

STUDY OF A FAST CONVOLUTION METHOD FOR SOLVING THE SPACE CHARGE FIELDS OF CHARGED PARTICLE BUNCHES

Dawei Zheng*, Aleksandar Marković†, Gisela Pöplau‡, Ursula van Rienen,
 Universität Rostock, Rostock, Germany

Abstract

The kernel of beam dynamics simulations using the particle-in-cell (PIC) model is the solution of Poisson's equation for the electric potential. A very common way to solve Poisson's equation is to use the convolution of charge density and Green's function, the so-called Green's function method. Additionally, the integrated Green's function method is being used in order to achieve a higher accuracy. For both methods, the convolutions are done using fast Fourier transform based on the convolution theorem. However, the construction of the integrated Green's function and the further convolution is still very time-consuming. The computation can be accelerated without losing precision if the calculation of Green's function values is limited to that part of the computational domain with non-zero grid charge density. In this paper we present a general numerical study of these Green's function methods for computing the potential of different bunches: The results can also be used in other simulation codes to improve efficiency.

INTRODUCTION

Inside a particle accelerator chamber, regardless of the accelerating RF electromagnetic field, there is also another important source of electromagnetic field to study: the beam itself, which produces both space charge and wake fields. These fields change variously, due to the total current, the bunch shape, beam pipe and surrounding residual materials. In modern accelerators with very high bunch charge, the space charge force calculation becomes even more crucial and often lack to agree with the experimental results. A common approach numerically convolutes the charge density with Green's function (GF) as one of the standard solution techniques for Poisson's equation in order to derive the electric self-field. However, this numerical strategy may suffer from errors in the Green's function values. This happens when the considered bunch has an extremely long cigar-shape or short pancake-shape. A highly accurate way to overcome this issue is to use the so-called integrated Green's function (IGF) method, which deals with the analytical integration rather than a numerical evaluation. However, the restriction of IGF is also obvious in that the calculation of the analytical integration value is very time-consuming. This can cost the most part of the computing time in space charge calculation when parallel implementation is not used.

There are several practical simulations which heavily rely on space charge calculation in beam dynamics. For instance,

beam tracking, the beam-beam interaction [4], the positron beam and electron clouds interaction as well as the simulation of the interaction between an electron bunch and ion clouds, etc. To study these different types of simulation, the space charge force calculation can be classified into two groups based on the computational domain. We denote it as the near-bunch domain calculation and the far-bunch domain calculation. As indicated by its name, the near-bunch domain calculation discretizes a cubic domain just covering the bunch and then calculates the self-field. In this case, no extra field outside of the bunch needs to be calculated. The basic beam tracking and beam-beam interaction simulation belong to this type. While the far-bunch domain calculation means the extra field out of bunch should be calculated, since this field acts on the electron or ion clouds in the simulation of the interaction between the bunch and charged clouds. These clouds are not shaped as an inerratic and concentrate area, but distributed widely spread.

In this paper, we present a less time-consuming method called cutting Green's function method (CGF), but showing the same accuracy as IGF for far-bunch domain space charge calculation. This new method brings a great benefit for the calculation time for beam tracking in a far-bunch domain and for the interaction simulation between particle bunches and charged clouds.

NUMERICAL SOLUTION OF POISSON'S EQUATION

The solution of Poisson's equation in free space [2] reads as:

$$\varphi(x, y, z) = \frac{1}{4\pi\epsilon_0} \cdot \iiint \rho(x', y', z') G(x, x', y, y', z, z') dx' dy' dz', \quad (1)$$

with Green's function

$$G(x, x', y, y', z, z') = \frac{1}{\sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}} \quad (2)$$

GF integral: With the well-known midpoint rule for the numerical integral in Eq.(1), the discretized GF formula is given by

$$\varphi(x_i, y_j, z_k) \approx \frac{h_x h_y h_z}{4\pi\epsilon_0} \cdot \sum_{i'=1}^{N_x} \sum_{j'=1}^{N_y} \sum_{k'=1}^{N_z} \rho(x_{i'}, y_{j'}, z_{k'}) G(x_i, x_{i'}, y_j, y_{j'}, z_k, z_{k'}). \quad (3)$$

* dawei.zheng@uni-rostock.de, supported by China Scholarship Council

† supported by BMBF 05K2013

‡ supported by BMBF 05K10HRC

IGF integral: With the summation of integrals for Green's function over each grid cell $[x_i - \frac{h_x}{2}, x_i + \frac{h_x}{2}] \times [y_j - \frac{h_y}{2}, y_j + \frac{h_y}{2}] \times [z_k - \frac{h_z}{2}, z_k + \frac{h_z}{2}]$, the discrete IGF formula is given by

$$\varphi(x_i, y_j, z_k) \approx \frac{1}{4\pi\epsilon_0} \cdot \sum_{i'=1}^{N_x} \sum_{j'=1}^{N_y} \sum_{k'=1}^{N_z} \rho(x_{i'}, y_{j'}, z_{k'}) \tilde{G}(x_i, x_{i'}, y_j, y_{j'}, z_k, z_{k'}), \quad (4)$$

where $\tilde{G}(x_i, x_{i'}, y_j, y_{j'}, z_k, z_{k'})$ can be calculated for the Green's function in Eq.(2) like :

$$\tilde{G}(x_i, x_{i'}, y_j, y_{j'}, z_k, z_{k'}) = \int_{x_{i'}-h_x/2}^{x_{i'}+h_x/2} \int_{y_{j'}-h_y/2}^{y_{j'}+h_y/2} \int_{z_{k'}-h_z/2}^{z_{k'}+h_z/2} G(x_i, x', y_j, y', z_k, z') dx' dy' dz'. \quad (5)$$

This integral can be calculated from the primitive function (antiderivative) of Eq.(2) derived by MATHEMATICA, its formal expression can be found in [3]. In order to make the calculation of (3), (4) more efficient, we should implement it as cyclic convolution, for which expansions \tilde{G}_{ex} , ρ_{ex} of \tilde{G} and ρ are needed. The charge density ρ_{ex} is padded with zeros in all expansion grid points, the tilde Green's function \tilde{G} is expanded to be symmetric. The details are introduced in [1] [2]. Generally, using 3D discrete Fourier transformation \mathfrak{F} and convolution theorem, the expanded potential expression is:

$$[\varphi_{ex}]_{i,j,k} = \frac{1}{4\pi\epsilon_0} \mathfrak{F}^{-1} \{ [\mathfrak{F}\tilde{G}_{ex}]_{i,j,k} \cdot [\mathfrak{F}\rho_{ex}]_{i,j,k} \}_{2N_x, 2N_y, 2N_z}. \quad (6)$$

Finally, the potential at each grid point equals the first N_x, N_y, N_z values of the expanded potential expression on each axis.

THE CUTTING GREEN'S FUNCTION

However, if we use the IGF for the far-bunch domain calculation, most portion of the integrated Green's function is over-calculated:

As we read from Eq.(4) and Fig.1, suppose the bunch domain (surrounding cuboid) is located at the subdomain $[x_b, x_t] \times [y_b, y_t] \times [z_b, z_t]$ of the grid (corresponding to $[N_{xb}, N_{xt}] \times [N_{yb}, N_{yt}] \times [N_{zb}, N_{zt}]$), which is in the center of the computational domain $[x_1, x_{N_x}] \times [y_1, y_{N_y}] \times [z_1, z_{N_z}]$, the ratio between bunch domain and the complete computational domain is $1 : \alpha_x, 1 : \alpha_y, 1 : \alpha_z$ in x -, y - and z -direction, respectively. taking the sum of the discretized convolution, there is a large area, in which the charge density is zero. Therefore we may introduce the

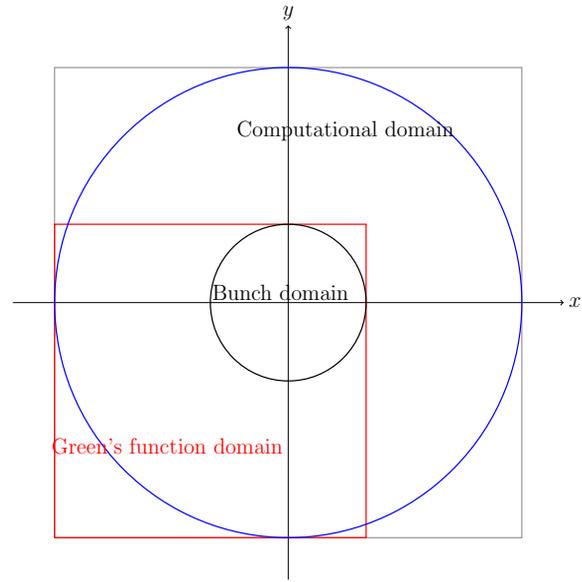


Figure 1: A schematic plot of cutting Green's function domain for Cartesian coordinates.

approximation

$$\varphi(x_i, y_j, z_k) \approx \frac{1}{4\pi\epsilon_0} \cdot \sum_{i'=N_{xb}}^{N_{xt}} \sum_{j'=N_{yb}}^{N_{yt}} \sum_{k'=N_{zb}}^{N_{zt}} \rho(x_{i'}, y_{j'}, z_{k'}) \tilde{G}(x_i, x_{i'}, y_j, y_{j'}, z_k, z_{k'}). \quad (7)$$

In Eq. (7), we neglect some portion of Green's function in the calculation: As the domain bounded by the red line (Fig.1) is sufficient to compute exactly, the remaining domain can be simply set to zeroes. Still, the results stay exactly the same. This means: The Green's function value \tilde{G} outside of the subdomain bounded by the red line does not contribute to the discretized convolution at all. The discretized convolution is done using the convolution theorem, which multiplies the discrete Fourier transforms of both Green's function and charge density. Therefore, the Green's function values should be calculated in advance. We define the ratio between the Green's function domain and the total computational domain as $(1 + \alpha_{x,y,z}/2) : \alpha_{x,y,z}$. The corresponding mesh number of calculated Green's function values is $M_{x,y,z} = \lceil \frac{2+\alpha_{x,y,z}}{2\alpha_{x,y,z}} N_{x,y,z} \rceil$ and the subdomain $[1, M_x] \times [1, M_y] \times [1, M_z]$ cut out of the original domain $[1, N_x] \times [1, N_y] \times [1, N_z]$. We call it cutting integrated Green's function (CIGF) $\tilde{G}_c(x_i, y_j, z_k)$.

$$\tilde{G}_c(x_i, y_j, z_k) = \begin{cases} \tilde{G}(x_i, y_j, z_k), & (1, 1, 1) \leq (i, j, k) \leq (M_x, M_y, M_z); \\ 0, & \text{otherwise;} \end{cases}$$

As GF and IGF method, we extend \tilde{G}_c and ρ to \tilde{G}_{cex} and ρ_{ex} . Using 3D discrete Fourier transformation \mathfrak{F} and convolution theorem as Eq. (6) to calculate the potential the same way.

VERIFICATION

We use an ideal uniform ellipsoidal beam as an example. $\alpha_x = \alpha_y = \alpha_z = 5$. The relative errors we used here are defined as:

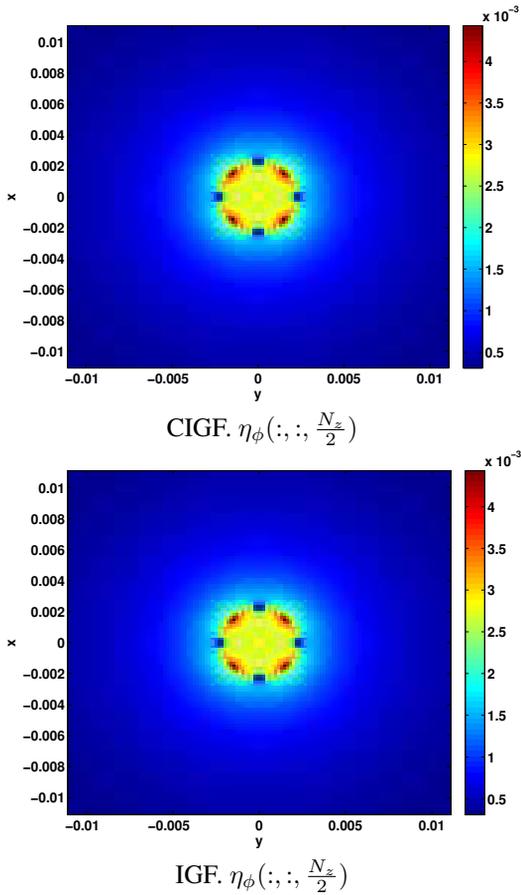


Figure 2: Comparison of $\eta_\phi(\cdot, \cdot, \cdot)$ for an ideal uniform ellipsoidal beam.

$$\begin{aligned} \eta_\phi(i, j, k) &:= \frac{|\varphi_{i,j,k} - \varphi_{true_{i,j,k}}|}{\max_{i,j,k} |\varphi_{true_{i,j,k}}|}, \text{ and} \\ \hat{\eta}_\phi &:= \max_{i,j,k} (\eta_\phi(i, j, k)). \\ \eta_{\mathbf{E}}(i, j, k) &:= \frac{\|\mathbf{E}_{i,j,k} - \mathbf{E}_{true_{i,j,k}}\|_2}{\max_{i,j,k} \|\mathbf{E}_{true_{i,j,k}}\|_2}, \text{ and} \\ \hat{\eta}_{\mathbf{E}} &:= \max_{i,j,k} (\eta_{\mathbf{E}}(i, j, k)). \end{aligned}$$

Here, the notations are, $\eta_\phi(i, j, k)$, $\hat{\eta}_\phi$, $\varphi_{i,j,k}$ and $\varphi_{true_{i,j,k}}$ as the relative error of the potential at index (i, j, k) , the global relative error of the potential, the computed potential at index (i, j, k) and the true potential for the same index, respectively. So does the electric field: $\eta_{\mathbf{E}}(i, j, k)$, $\hat{\eta}_{\mathbf{E}}$, $\mathbf{E}_{i,j,k}$ and $\mathbf{E}_{true_{i,j,k}}$.

DISCUSSION

This CIGF routine is particularly efficient for far-bunch domain simulation. As we see from Table 1, we could cut

Table 1: Comparison between IGF and CIGF

N	$\hat{\eta}_\phi$	$\hat{\eta}_{\mathbf{E}}$	IGF Time	CIGF Time
32	0.0587	0.0619	1.5175 s	0.6233 s
64	0.0130	0.0334	10.1015 s	3.6115 s
128	0.0045	0.0290	78.5222 s	27.6219 s

a valid Green's function domain, the volume is as small as $\frac{(2+\alpha_x)(2+\alpha_y)(2+\alpha_z)}{8\alpha_x\alpha_y\alpha_z}$ of the computational domain, compare Fig.1. Free boundary conditions are used for an open-ended round pipe, which is embedded into the cuboid computational domain. Even though one could set up a constant grid in advance, we suggest to cyclically adapt the grid, due to the grid dispersion and the need of fine grid resolution with the Debye length.

For near-bunch domain simulation, we recommend another fast IGF called reduced integrated Green's function (RIGF) from our former work [6], which uses a mixed GF and IGF to achieve a high efficiency.

CONCLUSION

A fast convolution approach for an FFT-based Poisson solver is presented. The potential calculated by the cutting Green's function method introduced above can be used for beam dynamics simulations in open-ended circular pipes. The idea can be enhanced to any type of Green's function for far-bunch domain calculation. For instance, the same cutting approach to another integrated Green's function from [7] suits for an open-ended rectangular pipe. In general, we showed an efficient numerical convolution method for Green's function method, bringing benefit in far-bunch calculation, which can be used in the calculation of the electric field for the bunch in electron (ion) clouds simulation as well as in other simulations.

REFERENCES

- [1] R.W. Hockney and J. W. Eastwood. Computer Simulation Using Particles. Institut of Physics Publishing, Bristol, (1992).
- [2] J. Qiang, S. Lidia, R.D. Ryne, and C. Limborg-Deprey, Phys. Rev. ST Accel. Beams, vol 9, 044204 (2006).
- [3] J.Qiang, S. Lidia, R.D. Ryne, and C. Limborg-Deprey, Phys. Rev. ST Accel. Beams, vol 10, 129901 (2007).
- [4] J. Qiang, M.A. Furman, and R.D. Ryne, A parallel particle-in-cell model for beam-beam interaction in high energy ring colliders, "J. Comput.Phys." 198, 278 (2004).
- [5] A. Marković, Simulation of the interaction of positively charged beams and electron clouds. PhD thesis, Rostock University (2013).
- [6] D. Zheng, G. Pöplau, U. van Rienen, Reduced integrated Green's function method for fast Poisson solver in beam dynamics simulation. submitted to Phys. Rev. ST Accel. Beams.
- [7] R. D. Ryne, An integrated Green function Poisson solver for rectangular waveguide. IPAC (2012).