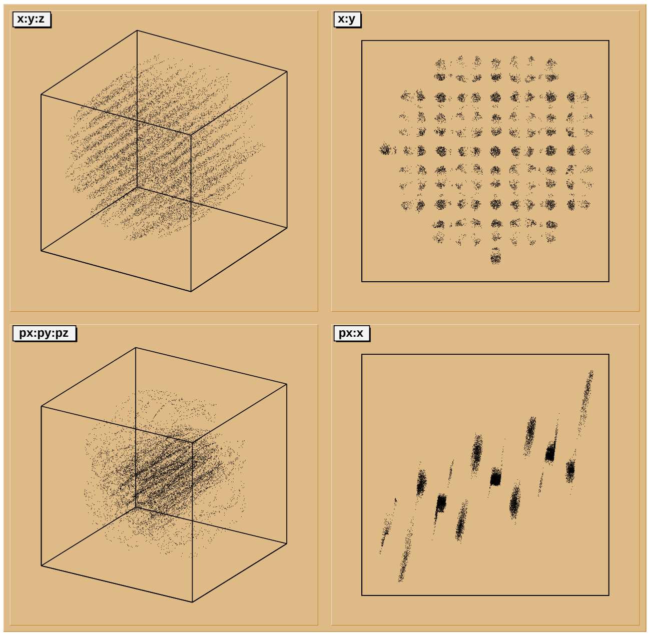

Fig. 8: *Selection of phase space plots of electron macroparticles after emission from field emitter array.*

3D static field solver

In order to supply the initial accelerating and focusing fields for the PIC module, which also should be a self-consistent solution of Maxwell's equations on the PIC grid itself, parallel static 3D field solvers for electric and magnetic fields are needed. The electrostatic solver is mostly completed. Current work concentrates on the evaluation of the parallel performance as well as the coupling with the PIC module.

Conclusion and Outlook

Development of the simulation code is progressing well. A parallel high-performance 3D Maxwell PIC simulation program with many features has been implemented from scratch. The POOMA II framework seems to be well-suited and leads to nice, efficient and easily extensible code. Thanks to compatibility to MAFIA, rigorous testing of the implemented features was possible. Several post-processing tools for visualization of arbitrary 1D, 2D and 3D field and particle data have been employed.

Further work will include completion of the PIC and static solver parts with strong focus on efficient parallelization. Reaching the aim of evaluating the ideal electron source setup will soon be possible.

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