ISBN: 978-3-95450-227-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2022-MOPOTK059

IMPLEMENTATION OF THE VICO-GREENGARD-FERRANDO POISSON SOLVER IN SYNERGIA2 *

Chong Shik Park†, Korea University, Sejong, South Korea

Abstract

Computation of space charge fields in accelerator simulations is one of the most challenging tasks. The algorithm proposed by Hockney and Eastwood is the fastest method for numerically solving Poisson equations with open boundaries and has been implemented in various accelerator simulation codes. Recently, Vico-Greengard-Ferrando proposed a new hybrid fast algorithm for computing volume potentials. The new algorithm is promising higher accuracy and faster error convergence than that of Hockney-Eastwood. This study presents the implementation of the Vico-Greengard-Ferrando solver in Synergia and shows a comparison of results with these Poisson solvers.

INTRODUCTION

Particle-in-Cell (PIC) methods are commonly used to compute space charge effects, beam-beam effects, etc. in high-intensity accelerator modeling. In PIC calculations, particles are deposited on a spatial grids and the electrostatic field on these grids is calculated by solving the Poisson equation. Finding solutions of Poisson's equations for all time steps is the most time-consuming part of full-beam dynamics simulation. Several numerical methods for solving Poisson equations in multi-particle simulations have been developed and are widely used, such as FFT-based methods [1,2], spectral finite difference methods [3], and multi-grid spectral finite difference methods [4,5].

Among them, the FFT-based Green's function method is widely used to solve the Poisson equation in the open boundary condition when the size of the beam is generally smaller than the radius of the vacuum pipe. The Green's function and charge density are computed in the doubled-domain with zero-padding [1]. In order to calculate the Green's function efficiently with high accuracy, several techniques were developed, such as the integrated Green's function [6] and the shifted Green's function [7].

Recently Vico *et al.* developed a new Green function technique for fast convolution computation [8]. This method introduces a truncated Green's function by cutting of a region beyond the domain of interest. The Fourier transform of this Green function can be solved analytically and shows higher accuracy at the cost of the additional FFT. In this study, the Vico-Greengard-Ferrando algorithm was implemented for FFT-based Green function calculation. Numerical simulations show improved accuracy with smaller grid sizes.

* Work supported by the National Research Foundation of Korea (NRF) grant funded by the Korea Government (MSIT) (No. 2020R1A2C1014675)
† kuphy@korea.ac.kr

POISSON SOLVERS

For a given charge distribution, ρ, the Poisson equation of an open boundary condition:

$$\vec{\nabla}^2\phi = -\frac{\rho}{\epsilon_0}$$

has a solution expressed with Green's function as

$$\begin{aligned}\phi(\vec{r}) &= \frac{1}{\epsilon_0}\int G(\vec{r},\vec{r}')\,\rho(\vec{r}')d^3\vec{r}' \\ &= \frac{1}{4\pi\epsilon_0}\int \frac{1}{|\vec{r}-\vec{r}'|}\,\rho(\vec{r}')d^3\vec{r}'\end{aligned}$$

The electric fields can be easily computed using $\vec{E} = -\vec{\nabla}\phi$. However, the Green's function above is defined in long range and has singular at $\vec{r} = \vec{r}'$. These make it difficult to calculate accurate solution of the potential in Particle-in-Cell simulations, and require fast algorithms and special and accurate quadrature techniques.

One of most popular techniques in accelerator physics codes is Hockney-Eastwood(HE) algorithm, which uses the Fast Fourier Transform(FFT) with zero-padding. In this algorithm, the charge distribution is zero-padded in the doubled domain, and then aperiodic convolution is applied using FFT as in Eq. (1).

$$\phi(\vec{r}) = \frac{1}{\epsilon_0}h_x h_y h_z \mathscr{F}^{-1}\left\{\mathscr{F}\{\hat{G}\}\mathscr{F}\{\hat{\rho}\}\right\}, \qquad (1)$$

where $\hat{G}$ is the Green's function on the extended domain, $\hat{\rho}$ is the padded charge distribution, h_x, h_y, and h_z are grid spacings on each spatial dimensions. Here, $\mathscr{F}\{\cdot\}$ represents a Fourier transformation in all spatial dimensions, whereas $\mathscr{F}^{-1}\{\cdot\}$ represents an inverse Fourier transformation in all spectral dimensions. This algorithm is scaled like $\mathcal{O}\left((2N)^d(\log(2N))^d\right)$, where N is the number of grid points in each direction before padding and d is the dimension size.

Vico *et al.* introduced a truncated spectral kernel for Green's function by replacing it as follows [8,9]:

$$G(\vec{r}) \Rightarrow G^L(\vec{r}) = G(\vec{r})\mathrm{rect}\left(\frac{r}{2L}\right),$$

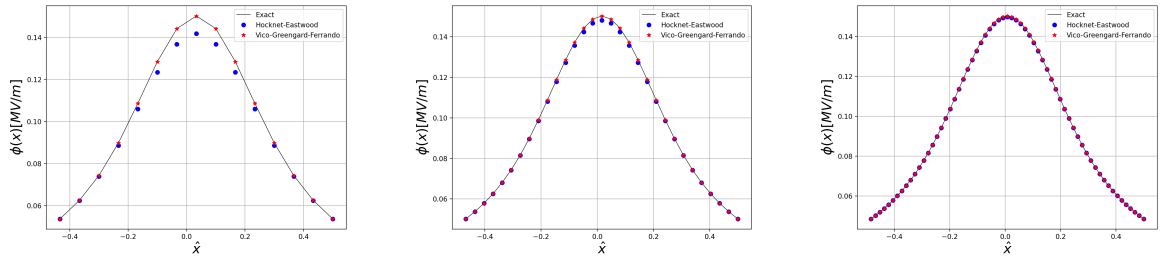
where $L > \sqrt{d}$ and the indicator function, $\mathrm{rect}(x)$, is defined as

$$\mathrm{rect}(x) = \begin{cases} 1 & \text{for} \quad |x| < 1/2 \\ 0 & \text{for} \quad |x| > 1/2. \end{cases}$$

Then, the potential solution can be rewritten as

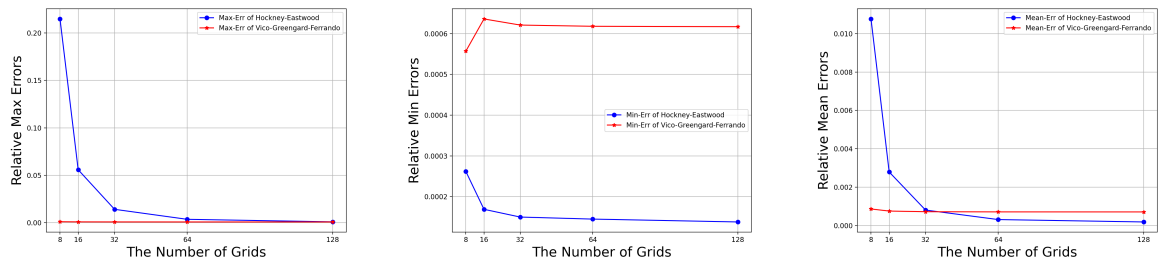
$$\phi(\vec{r}) = \frac{1}{\epsilon_0}\int G^L(\vec{r},\vec{r}')\,\rho(\vec{r}')d^3\vec{r}'.$$

ISBN: 978-3-95450-227-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2022-MOPOTK059



(a) $N = 16$ (b) $N = 32$ (c) $N = 64$

Figure 1: The electric potentials along the longitudinal beam axis with the different number of grids.



(a) Maximum Relative Errors (b) Minimum Relative Errors (c) Mean Relative Errors

Figure 2: The relative errors to the exact solution with the different number of grids.

In this Vico-Greengard-Ferrando Poisson solver, the Fourier transform of the truncated Green's function can be solved analytically and computed in the truncated dimensions, and the solution is characterized by fast convergence of smooth data with higher accuracy. For example, in three dimensions,

$$\mathscr{F}\left\{G^L\right\} = \frac{2}{\epsilon_0}\left[\frac{\sin\left(\frac{L|\vec{k}|}{2}\right)}{|\vec{k}|}\right]^2$$

Therefore, the solution of the Poisson equation is

$$\phi(\vec{r}) = \frac{2}{(2\pi)^3\epsilon_0}\int e^{i\vec{k}\cdot\vec{r}'}\left[\frac{\sin\left(\frac{L|\vec{k}|}{2}\right)}{|\vec{k}|}\right]^2 \rho(\vec{r}')d^3\vec{k}.$$

One drawback of this algorithm is that the charge distribution is zero-padded to a grid size of $(4N)^d$ compared to HE's $(2N)^d$. Vico *et al.* showed that the potential solution requires FFT's on a grid size of $(2N)^d$ after a pre-computation step of the inverse FFT of $\mathscr{F}\{G^L\}$on a grid of size $(4N)^d$. The computational time of this pre-computation step can be easily reduced by using vectorization algorithms. One can also note that the singular point ($r = 0$) is avoided without any special quadrature techniques as can be seen in the spectral integration above.

NUMERICAL IMPLEMENTATION AND TESTING

`Synergia2` is an accelerator modeling framework for combining physical effect modules for the simulation of single or multiple bunch utilizing Particle-in-Cell methods [10]. In `Synergia2`, various space solvers are included, such as 2.5 D and 3 D Hockney-Eastwood solvers, 2 D Bassetti-Erskine solver, 2 D Kapchinskij-Vladimirskij solver (all of these with open boundary conditions), and Rectangular Grid solver with rectangular boundary conditions. In this study, we implemented a new space charge solver in `Synergia2` with the Vico-Greengard-Ferrando algorithm, and compare simulation results with the Hockney-Eastwood solver.

The main difference between HE and VGF is that the computation of the truncated Green's function is done in the quadruple domain, so it was easy to implement in `Synergia2`. A uniform Gaussian distribution was used in all 3 dimensions to simplify the simulation model:

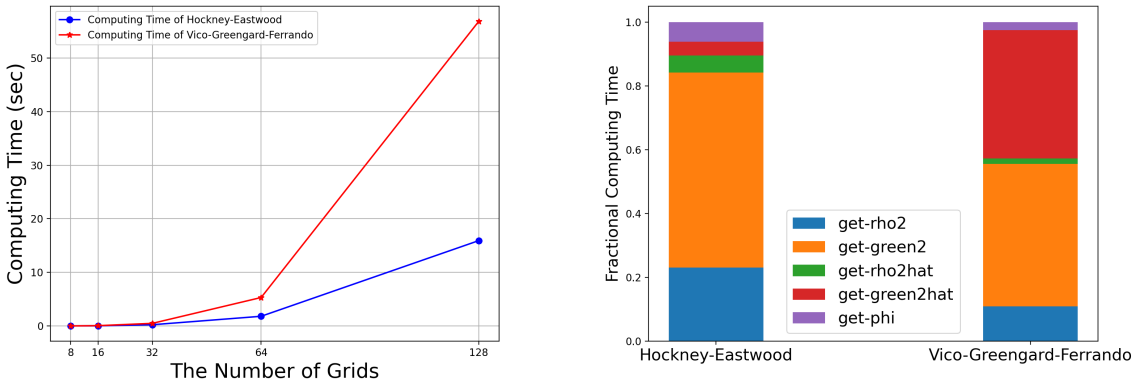
$$\rho(\vec{r}) = \frac{Q}{\sigma^3(2\pi)^{3/2}}\exp\left(-\frac{r^2}{2\sigma^2}\right),$$

where $Q = 27.24$ nC is the total charge of the beam, $\sigma = 1$ (mm) is the standard deviation for all 3 dimensions, and $r = |\vec{r}|$.

The exact solution of the Poisson equation with the above uniform Gaussian charge distribution is well known as:

$$\phi(\vec{r}) = \frac{Q}{4\pi\epsilon_0}\frac{1}{r}\mathrm{erf}\left(\frac{r}{\sqrt{2}\sigma}\right). \quad (2)$$

ISBN: 978-3-95450-227-1 ISSN: 2673-5490 doi:10.18429/JACoW-IPAC2022-MOPOTK059



(a) Maximum Relative Errors

(b) Minimum Relative Errors

Figure 3: Comparisons of computational time.

The number of grids in each dimension is the same, i.e., $[N, N, N]$. By increasing N from 8 to 128, we computed the electric potentials using HE and VGF solvers. Fig. 1 shows the electric potentials along the longitudinal beam axis for each algorithm with the different number of grids. With small N, the potential with the HE algorithm has large deviation at the center of the beam. As N is increased, this deviation is decreased.

The relative errors to the exact solutions in both algorithms are compared in Fig. 2. The VGF algorithm has smaller maximum and mean errors for small grid sizes, but larger minimum errors for all grid sizes. The maximum relative error for VGF occurs at the edge of the grid, but at the center for HE. In the case of minimum relative error, the opposite is true. Moreover, unlike HE, the accuracy of the VGF algorithm does not depend significantly on the number of grid sizes. This means that VGF can achieve high accuracy with a small grid size.

As expected, the computation time of the VGF algorithm is relatively long with a large number of grids, as shown in Fig. 3(a). This can be mitigated using advanced vectorization algorithms. However, similar accuracies for VGF can be achieved with lower N and computation time is much shorter than for HE.

Fig. 3(b) shows fractional computation time in each step for both algorithms. The computation time for charge density and Green's function is a large part of the HE solver. For the VGF algorithm, Green's function computation time is relatively longer due to the extended domain size.

CONCLUSION

The Vico-Greengard-Ferrando algorithm shows faster convergence and higher accuracy than the Hockney-Eastwood algorithm. A high degree of accuracy can be achieved, especially at the center of the distribution. In the VGF algorithm, the computation time increases significantly as the number of grids increases. However, one can easily compensate for the computation time by showing fast convergence with a smaller grid and by using vectorization techniques.

REFERENCES

[1] R.W. Hockney and J.W. Eastwood, *Computer Simulation Using Particles*, New York: McGraw-Hill Book Company, 1985.

[2] J. Qiang and S. Paret, "Poisson solvers for self-consistent multi-particle simulations," CERN Yellow Report CERN-2014-004, pp.51–55, contribution to the *ICFA Mini-Workshop on Beam-Beam Effects in Hadron Colliders*, CERN, Geneva, Switzerland, 18–22 Mar 2013. doi:10.5170/CERN-2014-004.51

[3] J. Qiang and R. Ryne, "Parallel 3D Poisson solver for a charged beam in a conducting pipe," *Computer Physics Communications*, vol. 138, no. 1, pp. 18–28, 15 July, 2001. doi:10.1016/S0010-4655(01)00185-0

[4] W. Hackbusch, *Multi-Grid Methods and Applications*, New York: Springer-Verlag, 1985.

[5] P. Wesseling, *An Introduction to Multigrid Methods*, Chichester: John Wiley & Sons, 1992.

[6] J. Qiang, S. Lidia, R.D. Ryne, and C. Limborg-Deprey, "Three-dimensional quasistatic model for high brightness beam dynamics simulation," *Phys. Rev. ST Accel. Beams*, vol. 9, p. 044204, 2006. doi:10.1103/PhysRevSTAB.9.044204

[7] J. Qiang, M. Furman, and R. Ryne, "Strong-strong beam-beam simulation using a Green function approach," *Phys. Rev. ST Accel. Beams*, vol. 5, p. 104402, 2002. doi:10.1103/PhysRevSTAB.5.104402

[8] F. Vico, L. Greengard, and M. Ferrandoa, "Fast convolution with free-space Green's functions," *Journal of Computational Physics*, vol. 323, pp. 191–203, 15 October 2016. doi:10.1016/j.jcp.2016.07.028

[9] J. Zou, E. Kim, A.J. Cerfon, "FFT-based free space Poisson solvers: why Vico-Greengard-Ferrando should replace Hockney-Eastwood," *arXiv preprint*, 15 Mar, 2021. doi:10.48550/arXiv.2103.08531

[10] Synergia2. https://synergia.fnal.gov