INVESTIGATION OF NUMERICAL NOISE IN PIC-CODES

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Abstract

For a detailed analysis of the dynamics of space charge dominated beams a combination of Particle-in-Cell methods with efficient FDTD schemes is widely used. Besides the calculation of the forces acting on the particles the interaction of the beam itself with the surrounding geometries is taken into account. A drawback of this method is its sensitivity to numerical noise in the spectral range nearby the grid cutoff frequency. In this paper we will present results of detailed studies of the impact of the bunch shape on the level of the numerical noise. Furthermore an a priori scheme for efficient noise suppression is derived which does not affect the FDTD update algorithm.

INTRODUCTION

The arising of numerical noise in calculations using FDTD methods interacting with Particle-in-Cell codes has been reported. The noise level quickly increases with the number of computational steps, leading to a domination of unphysical fields. An example for this behaviour is shown on the left hand side of Fig. 1. MAFIA TS2 is a FDTD based program whereas ASTRA computes the space charge effects in an analytical way. Performing a Fast Fourier Transformation (*FFT*) of the fields yields an accumulation of field energy near the grid cutoff frequency f_c, which corresponds to the frequency of the highest resolved mode

$$f_c = \frac{c}{\pi}\sqrt{\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2}}, \tag{1}$$

Δx, Δy, and Δz being the grid step sizes. In Fig. 1 this circumstance is shown. To eliminate this problem a continuous filtering of the field components via *Finite Impuls Response (FIR)*-Filters as well as dissipative time integration schemes [1] have been proposed already. In this paper a different approach of an a priori scheme will be presented.

CAUSES OF NUMERICAL NOISE

During all investigations a simplified rectangular drift tube was considered. To ease analysis some further simplifications were introduced.

Since the FDTD Leapfrog-Algorithm is stable within correct timestep settings it is clear that numerical noise can't arise from accelerating or focusing fields in the beam tube. The computational area was therefore free of any fields at the beginning of every run. So all observed fields

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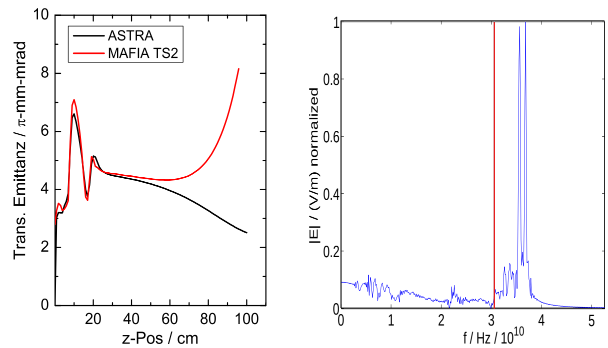

Figure 1: Physical (ASTRA) and unphysical (TS2) emittance development (left). Accumulation of field energy near the marked grid cutoff frequency (right).

are due to the bunch movement through the grid. For further simplification the particle motion was set parallel to the z-axis. Additionally the bunch was assumed to have very small transversal extensions so that it can be considered to be punctual. It therefore results in a z-directed line current. Finally the retroacting forces of excited fields on the particles as well as space charge forces weren't taken into account which can be justified by the relativistic velocity.

For the mapping of the particles to the grid a first order PIC-scheme was used. First investigations with gaussian shaped bunches showed a strong correlation of bunch length and noise level. In the upper drawing of Fig. 2 the frequency spectra of three gaussian bunches are shown. Each bunch has a total length of six standard deviations σ with the value of σ varying from the length of three mesh steps (in z-direction) to 2/3 mesh steps. There is an obvious dependency of the noise level on the frequency distribution of the exciting grid current caused by the travelling bunch. In effect the appearance of high-frequency numerical noise during simulations is due to a violation of the sampling theorem.

AN A PRIORI-FILTER FOR HF-NOISE SUPPRESSION

Since it was shown that the numerical noise originates from energy fractions with higher frequencies than f_c in the grid current it is convincing to apply a HF-filter that a priori adapts the bunch shape. The simplest algorithm for such a filter consists of just three steps:

1. Transformation of bunch signal into frequency domain by FFT
2. Erasing frequency fractions above grid cutoff
3. Backtransformation via inverse FFT.

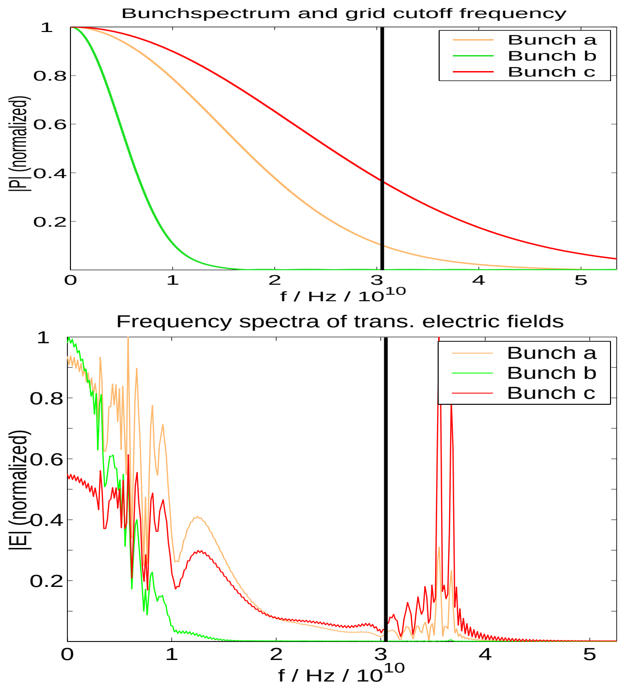

Figure 2: Frequency spectra of three gaussian bunches with different sigma and spectra of the resulting longitudinal electrical fields.

The number of particles in the bunch corresponds to the number of points used in the FFT. Since the number of supporting points in time- and frequency-domain are equal when using the FFT the bunch spectrum may be too coarse to resolve the grid cutoff frequency to satisfying accuracy especially because half of the points are allocated to the mirror spectrum and do not give new information.

In such cases the filtering quality can be improved by attaching a number of zeros to the signal which is reffered to as the zero-padding technique [2]. As the number of points is invariant during transformation the frequency spectrum will be sampled with a higher resolution. This does not introduce new information since the spectrum of a N-point signal is comletely described by a N-point spectrum but it will raise the resolution.

This filter was tested with different rectangular bunches. In the drawing on the left of Fig. 3 there is an example for an original and a modified rectangular bunch. Since the total bunch charge remains constant the maximum charge per macroparticle decreases. The extension of the bunch and simultaneously the number of macroparticles shouldn't be increased strongly because of computational costs. Therefore a limit Q_{low} for the macroparticle charge is introduced. This limit refers to the local maxima that arise at the bunch endings. All particles beside the first local maximum with less charge than Q_{low} are deleted. This approach leads to a small amount of energy in the region above the grid cutoff frequency again. Therefore a second parameter res is defined. It specifies a reserve in the frequency domain. The truncation frequency used is res percent lower than the grid cutoff frequency f_c. The truncation frequency f_t is therefore:

$$f_t = (1 - res/100) \cdot f_c. \qquad (2)$$

As may be seen in the drawing on the right side of Fig. 3 there is still some energy in the region above f_c. In this example the value of res was chosen to 10 %.

USING WINDOWING FUNCTIONS TO ENHANCE FILTER CHARACTERISTICS

The selection of several values out of a longer series is referred to as windowing. The windowing functions differ in their properties in time and frequency domain. The most commonly used window is the rectangular one which extracts a number of unmodified values according to its length. The Fourier Transformation of the rectangular window shows a high selectivity in the pass-band and a poor attenuation in the blocking-zone. Since the window is applied in the frequency domain, its transformed "spectral"

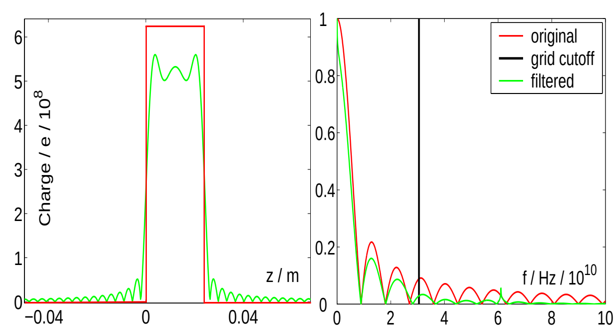

Figure 3: Shapes (left) and spectra (right) of a filtered and an original rectangular bunch using zeropadding.

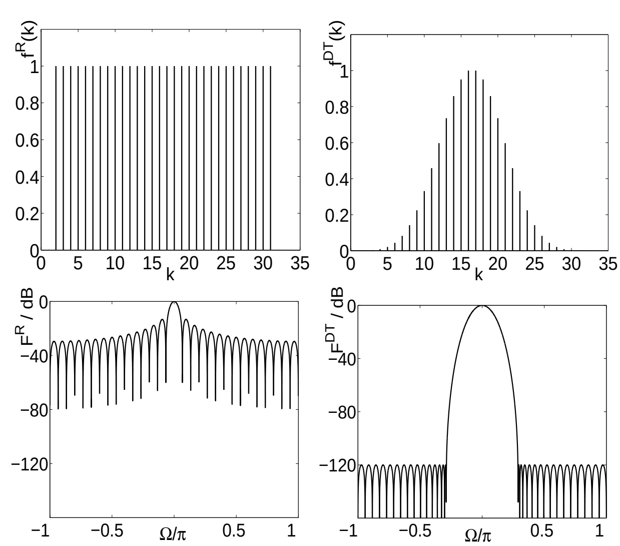

Figure 4: 32-point Rectangular (left) and Dolph-Tschebyscheff-Window (right) in time and frequency domain

properties will affect the time signal of the bunch. The rectangular window is therefore not the first choice because the ripples at the bunch endings should be suppressed as effective as possible.

The Dolph-Tschebyscheff window [2] was considered to be most suitable for the given problem. In Fig. 4 the time and frequency domain representation of a 32-point rectangular and Dolph-Tschebyscheff window are given. The most descriptive definition of the Dolph-Tschebyscheff window can be given in the frequency domain:

$$F^{DT}(e^{j\Omega}) = \frac{1}{A_0} \cdot \begin{cases} \cosh\left[k \cdot \operatorname{arcosh}\left(\frac{\cos(\Omega/2)}{\cos(\Omega_S/2)}\right)\right], & 0 \le \Omega \le \Omega_S, \\ \cos\left[k \cdot \arccos\left(\frac{\cos(\Omega/2)}{\cos(\Omega_S/2)}\right)\right], & \Omega_S \le \Omega \le \pi, \end{cases} \tag{3}$$

where A_0 is a constant for the normalization to the value of 1 at $\Omega = 0$ and k denotes the window length. As can be seen, the achievable attenuation is only dependent on the value of k which is because of zero-padding usually large enough to allow attenuations of -120 dB and more.

TESTING THE HF-FILTER ON PITZ-BUNCHES

The purpose of the PITZ (*Photo Injektor Teststand Zeuthen*)- project is the development of an injector which emits very short bunches. The design shape of the particle bunches is a symmetric trapezoid with a FWHM of 22 ps at c_0 and a rise time of 2 ps. The total charge should be 1 nC (see red bunch in Fig. 6 up-right). It should be noted that by the application of the described filter almost every bunch can be simulated noisefree. So it has to be ensured that the filtered bunch shape is still representative for its original. In Fig. 5 the result of the filtering of a bunch on a very coarse grid is shown. This of course isn't representative for the original problem anymore. On the other hand, as described, numerical noise is a problem of the sampling in space. So noise can also be reduced or avoided by refining the grid. It is therefore of interest how much computational costs considering the reduction of grid points can be saved by the appliance of the a priori-filter. In Fig. 6 two modified bunches are shown which are considered to be representativ for the original problem. In this example the original bunch was sampled by 11 grid points. To reach the same minimal noise level as achieved by the filter using

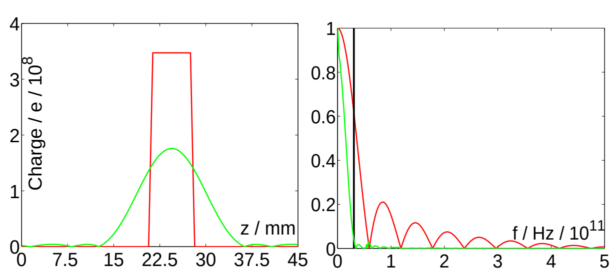

Figure 5: Example for a non-representative bunch after filtering.

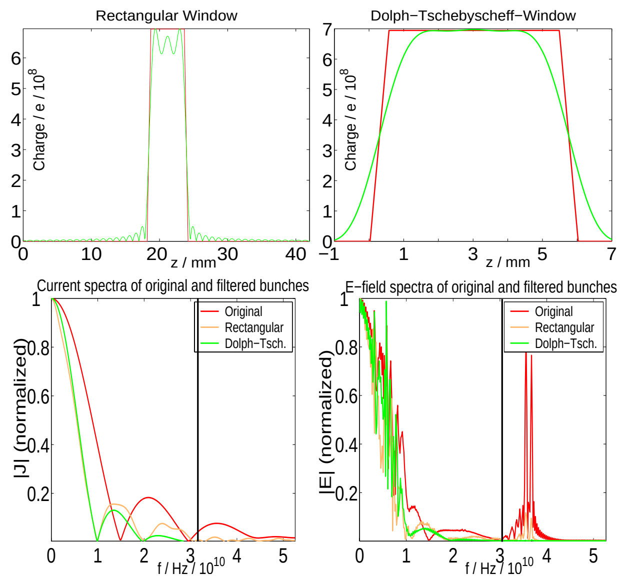

Figure 6: Effect of the a priori-filter on the bunch shape in representative examples (upper row). Grid current spectra and resulting e-field spectra (below).

a Dolph-Tschebyscheff window with the unmodified bunch the number of grid points had to be increased to 25. This is equal to a reduction of 56 % in this one-dimensional case. It has to be marked that also real PITZ bunches may not have the design shape as an effect of the bandwidth of the exciting laser.

BENEFITS AND LIMITATIONS

The presented scheme is a simple and efficient solution for the reduction of numerical noise in Particle-in-Cell simulations. By the application of this filter it is possible to save half of the necessary grid points (in one dimension) that are needed to achieve noisefree results. If the bunch dimensions get very small in comparison to the computational domain however, the effect isn't ample to allow the simulation of large accelerator sections. Here a combination of the a priori-filter and some effective dynamic subgrid or graded mesh may be inevitable.

In contrast to *FIR*-filtering or dissipative time integration schemes the modifications to the bunch shape are well-known which is of great advantage. Unfortunately, the current implementation of the filter is no longer usable if a bunch compression occurs in the simulated section.

REFERENCES

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