PROGRESS IN 3D SPACE-CHARGE CALCULATIONS IN THE GPT CODE

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Abstract

The mesh-based 3D space-charge routine in the GPT (General Particle Tracer, Pulsar Physics) code scales linearly with the number of particles in terms of CPU time and allows a million particles to be tracked on a normal PC. The crucial ingredient of the routine is a non-equidistant multigrid Poisson solver to calculate the electrostatic potential in the rest frame of the bunch. The solver has been optimized for very high and very low aspect ratio bunches present in state-of-the-art high-brightness electron accelerators. In this paper, we introduce a new meshing strategy based on a wavelet decomposition of the space-charge density. The numerical results show that the number of particles with large numerical error, typically located at the edges of the bunch, can be reduced with this new approach enormously.

INTRODUCTION

Progress in accelerator physics is measured in terms of brightness, scaling as the peak current divided by the emittance squared [8]. Space charge forces are the main limiting factor to reach ever higher brightness, and therefore extremely important for the high-brightness accelerator community. The most demanding applications in this field are SASE-FELs and colliders, such as currently under research and construction at DESY [2, 3]. In these devices, space-charge continues to play an important role to very high energies due to bunch compression systems that reduce bunch-length and thus increase charge density.

Our contribution to this field is the implementation of a fast 3D space-charge routine in the widely used General Particle Tracer (GPT) code [4]. It calculates the electrostatic potential by means of a multigrid Poisson solver on a non-uniform mesh. The space-charge model is written such that it can be used for injector design and subsequent acceleration to the GeV range, during a single run. This is accomplished by employing a very flexible multigrid Poisson solver, tailor-made for anisotropic meshes with extreme aspect ratios to cover all parts of the acceleration process [7].

An efficient distribution of mesh lines is still an open problem. Although the recent meshing technique works just fine for most 'normal' bunches, it is not optimal for the more exotic shapes such as after the DESY compression system. This paper presents first results of a new meshing strategy, based on wavelet decomposition of the discretized charge density function.

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WAVELET APPROACH

The current version of the 3D space-charge model uses a non-uniform meshing strategy based on the projected charge density to distribute the mesh lines. Bunches with very high or low aspect ratios require an improved mesh where additional mesh lines take care of discontinuities in the particle distribution. A well-established tool for the detection of such discontinuities is the wavelet decomposition. We give here only a short overview of the wavelet theory. Details can be found for instance in [1].

The main idea of a wavelet decomposition is to split a function f (in our application it is the space-charge density ρ) into a smooth part and details of a certain amplitude, the wavelet part [1]. This decomposition process is described by means of a *multiresolution analysis (MRA)*. A MRA is defined as a nested sequence of closed subspaces $V_m \subset L^2(\mathbb{R})$ ($L^2(\mathbb{R})$ is the space of square integrable functions over $\mathbb{R}$) of the form

$$\{0\} \subset \cdots \subset V_2 \subset V_1 \subset V_0 \subset V_{-1} \subset V_{-2} \subset \cdots \subset L^2(\mathbb{R})$$

with the properties

$$\overline{\bigcup_{m\in\mathbb{Z}} V_m} = L^2(\mathbb{R}),\ \bigcap_{m\in\mathbb{Z}} V_m = \{0\},$$
$$f(x) \in V_m \Leftrightarrow f(2^m x) \in V_0,\ x \in \mathbb{R}.$$

Further, there is a function $\varphi \in L^2(\mathbb{R})$, the so-called scaling function, such that the integer translates $\varphi(x-k)$ ($k \in \mathbb{Z}$) form a Riesz bases of V_0, i. e.

$$V_0 = \overline{\mathrm{span}\{\varphi(x-k),\ x \in \mathbb{R},\ k \in \mathbb{Z}\}},$$
$$A \sum_{k\in\mathbb{Z}} c_k^2 \le \left\| \sum_{k\in\mathbb{Z}} c_k \varphi(x-k) \right\|_{L^2}^2 \le B \sum_{k\in\mathbb{Z}} c_k^2$$

for all $\{c_k\}_{k\in\mathbb{Z}}$ with $\sum_{k\in\mathbb{Z}} c_k^2 < \infty$ and for positive constants A and B. Thus, the spaces V_m can be generated by scaled versions of φ which are given by

$$\varphi_{m,k}(x) := 2^{-m/2}\varphi(2^{-m}x - k), \qquad k,m \in \mathbb{Z}, x \in \mathbb{R}.$$

Now, the wavelet space W_m is introduced as orthogonal complement of V_m with respect to V_{m-1}, i. e.

$$V_{m-1} = V_m \bigoplus W_m,\ V_m \perp W_m.$$

For every MRA there exists a wavelet ψ, the translates and dilatations of which form an orthonormal basis of W_m:

$$\psi_{m,k}(x) := 2^{-m/2}\psi(2^{-m}x - k), \qquad k,m \in \mathbb{Z}, x \in \mathbb{R}.$$

The wavelet decomposition of a function $f \in L^2(\mathbb{R})$ requires first an approximation of f in V_m by means of an orthogonal projection $P_m f$ with

$$P_m f = \sum_{k\in\mathbb{Z}} c_k^m \varphi_{m,k},$$

where the coefficients c_k^m are given by $c_k^m = \int_{\mathbb{R}} f \overline{\varphi_k^m}\, dx$. Due to the decomposition $V_m = V_{m+1} \bigoplus W_{m+1}$ the projection $P_m f$ can be split as follows

$$\begin{aligned} P_m f &= P_{m+1} f + Q_{m+1} f \\ &= \sum_{k\in\mathbb{Z}} c_k^{m+1} \varphi_{m+1,k} + \sum_{k\in\mathbb{Z}} d_k^{m+1} \psi_{m+1,k}. \end{aligned}$$

The projection $P_{m+1} f$ represents the smooth part of f and $Q_{m+1} f$ the details with respect to V_m.

The three dimensional case can be considered as tensor product. Let $P_{m,x}$, $P_{m,y}$ und $P_{m,z}$ be the approximation with the scaling function in x-, y- and z-direction, respectively. The wavelet parts are analogously denoted by $Q_{m,x}$, $Q_{m,y}$ and $Q_{m,z}$. Than, the decomposition of $f \in L^2(\mathbb{R}^3)$ has the form

$$\begin{aligned} P_{m,z}P_{m,y}P_{m,x} f &= P_{m+1,z}P_{m+1,y}P_{m+1,x} f \\ &+ P_{m+1,z}P_{m+1,y}Q_{m+1,x} f \\ &+ P_{m+1,z}Q_{m+1,y}P_{m+1,x} f \\ &+ P_{m+1,z}Q_{m+1,y}Q_{m+1,x} f \\ &+ Q_{m+1,z}P_{m+1,y}P_{m+1,x} f \\ &+ Q_{m+1,z}P_{m+1,y}Q_{m+1,x} f \\ &+ Q_{m+1,z}Q_{m+1,y}P_{m+1,x} f \\ &+ Q_{m+1,z}Q_{m+1,y}Q_{m+1,x} f. \end{aligned}$$

Here $P_{m+1,z}P_{m+1,y}P_{m+1,x} f$ is the smooth part of f and all other terms with a wavelet part are regarded as representation of details. The wavelet coefficients are large at locations with a lot of detailed information, for instance discontinuities. Here additional mesh lines have to be added. The goal of these approach is, that we can start the mesh calculation with a relative small number of mesh lines using the recently implemented adaptive meshing strategy. By means of the wavelet decomposition mesh lines are only added at locations where a refinement is necessary. More detailed we have applied the following scheme:

The Wavelet Meshing Algorithm

1. Compute the mesh line distribution for a relatively coarse grid following the distribution of the particles and calculate the space-charge density ρ at the grid points.
2. Calculate the wavelet decomposition of $f = \rho$.
3. Add mesh lines at locations with large wavelet coefficients of the following parts:
   - mesh in x-direction: $P_{m+1,z}P_{m+1,y}Q_{m+1,x}\rho$,
   - mesh in y-direction: $P_{m+1,z}Q_{m+1,y}P_{m+1,x}\rho$,
   - mesh in z-direction: $Q_{m+1,z}P_{m+1,y}P_{m+1,x}\rho$.

NUMERICAL RESULTS

The model of very low or high aspect ratio bunches is a cylindrically shaped bunch with an aspect ratio A given by $A = R/\gamma L$, where R denotes the Radius, L the length of the cylinder and γ the Lorentz factor. With this definition high aspect ratio bunches have a pancake shape and low aspect ratio bunches have a cigar shape. Assuming a uniform particle distribution it is shown in [5] that the electrical field of those bunches are highly nonlinear with sharp peaks at the edges of the bunch.

In this paper we present numerical results from a cigar shaped bunch with $A = 0.01$ containing 10,000 macroparticles which are uniformly distributed. The wavelet decomposition has been performed with Haar wavelets. The adaptive non-uniform mesh with 33x33x33 mesh lines calculated following the particle distribution is presented in Figure 1. Figure 2 shows the wavelet mesh which has now 45x45x41 mesh lines. Corresponding to large wavelet coefficients mesh lines are added transversally inside the bunch, while longitudinally mesh lines are mainly added at head and tail of the bunch.

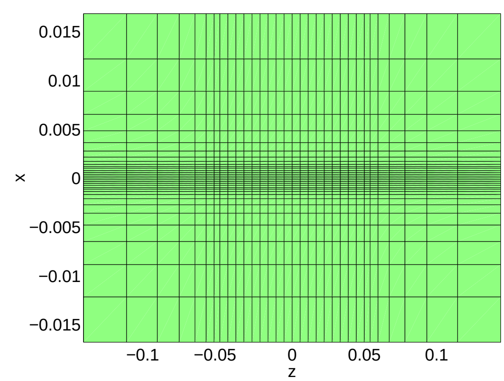

Figure 1: The discretization of a cigar shaped bunch ((x,z)-plane): grid with 33x33x33 mesh lines distributed following the particle distribution.

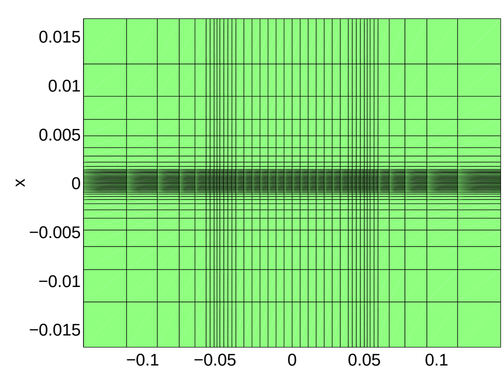

Figure 2: The discretization of a cigar shaped bunch ((x,z)-plane): wavelet mesh with 45x45x41 mesh lines.

Figures 3 and 4 show the distribution of the particles with relative error of the electric field greater than 0.1. Although the particles have uniform distribution the particles with large errors are located at the edges of the bunch and here for the cigar shaped bunch mainly at head and tail of the bunch. On the wavelet mesh only 308 particles with an error greater than 0.1 remain. Compared to 952 particles on the original grid this number is reduced enormously. This effect is achieved with the refined grid at head and tail of the bunch (see Figure 2).

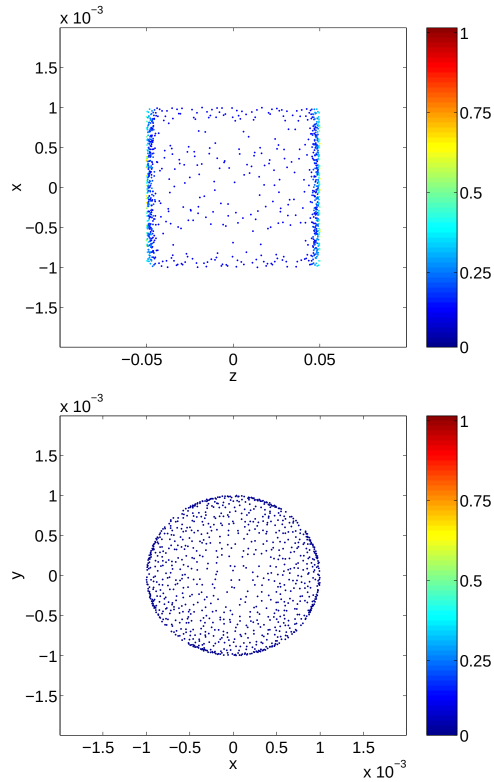

Figure 3: Cigar bunch with $A = 0.01$: Particles with relative error of the electrical field > 0.1 for a 33x33x33 mesh. Transversal direction (top), longitudinal direction (bottom).

CONCLUSIONS

The fast calculation of 3D space-charge fields requires not only an efficient Poisson solver but also an adaptive mesh with as few mesh lines as possible and as many mesh lines as necessary. Up to now the choice of an appropriate discretization is an open problem. In this paper we have investigated a new meshing technique based on the wavelet decomposition of the space charge density. This strategy allows to start the calculation with a relatively coarse mesh that follows the space-charge density. This mesh is than further refined only at distinct locations determined by means of the wavelet meshing algorithm. A main goal of the algorithm is that the wavelet coefficients detect discontinuities of the space charge density. Thus the wavelet mesh provides an improved approximation especially of bunches with very high or very low aspect ratio.

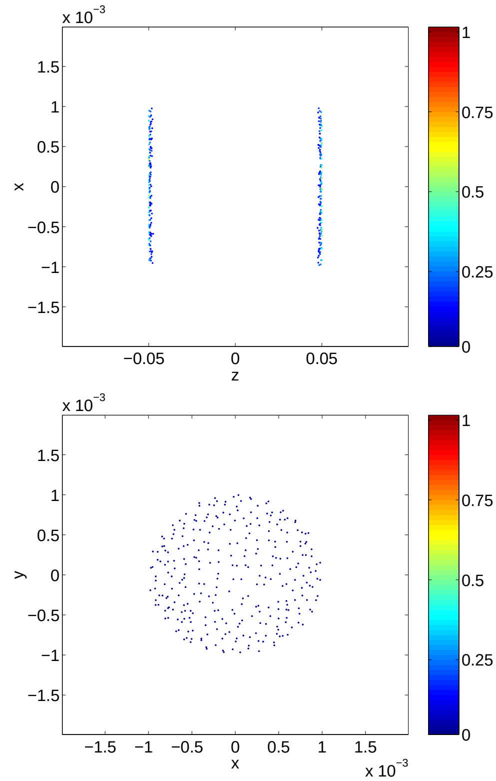

Figure 4: Cigar bunch with $A = 0.01$: Particles with relative error of the electrical field > 0.1 for a wavelet mesh with 45x45x41 mesh lines. Transversal direction (top), longitudinal direction (bottom).

REFERENCES

[1] I. Daubechies, “Ten Lectures on Wavelets”, SIAM, Philadelphia, 1992.

[2] DESY, Hamburg, Germany, `tesla.desy.de`, “The TESLA Project”.

[3] DESY, Hamburg, Germany, `xfel.desy.de`, “The European X-Ray Laser Project XFEL”.

[4] General Particle Tracer (GPT), release 2.52, Pulsar Physics, De Bongerd 23, Soest, The Netherlands, `www.pulsar.nl/gpt`.

[5] S.B. van der Geer, M.J. de Loos, O.J. Luiten, G. Pöplau, U. van Rienen, “3D Space-Charge Model for GPT Simulations of High-Brightness Electron Bunches”, TESLA-Report 2003-04, DESY, 2003.

[6] G. Pöplau, U. van Rienen, S.B. van der Geer, M.J. de Loos, “A Fast 3D Multigrid Based Space-Charge Routine in the GPT Code”, Proceedings of EPAC 2002 (Paris), pp. 1658-1660 (2002).

[7] G. Pöplau, U. van Rienen, S.B. van der Geer, M.J. de Loos, “Multigrid Algorithms for the Fast Calculation of Space-Charge Effects in Accelerator Design”, IEEE Transactions on Magnetics, 40(2), pp. 714–717 (2004).

[8] M.J. van der Wiel, Conf. Proc. 2nd ICFA Future Accelerator Workshop on “The Physics of High-Brightness Beams”, Los Angeles (1999).