ANALYSIS OF A PARTICLE-IN-CELL CODE BASED ON A TIME-ADAPTIVE MESH*

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Abstract

Several techniques are known for the coupled simulation of charged particles and electromagnetic fields. In order to achieve accurate results, various parameters have to be taken into account. In Particle-In-Cell (PIC) simulations, the number of macro particles per cell, the resolution of the computational grid, and other parameters strongly affect the accuracy of the results. In the code *tamBCI* [1], based on a time-adaptive mesh, additional variables related to the adaptive grid refinement have to be chosen appropriately. An analysis of these parameters is carried out and the results are applied to fully three-dimensional, self-consistent simulations of the injector section of FLASH [2].

INTRODUCTION

In space charged dominated problems the application of codes performing a self-consistent simulation of the charged particle beams is necessary. A large number of such codes is available: the *MAFIA TS* modules [3] being perhaps the most prominent examples. These codes use a fixed computational mesh. Taking into account the short bunches used, e.g., in FLASH (Free-electron LASer in Hamburg) [2] and the very high-frequency fields they excite, the choice of an appropriately small mesh spacing leads to memory demands which cannot be handled with the commonly available computational resources. Thus only self-consistent simulations of short sections for fully three-dimensional structures can be performed.

In previous works [4, 5] we reported on the self-consistent particle beam code *tamBCI* [1] based on a time-adaptive mesh refinement technique. After a short description of the underlying mesh adaptation algorithm this article will focus more on the choice of simulation parameters leading to sufficiently accurate results.

TIME-ADAPTIVE MESH REFINEMENT

For the purpose of a fast and efficient manipulation of the computational mesh a hierarchical data structure is used. The static refinement of the mesh in the transverse directions is applied beforehand. This approach is justified since we deal with injectors and linear accelerators where the transverse position of the bunches does not vary.

In the longitudinal direction the mesh is refined by hierarchical splitting of cells. In each refinement step one plane of base grid cells and their descendants are refined by bisection. Using this procedure no hanging nodes occur. The longitudinal mesh step size Δ decreases according to

$$\Delta = \Delta_{\text{base}}/2^N, \quad (1)$$

N being the refinement level. The organization of the refinement levels in binary trees is convenient and allows for an easy recombination of cells in the region left behind the particles. In order to keep numerical reflections at the transitions between different refinement levels low, the difference in the refinement levels of neighboring cells is limited to one.

Maxwell's equations are discretized in space according to the *Finite Integration Technique* (FIT) [6]. However, in order to apply the method, the values of field components have to be interpolated to new positions after each grid refinement or coarsening process. The interpolations are carried out utilizing a modified Akima subspline as interpolating function [4, 7].

In Fig. 1 two snapshots of the dynamically adapted meshes and the computed space charge fields are shown. The quality of the approximation of surfaces increases along with the mesh resolution.

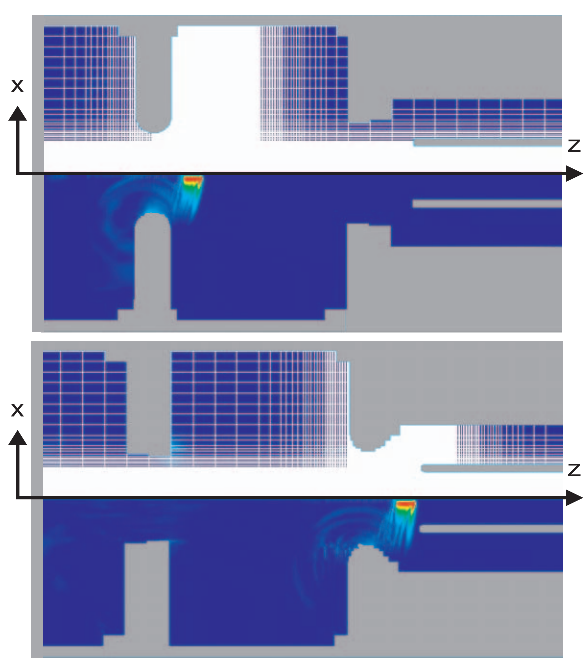

Figure 1: Combined view of the computational grid and the computed space charge fields at two instants in time for a simulation of the PITZ [8] gun (x-z cut).

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SIMULATION PARAMETERS

In this section we report on the experience gained with the choice of several critical parameters in the simulation of the injector section of FLASH. This photo injector is developed within the framework of the PITZ (Photo Injector Test Facility in DESY Zeuthen) project [8].

Mesh Step Sizes

The mesh step size is the most important parameter in the coupled simulation of electromagnetic fields and charged particles. It becomes even more critical in simulations starting from a cathode. After emission, the particles have very low energy and space charge forces are at their strongest influence. Neglecting these effects will lead to considerably deterioration of numerical accuracy downstream of the cathode.

In Fig. 2 (top) the result of a convergence study monitoring the RMS bunch length for different longitudinal mesh step sizes is shown. In order to separate the different discretization effects, a static and equidistant mesh was used to carry out this study. At a distance of 2.5 cm from the cathode the bunch has reached about 90 % of its final length. Reducing the step size from 10 μm to 5 μm the bunch length increases by only 0.01 μm . Thus, at a step size of 10 μm sufficient accuracy is reached.

Since the highest resolution is necessary in the immediate vicinity of the cathode only, a static mesh refinement in this area can be applied. For simulations over longer distances, the static discretization in the cathode area can be combined with the dynamical mesh refinement. In the lower part of Fig. 2 the results for static mesh refinements by a factor of 2 to 16 up to a distance of 1 cm from the cathode are shown. The results are, except for minor discrepancies, identical to the simulations utilizing an equidistant mesh.

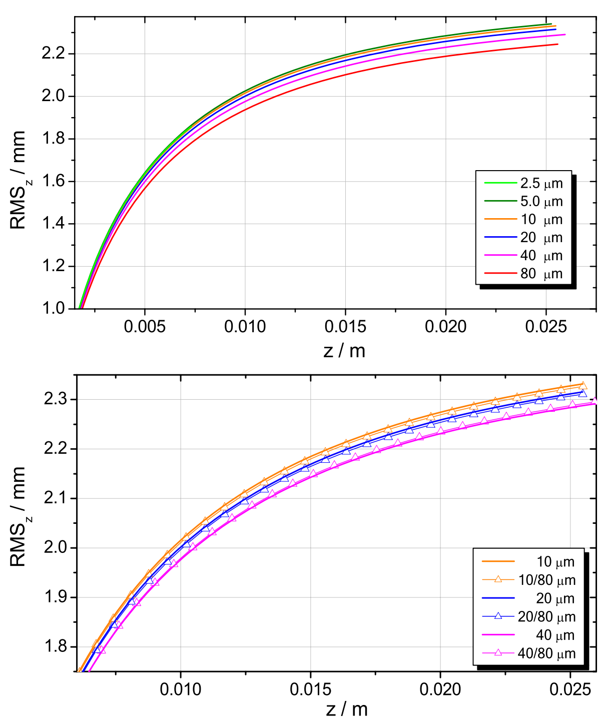

Figure 2: Convergence of the RMS bunch length with respect to the longitudinal mesh step size for an equidistant mesh (top). RMS bunch length for static mesh refinements up to a distance of 1 cm from the cathode by factors of 2 to 16 (bottom).

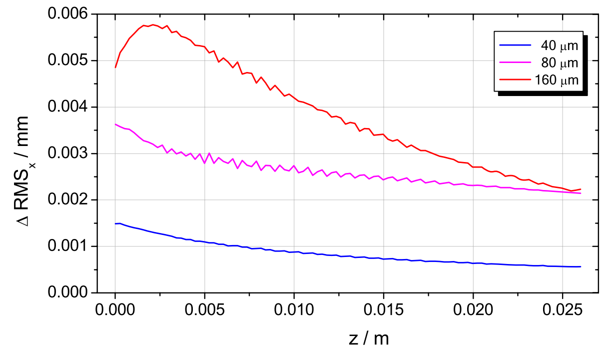

Figure 3: Differences in the transverse RMS bunch size for different transverse mesh step sizes with respect to the results obtained for a transverse step size of 20 μm .

To reach a deviation of less than 5 μm in the transverse bunch size a transverse mesh step of 80 μm is sufficient.

The bunch width is rather insensitive to changes in the transverse step size. In Fig. 3 the differences in the bunch RMS bunch width with respect to a result calculated using a transverse step size of 20 μm is shown. The deviations are in the μm-range corresponding to errors of some per mille.

Emission Samples Per Cell

As the bunch propagates, the computational particles (macro particles) induce currents. The smoothness of the temporal profile of the induced depends on the number of particles and the current-to-grid extrapolation scheme.

The average number of macro particles per cell determines how smooth the distribution of grid currents in the bunch region is. It is, in consequence, crucial concerning the level of numerical noise being excited. However, this number is difficult to fix prior to the simulation and moreover it depends on the size of the bunch. Hence, the number of emission samples placed in every cell on the cathode surface is chosen. For this study, particle emission took place in every time step using every sample. The total number of computational particles is, hence, linked to the transverse mesh resolution and the time step. Fig. 4 illustrates the convergence of the RMS bunch length and transverse size with respect to the number of samples per cell. Considering the transverse bunch size a number of two to four samples per cell are sufficient to reach convergence. For convergence in the computed bunch length, however, 8 samples per cell are necessary.

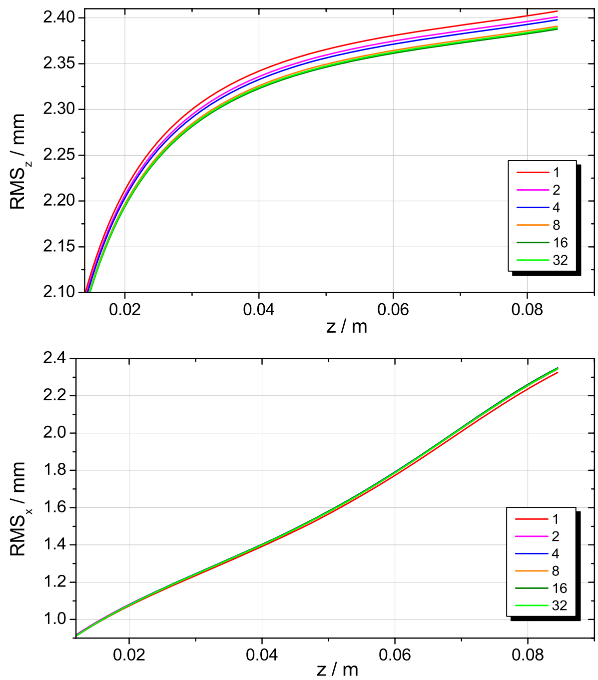

Figure 4: Computed longitudinal and transverse bunch size depending on the number of emission samples per cell.

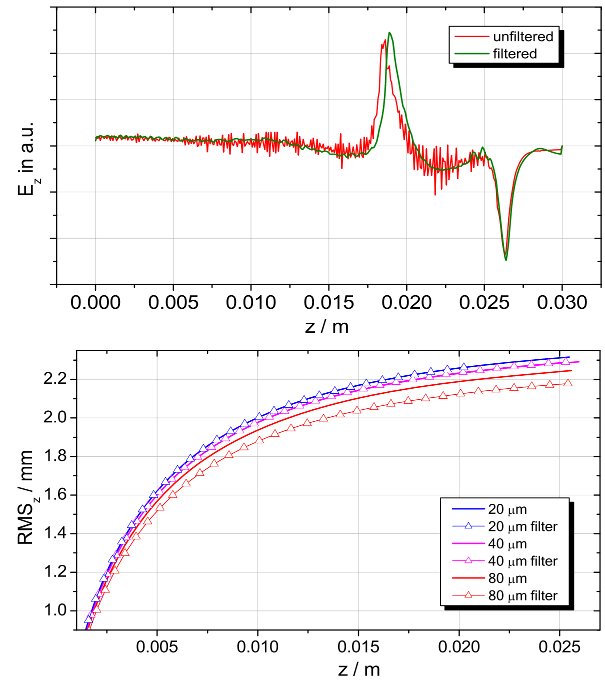

Figure 5: Effect of spatial current filtering on the excited electric field (top) and on the bunch length (bottom).

Spatial Current Filtering

The excitation of fields via moving point charges or localized charged clouds can lead to numerical noise in the frequency range near the grid cut-off frequency. This results in spurious fields which pollute the physical solution. This effect is demonstrated in Fig. 5 (top). In [9] a spatial filter of variable stencil width to suppress high-frequency noise was proposed. The green curve in Fig. 5 (top) illustrates the effect of the filter. For this example, a rather coarse mesh resolution of 80 μm in each direction has been chosen. The filter fulfills the continuity equation and does therefore not generate residual charges [10].

Filtering the current distribution involving neighboring cells, leads to a smoother distribution of currents in the bunch region. On the other hand it leads to a loss in accuracy in the calculation of space charge forces, especially for low mesh resolution. A stencil consisting of three points was found to be the best compromise dealing with noise suppression and space charge effects. In the lower part of Fig. 5, for a spacing of 80 μm the bunch length is significantly smaller when applying the filter, which is a clear indication of reduced space charge forces. Reducing the step size diminishes this effect.

CONCLUSIONS

A study of several important parameters in the coupled simulation of charged particles and electromagnetic fields has been carried out. The effects of the different parameters have been investigated separately. Explicit ranges of the discretization parameters are given for which accurate results are expected. In all simulations the setup of the PITZ injector was used. For any other setups the choice of the parameters under consideration can be different though they will approximately match for similar injectors.

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