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SELF-CONSISTENT MODELING USING A LIENARD-WIECHERT PARTICLE-MESH METHOD

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Abstract

In this paper we describe a parallel, large-scale simulation capability using a Lienard-Wiechert Particle-Mesh (LWPM) method. The approach is a natural extension of the convolution-based technique to solve the Poisson equation in space-charge codes. It provides a unified method to compute both Coulomb-like self-fields and radiative phenomena like coherent synchrotron radiation (CSR). The approach brings together several mathematical and computational capabilities including the use of integrated Green function (IGF) methods and adaptive quadrature methods. We will describe the theoretical model and our progress to date.

INTRODUCTION

The simulation of beam dynamics in particle accelerators has undergone tremendous advances in recent years. There now exist several massively-parallel multi-physics codes that include 3D space-charge effects. Despite advances in space-charge modeling, the simulation of 3D radiative phenomena such as coherent synchrotron radiation (CSR) has remained an outstanding problem. Yet the ability to accurately model CSR has become a key issue due to the growing importance of accelerators involving bright electron beams, *e.g.*, the drivers for X-ray Free Electron Lasers (XFELs).

Previously the authors have reported on a Lienard-Wiechert (LW) method to compute electromagnetic fields [1,2]. In this paper that method is extended to self-consistent modeling using a technique we call the Lienard-Wiechert particle-mesh (LWPM) method. As will be shown the method is a natural extension of techniques that have previously been used to model 3D space-charge effects.

SPACE-CHARGE SIMULATION

Existing space-charge codes typically solve Poisson's equation in the bunch frame by some method, compute the self-fields, and transform back to the lab frame. The self-fields are then used along with external fields to advance the particles. The most widely used approach to compute the self-fields is a convolution method with free-space boundary conditions [3]. The scalar potential in the bunch frame is,

$$\phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_o}\int d\mathbf{r}'\rho(\mathbf{r}')G(\mathbf{r}-\mathbf{r}'), \quad (1)$$

where ρ is the charge density and where the free-space Green function for ϕ is,

$$G(\mathbf{r}-\mathbf{r}') = \frac{\mathbf{1}}{|\mathbf{r}-\mathbf{r}'|}. \quad (2)$$

A simple discretization of Eq. (1) leads to,

$$\phi_{i,j,k} = \frac{\delta_x\delta_y\delta_z}{4\pi\epsilon_o}\sum_{i'=1}^{i'_{max}}\sum_{j'=1}^{j'_{max}}\sum_{k'=1}^{k'_{max}}\rho_{i',j',k'}G_{i-i',j-j',k-k'}, \quad (3)$$

where $(\delta_x, \delta_y, \delta_z)$ is the grid cell size, $\rho_{i,j,k}$ is the charge density at the grid points, and $G_{i-i',j-j',k-k'}$ denotes G at values of grid point separation. Fast Fourier transforms (FFTs) can then be used to efficiently compute the convolution by appropriate zero-padding [4]. Hence the solution of Eq. (3) is,

$$\phi_{i,j,k} = \frac{\delta_x\delta_y\delta_z}{4\pi\epsilon_o}\mathcal{F}^{-1}\{(\mathcal{F}\rho_{i,j,k})(\mathcal{F}G_{i,j,k})\} \quad (4)$$

where $\mathcal{F}$ denotes a forward FFT and $\mathcal{F}^{-1}$ denotes an inverse FFT.

The discrete convolution, Eq. (3), is a simple approximation to Eq. (1). It makes use of G only at the grid points even though it is known everywhere analytically. This can lead to serious inaccuracy when ρ and G have disparate spatial variation, as is often the case with high aspect ratio grids. There may also be difficulties dealing with the singularity.

These problems are solved by using integrated Green functions (IGF's) [5–8]. In this approach a simple analytical form is assumed for the variation of ρ within a cell, and the convolution integral is performed analytically for each cell of the problem. As a result, the accuracy is controlled by how well the discretization resolves ρ, not G.

To summarize, the usual treatment of space charge involves solving the Poisson equation in the bunch frame using a convolution method with an IGF. Similarly, one may obtain the fields directly (not from the potential) by replacing Eq. (2) with the Green function for the fields,

$$\mathbf{G}(\mathbf{r}-\mathbf{r}') = \frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^{3/2}}. \quad (5)$$

at the expense of performing more FFTs.

LIENARD-WIECHERT SIMULATION

Now consider the Lienard-Wiechert (LW) fields,

$$\begin{aligned}\vec{E} &= \left[\frac{q}{\gamma^2\kappa^3R^2}\left(\hat{n}-\vec{\beta}\right)+\frac{q}{\kappa^3Rc}\hat{n}\times\left\{\left(\hat{n}-\vec{\beta}\right)\times\frac{\partial\vec{\beta}}{\partial t}\right\}\right]_{ret}\\ \vec{B} &= (1/c)\hat{n}_{ret}\times\vec{E}. \quad (6)\end{aligned}$$

where $\hat{n} = \vec{R}/|R|$ is a unit vector pointing from the retarded emission point to the observation point, $\vec{\beta} = \vec{v}/c$, c is the speed of light, $\gamma = 1/\sqrt{1-\beta^2}$, and $\kappa = 1 - \hat{n}\cdot\vec{\beta}$.

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The transition to LW modeling begins by noticing that the space-charge method is equivalent to using a LW approach, ignoring the radiation term, and replacing the velocity term involving retarded quantities with the Heaviside expression involving instantaneous quantities. The Heaviside expression is,

$$\mathbf{E} = \frac{1}{\gamma^2 r^2} \frac{\hat{\mathbf{r}}}{\left(1 - |\beta \times \hat{\mathbf{r}}|^2\right)^{3/2}}, \quad (7)$$

where $\hat{\mathbf{r}}$ points from the (instantaneous) emission point to the observation point.

In other words, convolution-based codes that solve Poisson's equation in the bunch frame and transform back to the lab frame are using the same physical model as if they used Eq. (7) in the lab frame. These codes have two omissions: First, they ignore the radiation term. Second, they don't correctly calculate the Coulomb term in dipole magnets, because the Heaviside expression assumes a particle moving in a straight line at constant velocity.

To remedy these omissions we use the full LW expression for the fields of a point charge. The solution of Poisson's equation in free space can be expressed exactly as a convolution involving difference variables. But in a particle-mesh (PM) code it's approximate since, to be exact, all particles would have to be moving exactly in the same direction at the same energy, as is evident by γ and β appearing in Eq. (7). In the LWPM method we approximate the fields as a convolution although strictly speaking this is an approximation whose validity is problem dependent. Furthermore, we take the convolution kernel to be the LW field of the bunch centroid. As a result it is necessary to keep track of the history of just the centroid, not all the simulation particles. This represents a significant savings in memory compared with a point-to-point (with history) LW code.

THE LW3D CODE

We have developed a prototype of a code, called LW3D, for 3D self-consistent simulation using the LWPM method. It makes use of several algorithmic and computational technologies:

- Domain decomposition
- Parallel FFT of distributed data [9]
- Integrated Green function (IGF) methods
- Numerical IGFs
- Efficient trajectory integration with adaptive step size (for retarded quantities)
- Adaptive quadrature [10]

Traditionally, the use of an IGF has been possible because the integral over a computational cell of the free-space Coulomb Green function or the Green function for the fields can be found analytically. This is not possible for the LW Green function. To deal with this, we use a numerically integrated Green function (nIGF) method. In this method an adaptive quadrature package (also known as adaptive cubature in the multi-dimensional case) is used to perform the definite integrals of the Green function over the problem cells.

In a space-charge code the computational bottleneck will depend on the problem parameters but often it is associated with inter-node communication in the space-charge computation. The time spent calculating the Green function, Eq. (7), at all values of grid point separation, is minor. If the IGF is used the effort is somewhat larger but still not dominant. In contrast, an LWPM code must evaluate Eq. (6). This is computationally demanding due to the need to find the retarded quantities for every tabulated value of the LW Green function based on the history of the centroid. Domain decomposition is essential to distribute the computational load. The calculation in Eq. (6) requires no communication, so an LWPM code is ideally suited to computer architectures that favor high FLOPS with little data movement.

RESULTS

Consider a 1 nC, 1 GeV cold Gaussian bunch propagating in a drift space and expanding due to it's space-charge field. The bunch has rms size $\sigma_x = \sigma_y = \sigma_z = 1$ mm in the bunch frame. Using the convolution, Eq. (3), we have modeled this using the following different methods for computing the Green function:

- Analytic IGF: Using the IGF for Eq. (7)
- Heaviside nIGF: Using Eq. (7) with adaptive quadrature
- LW nIGF: Using Eq. (6) with adaptive quadrature

Analytic IGF is what is used in existing space-charge codes such as IMPACT. Heaviside nIGF is essentially a test of the adaptive quadrature package. LW nIGF tests both the quadrature package and tests the software that computes retarded quantities and the resulting LW field, Eq. (6). Note that the LW nIGF method is used here only as a test of the software, *i.e.*, one would never use retarded quantities (that are time-consuming to compute) when one could use instantaneous quantities, as is the case when the Heaviside approximation is valid. But as a test of the computational method, this is a challenging regime for the LW nIGF model. The computation of retarded quantities in this 1 GeV example involves retarded positions that are more than 100 ns (i.e. more than 30 m) behind the bunch.

Figure 1 shows the horizontal rms beam size, x_{rms}, as a function of z. All three methods exhibit the same growth in beam size. (The analogous plots for y and z look the same.) This gives confidence in the adaptive quadrature method for the IGF and in the calculation of retarded quantities. Rather than looking at rms size, the rms emittance provides a more sensitive diagnostic. Figure 2 shows the horizontal rms emittance growth. Again, all three methods agree. This is an important test since one of the primary purposes of such simulations is to estimate rms emittance growth. This demonstrates that, in this example for which the a space-charge model and the LWPM should agree, the two methods predict the same rms emittance growth.

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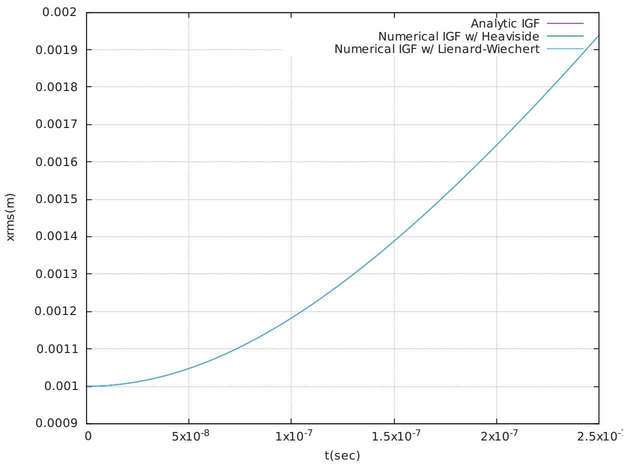

Figure 1: x_{rms} versus t for a 1 GeV, initially cold Gaussian electron beam in a drift space. The Green function was calculated three different ways as described in the text. All the curves lie on top of each other.

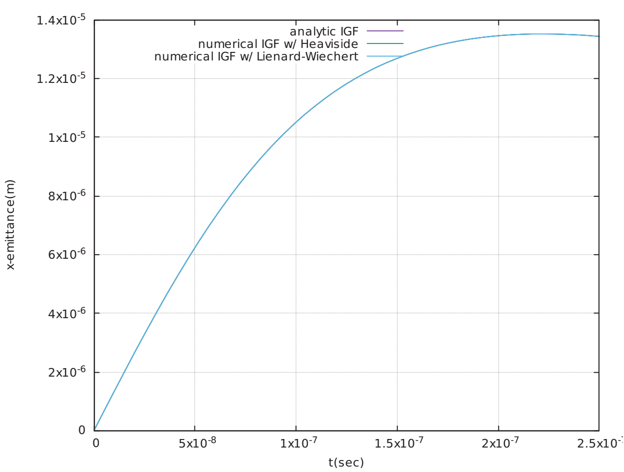

Figure 2: ϵ_x versus t for a 1 GeV, initially cold Gaussian electron beam in a drift space. The Green function was calculated three different ways as described in the text. All the curves lie on top of each other.

FUTURE WORK

Having verified that the LWPM method works for a beam expanding in free space, we are now in the process of testing it for a steady-state dipole model and for a chicane model. We expect that the singularity in the LW radiation term at high γ will have to be treated with care. However, previous results have already shown that that a convolution-based approach agrees with brute force LW summation in certain test cases [2]. We have now begun to implement a 3D, self-consistent simulation of the Berlin-Zeuthen benchmark using the LWPM method [11].

CONCLUSION

The 3D simulation of radiative phenomena like CSR remains an outstanding problem despite the major advances in 3D space-charge modeling. In this paper we have described an approach – the LWPM method – that is a natural extension of the space-charge approach. We have shown that a simulation based on calculation of LW retarded quantities produces essentially the same results as a Heaviside model (the space-charge model) for a beam expanding in free space. This is the case even at high γ, where the computation of retarded quantities is potentially difficult and where the Green function is highly singular. Given these results, the LWPM method holds great promise for the simulation of 3D phenomena in more complex systems like bunch compressors. At this time we are preparing to perform 3D simulations of the Berlin-Zeuthen benchmark chicane.

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