AN INTEGRATED GREEN FUNCTION POISSON SOLVER FOR RECTANGULAR WAVEGUIDES

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Abstract

A new method is presented for solving Poisson's equation inside a rectangular waveguide. The method uses Fast Fourier Transforms (FFTs) to perform mixed convolutions and correlations of the charge density with an integrated Green function. Due to its similarity to the widely used Hockney algorithm for solving Poisson's equation in free space, this capability can be easily implemented in many existing particle-in-cell beam dynamics codes.

INTRODUCTION

The solution of Poisson's equation is an essential component of any beam dynamics code that models the transport of intense charged particle beams, subject to the assumption that the motion is nonrelativistic in the beam frame. If the bunch is small compared to the transverse size of the beam pipe, the conducting walls are usually neglected. In this case the potential can be found using the Hockney algorithm, where the continuous convolution-based solution is replaced by a discrete convolution on a doubled grid [1]. The resulting discrete convolution can be performed using Fast Fourier Transform (FFT) techniques, with the computational effort scaling as $(2N)^d(log_2 2N)^d$, where N is the number of grid points in each dimension of the physical mesh and where d is the dimension of the problem.

When the bunch fills a substantial portion of the beam pipe transversely, or when the bunch length is long compared with the pipe transverse size, the conducting boundaries cannot be ignored. Poisson solvers have been developed to treat a bunch of charge in an open-ended pipe with various geometries [2, 3]. Another approach is to use a Poisson solver with periodic, Dirichlet, or Neumann boundary conditions on the pipe ends, and to extend the pipe in the simulation to be long enough so that the field is essentially zero there.

Here a new algorithm is presented for the open-ended rectangular pipe. Since its structure is similar to the FFT-based free-space method, it is straightforward to add this capability to codes that already have the free space solver. Also, since it is Green-function based, it does not require modeling the entire transverse pipe cross section, *i.e.*, if the beam is of small transverse extent one can model only a small transverse region around the axis. Since it is based on convolutions and correlations involving Green functions, one can use integrated Green function (IGF) techniques. These techniques have the potential for higher efficiency and/or accuracy than non-IGF methods [4, 5, 6, 7, 8, 9].

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POISSON'S EQUATION IN AN OPEN RECTANGULAR PIPE

The FFT-based free-space algorithm can be adapted to treat a beam bunch in an open-ended rectangular pipe as follows: The Green function for a point charge in an open rectangular pipe with transverse size $(0, a) \times (0, b)$ is given by, $G =$

$$\frac{1}{2\pi ab}\sum_{m,n=1}^{\infty}\frac{1}{\kappa_{mn}}\sin\frac{m\pi x}{a}\sin\frac{m\pi x'}{a}\sin\frac{n\pi y}{b}\sin\frac{n\pi y'}{b}e^{-\kappa_{mn}|z-z'|}, \quad (1)$$

where $\kappa_{mn}^2 = (\frac{m\pi}{a})^2 + (\frac{n\pi}{b})^2$. Equivalently, it is given by

$$G = R(x-x', y-y', z-z') - R(x-x', y+y', z-z') - R(x+x', y-y', z-z') + R(x+x', y+y', z-z'), \quad (2)$$

where

$$R(u,v,w) = \frac{1}{2\pi ab}\sum_{m,n=1}^{\infty}\frac{1}{\kappa_{mn}}\cos\frac{m\pi u}{a}\cos\frac{n\pi v}{b}e^{-\kappa_{mn}|w|}. \quad (3)$$

Since FFT-based methods can be used to treat both convolutions and correlations [9], the solution of the Poisson equation in an open rectangular pipe follows immediately from Eq. (2): $\phi_{i,j,k}/(h_x h_y h_z) =$

$$\mathcal{F}^{bbb}\{(\mathcal{F}^{fff}\rho_{i,j,k})(\mathcal{F}^{fff}R_{i,j,k})\} - \mathcal{F}^{bfb}\{(\mathcal{F}^{fff}\rho_{i,j,k})(\mathcal{F}^{bfb}R_{i,j,k})\} - \mathcal{F}^{fbb}\{(\mathcal{F}^{fff}\rho_{i,j,k})(\mathcal{F}^{bff}R_{i,j,k})\} + \mathcal{F}^{ffb}\{(\mathcal{F}^{fff}\rho_{i,j,k})(\mathcal{F}^{bbf}R_{i,j,k})\} \quad (4)$$

In the following section it will be shown how integrated Green functions can be used to efficiently discretize the above continuous convolutions and correlations.

INTEGRATED GREEN FUNCTION

The simplest method of discretizing a continuous convolution of a charge density ρ with a Green function G involves using values of ρ and G at the grid points. This can lead to serious inaccuracy when ρ and G have a disparate spatial variation. This can happen in a variety of situations (free space, open-ended pipe, *etc.*) depending on the problem geometry and the number of grid cells in each dimension. For example, inside a conducting pipe the beam might be long and slowly varying, whereas the pipe Green function decays exponentially with z.

Integrated Green functions (IGF's) provide a means to approximate continuous convolutions accurately when certain integrals involving G can be obtained analytically [4]. IGFs have been applied to simulations involving space-charge, beam-beam effects, and coherent synchrotron radiation [5, 6, 7, 8]. This is accomplished by assuming a simple analytical form for the variation of ρ within a cell, and computing certain definite integrals within each cell of the problem. As a result, the accuracy is controlled by how well the discretization resolves ρ, not G.

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For illustration, consider a 1D problem with isolated boundary conditions. Suppose that linear basis functions are used to approximate ρ within each cell. Then

$$\phi(x_i) = \frac{1}{h_x}\sum_{i'}\rho_{i'}\int_0^{h_x} dx'\,(h_x - x')G(x_i - x_{i'} - x') + \frac{1}{h_x}\sum_{i'}\rho_{i'+1}\int_0^{h_x} dx'\,x'G(x_i - x_{i'} - x',). \quad (5)$$

Shifting the indices in the last sum above, collecting terms, and factoring out h_x, the IGF is the coefficient of $h_x\rho_{i'}$,

$$\phi(x_i) = h_x\sum_{i'}\rho_{i'}G^{int}_{i-i'}. \quad (6)$$

Returning to the problem of the open-ended rectangular pipe, here we will use the IGF approach to treat the longitudinal dimension. Suppose that, inside the k^{th} cell, the longitudinal dependence of the charge density is given by,

$$\rho(z) = \frac{1}{h_z}\left[\rho_k(h_z - (z - z_k)) + \rho_{k+1}\,(z - z_k)\right]. \quad (7)$$

The longitudinal dependence of the IGF is, $g_z = \frac{1}{h_z^2}\times$

$$\int_{z_k}^{z_{k+1}} dz'\left[\rho_k(h_z - (z' - z_k)) + \rho_{k+1}\,(z' - z_k)\right]e^{-\kappa_{mn}|z-z'|}. \quad (8)$$

Integrating and summing over cells, 2 terms from adjacent cells contribute, with the result, $g_z(w) = \frac{1}{h_z^2\kappa_{mn}^2}\times$

$$\left[2h_z\kappa_{mn}\delta_{w,0} + \left(e^{-\kappa_{mn}|w+h_z|} - 2e^{-\kappa_{mn}|w|} + e^{-\kappa_{mn}|w-h_z|}\right)\right], \quad (9)$$

where $w = z - z_k$. In summary, in analogy to Eq. (3), the integrated Green function, R_{int}, integrated in just the longitudinal coordinate, for a distribution of charge in an open-ended rectangular pipe, is given by,

$$R_{int}(u,v,w) = \frac{1}{2\pi ab}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{1}{\kappa_{mn}}\cos\frac{m\pi u}{a}\cos\frac{n\pi v}{b}g_z(w). \quad (10)$$

NUMERICAL EXAMPLE

Consider a rectangular waveguide of full width and height $a = b = 4$ cm. The functions R and R_{int} will be calculated using $m, n = 1, \ldots, 20$. Consider a 3D Gaussian charge distribution with transverse rms sizes $\sigma_x = 6$mm, $\sigma_y = 6$mm, and longitudinal rms size σ_z. The distribution is set to zero at $x^2/\sigma_x^2 + y^2/\sigma_y^2 + z^2/\sigma_z^2 > 3^2$.

Figures 1, 2, and 3 show convolution results for the three different bunch lengths, $\sigma_z = 1.2$ cm, $\sigma_z = 12$ cm, and $\sigma_z = 1.2$ m, respectively, for grid sizes $64 \times 64 \times 128$ up to $512 \times 512 \times 1024$. The upper plot of each figure shows the potential as a function of z on-axis for various grid sizes, comparing results based on the ordinary Green function and the integrated Green function. The lower plot shows the relative error of the calculated potential. In Fig. 1, σ_z is less than the pipe transverse size (1.2 cm vs. 4 cm); both the ordinary Green function and the IGF are accurate to better than 1% for all the grid sizes shown. In Fig. 2, σ_z is somewhat larger than the pipe transverse size (12 cm vs. 4 cm); when the grid is coarse, the ordinary Green function has significant errors (a few percent to several tens of percent), while the IGF accuracy is 1% or better. In Fig. 3, σ_z is much larger than the pipe transverse size (1.2 m vs. 4 cm); in this case when the grid is coarse the ordinary Green function results exhibit huge errors (more than 100%), while the IGF accuracy is still 1% or better. As mentioned above, the accuracy of the IGF results depends on how well the grid resolves *just* ρ. For the non-IGF results, the accuracy depends on resolving *both* the ρ and G, and, due to the exponential fall-off of the G, a coarse grid gives unusable results. The relative error in the potential is shown in the lower plots. These were obtained be plotting $(\phi - \phi_{highres})/\phi_{highres}$), where $\phi_{highres}$ is the highest resolution result, obtained using the IGF with a $512 \times 512 \times 1024$.

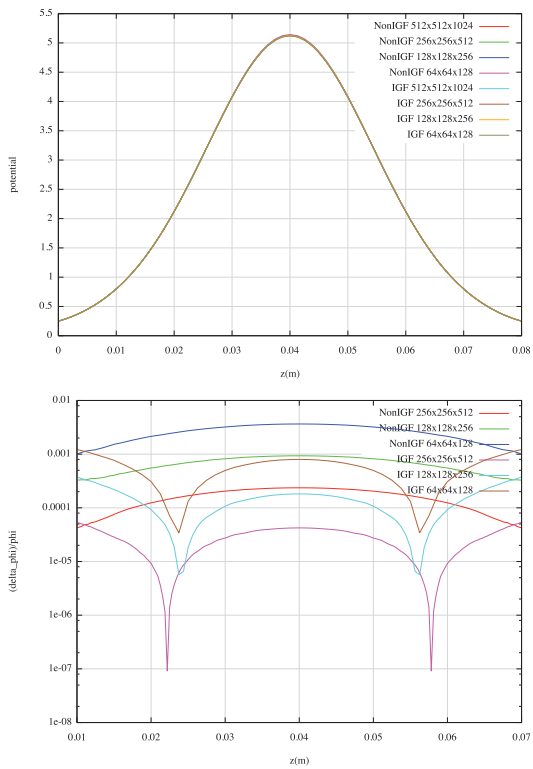

Figure 1: Top: On-axis potential vs. z showing the ordinary Green function result and the Integrated Green function (IGF) result for various grid sizes. The bunch is a Gaussian distribution with $\sigma_x = \sigma_y = 6$mm, $\sigma_z = 1.2$ cm. Bottom: Relative error of the on-axis potential vs. z for grid sizes $64 \times 64 \times 128$, $128 \times 128 \times 256$, and $256 \times 256 \times 512$.

DISCUSSION AND CONCLUSION

A new method has been presented for solving Poisson's equation in an open-ended rectangular pipe. Compared with the Hockney method for isolated systems which can be computed with a single FFT-based convolution, the new

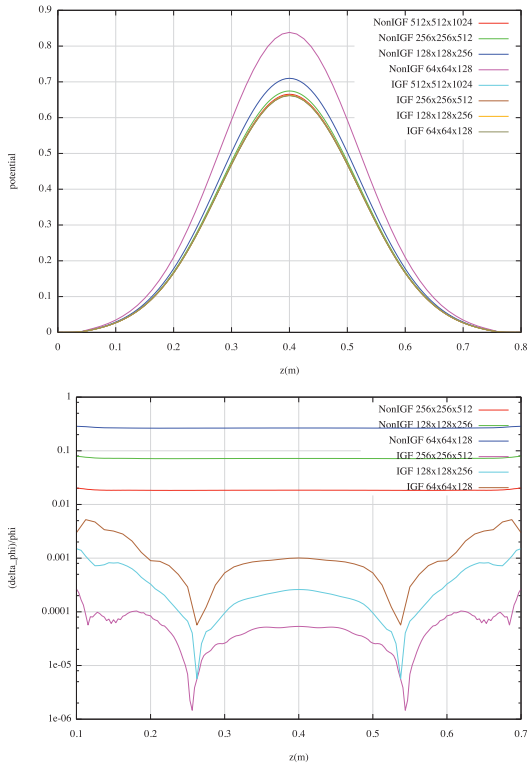

Figure 2: Top: On-axis potential vs. z showing the ordinary Green function result and the IGF result for various grid sizes. $\sigma_x = \sigma_y = 6\text{mm}$, $\sigma_z = 12$ cm. Bottom: Relative error of the on-axis potential vs. z.

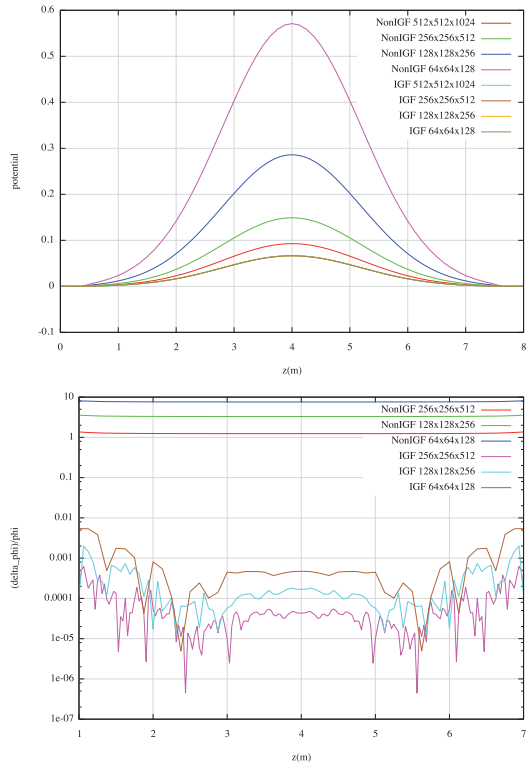

Figure 3: Top: On-axis potential vs. z showing the ordinary Green function result and the IGF result for various grid sizes. $\sigma_x = \sigma_y = 6\text{mm}$, $\sigma_z = 1.2$ m. Bottom: Relative error of the on-axis potential vs. z.

method involves 4 mixed convolutions and correlations (Eq. (4)). Starting with the Green function for a charge in an open-ended rectangular pipe (Eqs. (2-3)), an Integrated Green function (IGF) was derived (Eqs. (9-10)). Simulations of a Gaussian beam in an open-ended pipe showed that the IGF approach is more robust, *i.e.,* it retains much better accuracy than the non-IGF method over a wide range of bunch lengths. This is because the accuracy of the IGF approach depends only on having a fine enough grid resolve the spatial variation of the charge density. In contrast, the non-IGF approach is sensitive to disparities between the spatial variation of the Green function and the density.

In theory the calculation of the IGF, which is represented as an infinite series in Eq. (10), could make the simulation much more time consuming than for free-space boundary conditions. But in practice this is unlikely since free-space simulations often re-grid at every time step (or as needed) to account for the changing beam size. This would not be the case for the rectangular pipe solver if the beam filled most of the pipe transversely, since the IGF would be computed once, Fourier transformed 4 ways, stored, and reused.

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