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Numerical approaches for space charge calculations in intense proton beams

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Abstract

Charged particle beams in modern particle accelerators are becoming increasingly intense, with the number of particles per bunch reaching 10^{11}-10^{14}. Examples of relevant systems include synchrotrons and particle storage rings for high-energy colliders. Mathematical modeling is widely used in modern particle accelerator design to predict the long-term evolution of particle position-momentum phase space that reflects the physics of the problem. In order to understand collective particle dynamics, one needs reliable predictions for the forces exerted on the particles due to the interactions among them.

Due to the very high number of particles in beams, direct computation of particle-particle interaction requires prohibitively long computation times. Therefore, macroparticle-based approximations to space charge distributions, coupled with numerical methods to compute the electric potentials and fields are used in order to make the computational complexity manageable. The total number of macroparticles can be reduced to tractable numbers (~10^6), and the numerical methods make use of implementations that require the lowest number of computer operations to solve for the electric field.

This paper compares the accuracy and convergence rates of two popular numerical algorithms used to solve the Poisson's equation, a) spectral solvers, used in Fermilab's Synergia 2.0 code, and b) fast Fourier transform – based finite-difference solvers. In particular, the Poisson solvers are compared based on their accuracy (convergence of the solution with respect to the grid resolution and the number of macroparticles used in the 'particle-in-cell' (PIC) approximation to the charge density). Various implementations of the PIC scheme itself are also tested for accuracy.

Introduction

Charged particles in particle beams interact with one another through electromagnetic forces. In practical accelerator systems, particles can have charges of the same sign, e.g., all protons, or of different signs, e.g., protons-antiprotons. Practical beams have of particles of the same sign charge close together, while particles of opposite signs interact only upon collision. The mutual repulsive forces that are felt by protons in beams cause the beams to diverge, therefore, a set of quadrupole magnets is typically used in accelerators to keep the beam focused as it travels in a synchrotron beampipe.

Particle dynamics in a proton accelerator, for instance, a synchrotron with multiple fodo cells connected sequentially, will be affected by the space charge repulsive forces in several ways, including the changes in the transverse profile of the beam, longitudinal spread of a particle bunch, and, more importantly, loss of synchronism between the accelerating RF pulses and the traveling proton bunch. The long-term effects of the space charge on particle dynamics, can cause significant variations in proton beam luminosity, spatial profile, and proton kinetic energy distributions. These, in their turn, lead to various instabilities in a single beam or during collisions between two bunches traveling in opposite directions. For this reason, the accurate prediction of long-term dynamics of particle beams is very important to the design of accelerators and their control systems.

Due to the ultimate complexity of the problem, space charge calculations can only be done using approximate numerical methods, rather than with analytical methods. The two most common classes of methods used are particle-based methods [1] and deterministic continuum methods such as 'rigid beam' approximation [2].

While the particle-based methods treat particle beams as collections of interacting macroparticles, thus allowing any space charge distributions to be included in dynamic calculations the rigid-beam methods make strict assumptions about the shape of the bunch and treat all collective oscillations and instabilities as perturbations of the fundamental modes of transverse and longitudinal oscillations in beam position. Thus, in many instances, particle-based simulations provide essential information about phase space evolution that is not available from continuum methods. Related phenomena include filamentation of proton bunches in phase space and departure of charge distributions from Gaussian due to bunch-bunch interactions [4]. Self-consistent calculations of space charge that reflect the actual evolution of the particle phase-space are, therefore, essential in order to capture such instabilities and distortions in particle beams.

Particle tracking codes for accelerators use a variety of approaches to solve for the electromagnetic forces due to self-fields, including: spectral methods [1], finite-difference time-domain (FDTD) and finite-difference (FD) methods [3]. Due to a very large number of individual charged particles (10^{11}-10^{14}), for example, protons coasting in a storage ring, direct particle-particle methods for computing the electric fields are prohibitively costly, and approximations, such as particle-in-cell (PIC) are used [3]. The discretization of the spatial computational domain and the assignment of charge density using PIC result in numerical errors, due to additional 'numerical' non-physical fluctuations in the electric self-fields. Estimates of these fluctuations can be used in predictive models that treat, for example, the emittance growth in a coasting particle bunch as a combination of physically observable effects and numerical errors [4].

Figuring out how the numerical errors in the simulated electric field are affected by the nature of the Poisson solver, parameters used by the solver, the choice of a PIC scheme, numbers of macroparticles used, is of high importance to understanding long-term particle dynamics, collective modes of oscillation, physical and numerical instabilities in particle beams.

Theory

In this analysis all calculations are done in the inertial frame of reference of the moving proton bunch. This is the standard approach used by beam dynamics modelers, allowing to later apply a Lorentz transformation to convert particle position-momentum trajectory to a stationary 'lab frame'. Another assumption that has proved itself accurate for most particle accelerator systems is that the dynamical changes in the electric and magnetic self-fields occur on a time scale that is considerably longer than the collective oscillations in the accelerated beams [5], so a static Poisson's equation approximation (1) is valid under those conditions to describe the beam space charge.

$$\nabla^2\Phi = -\frac{\rho}{\varepsilon_0} \qquad (1)$$

where Φ is the electric potential, ρ is the charge density, and ε_0 is the permittivity of free space.

The right-hand side of (1) is computed using a particle-in-a-cell (PIC) approach [1] using a set of 'macroparticles' representing interacting charges within a proton bunch. In the PIC methods, the Cartesian space occupied by the space charge is also discretized using a grid. Then, the continuous charge density at node p, located at position x_p is calculated by summing up weighted contributions of each macroparticle to the charge density:

$$\rho(\vec{x}_p) = \frac{q}{V}\sum_{i=1}^{N_p} W_M(\vec{x}_i - \vec{x}_p) \qquad (2)$$

where x_p and x_i is a the position vectors corresponding to p-th grid node and i-th particle position, W_M is a weighting function of order M, N_p is the number of macroparticles used, V is the volume of a grid cell.

In this paper, two methods are used to solve the particle-based Poisson equation: a) a spectral Hockney's method and b) a finite-difference matrix method, accelerated with the help of fast Fourier transforms. One of the reasons why this comparison is important is that due to the completely different nature of the methods, one of which, (a), implements the Green's function approach, and the other, (b), uses direct discretization of the Laplace operator and utilizes its explicit eigenfunctions and eigenvalues.

There exist multiple implementations of the finite difference electromagnetic solvers methods available. Some of them are finite-difference time-domain (FDTD) schemes, for instance, [6]. Since this paper makes an assumption that electric self-fields are well approximated as static, an FD Poisson solver is used to solve (1). The particular implementation was using in this article.

The spectral Poisson solver is based on the theoretical framework in [1], and its practical implementation bears a very close resemblance to that used by the developers of Synergia 2.0 code at Fermilab [6]. Under this approach, the electric potential is written as the discrete convolution of the charge density from (2) with the Green's function that satisfies the PDE of specific dimensionality (3a). Then the spectral convolution theorem is used to find the electric potential in reciprocal space (3b). Finally, the real-space electric potential is written as (3c). This potential distribution can now be utilized to find the electric field and the forces acting on individual macroparticles.

$$\Phi(\vec{x}_p) = V\sum_{p'=1}^{N} G(\vec{x}_p - \vec{x}_{p'})\rho(\vec{x}_{p'}) \tag{3a}$$

$$\widetilde{\Phi}(\vec{k}) = F(G(\vec{x}))F(\rho(\vec{x})) \tag{3b}$$

$$\Phi(\vec{x}) = F^{-1}(\widetilde{\Phi}(\vec{k})) \tag{3c}$$

where G is the Green's function of the Poisson's equation, F and F^{-1} are direct and inverse Fourier transforms, respectively, N is the number of nodes at which the charge density is interpolated.

Under the finite-difference approach, equation (1) is discretized on a finite grid and the partial derivatives in the Laplacian are replaced with finite differences. Then the Poisson equation is replaced with a system of finite difference equations. For instance, in two dimensions, these equations take the form:

$$4\Phi_{i,j} - \Phi_{i+1,j} - \Phi_{i-1,j} - \Phi_{i,j+1} - \Phi_{i,j-1} \approx -\frac{h^2\rho_{i,j}}{\varepsilon_0} \tag{4}$$

where i and j are nodal indices, h is the discretization step.

The resulting matrix equation can be rewritten as:

$$\Phi U = B,\ or\ \begin{bmatrix} S & T & 0 & 0 \\ T & S & 0 & 0 \\ 0 & 0 & S & T \\ 0 & 0 & T & S \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \end{bmatrix} = \begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ B_4 \end{bmatrix} \quad (5)$$

where U_1 to U_4 are electric potential column-vectors, B_1 to B_4 are column vectors that depend on charge distribution, matrices S and T are block matrices that are related to the eigenvectors Q and eigenvalue diagonal matrices D_S and D_T as follows:

$$S = Q^{-1} D_S Q, T = Q^{-1} D_T Q \quad (6a)$$

The combined eigenvalue matrix is then:

$$\Lambda = D_S + D_T \quad (6b)$$

The solution of the system of Poisson FD equations can be greatly accelerated by using singular value decomposition of Φ in (5) and the exploring the properties of the eigenvectors of the Poisson's operator:

$$Q_{j,l} = \sqrt{\frac{2}{m+1}} \sin\left(\frac{\pi j l}{m+1}\right),\ j,l = 1,2,...,m \quad (7a)$$

$$Q^{-1} = Q \quad (7b)$$

The presence of the index-dependent harmonic function in (7a) prompts the use of the sine transforms that can be evaluated using fast Fourier transform algorithms, thus reducing the complexity of matrix inversion from $O(N^3)$ to $O(N\log_2(N))$, where N is the rank of the matrix in (5).

In order to compute the vector of nodal potentials U, steps (8a) to (8c) are utilized:

$$\bar{B} = QBQ \quad (8a)$$

$$U(j,k) = \bar{B}(j,k)/(\Lambda(j,j) + \Lambda(k,k)) \quad (8b)$$

$$U = Q\bar{U}Q \quad (8c)$$

The electric field can be then computed from the electric potential using a gradient the latter, evaluated numerically.

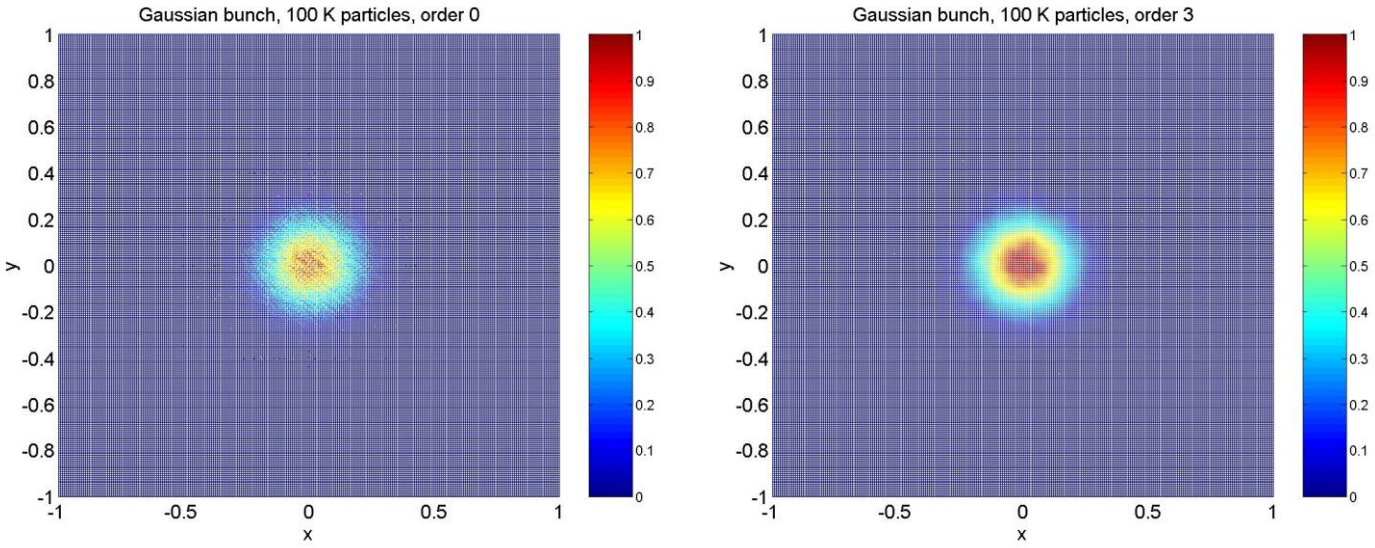
An integral part of any particle-mesh space charge solver is a PIC scheme that assigns spatial distributions of charge density using macroparticle positions at each time step. PIC was also implemented in two versions – with flat-top (zero-order b-spline) weighting functions and order 3 b-splines. Order 3 b-splines have smoother shapes [3], they are computed by convolving two order 1 b-splines, which are, in their turn, computed by finding a convolution of order 0 (flat-top) b-splines.

The two types of particle charge distributions considered in this paper are the 2-D Gaussian bunch (GB) and 2-D Kapchinski-Vladimirski (KV) beam [5]. Both ideal cases allow the electric field to be calculated from the charge density analytically [4], [5], [9]. In order to simulate the deposition of

charged macroparticles onto a numerical grid, the PI used a Monte Carlo approach with uniform and Gaussian p.d.f.'s, generated using Sobol sets.

Results

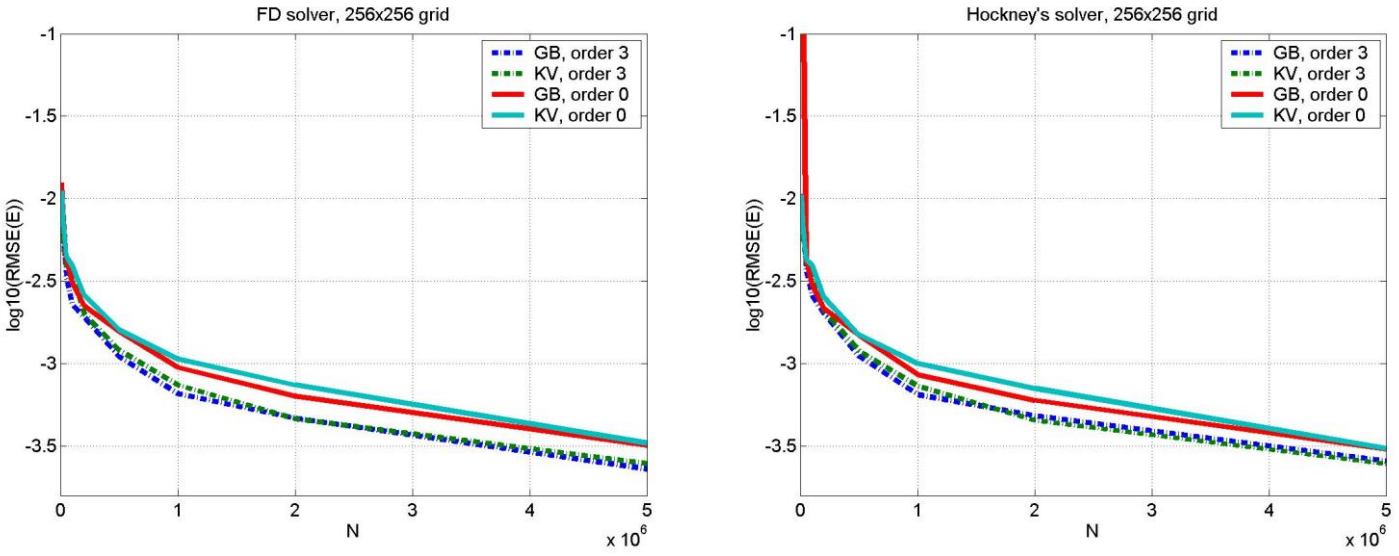
The rest of this section presents simulation results. Figure 1 shows comparisons between the 2-D space charge density generated using a PIC with flat-top and b-spline of order 3 macroparticles [1] for a reasonably large number of macroparticles (N_m=100,000).



a) b)

Figure 1. Space charge density calculated by the PIC algorithm for a Gaussian bunch using 100,000 macroparticles, a) order 0 b-splines, b) order 3 b-splines.

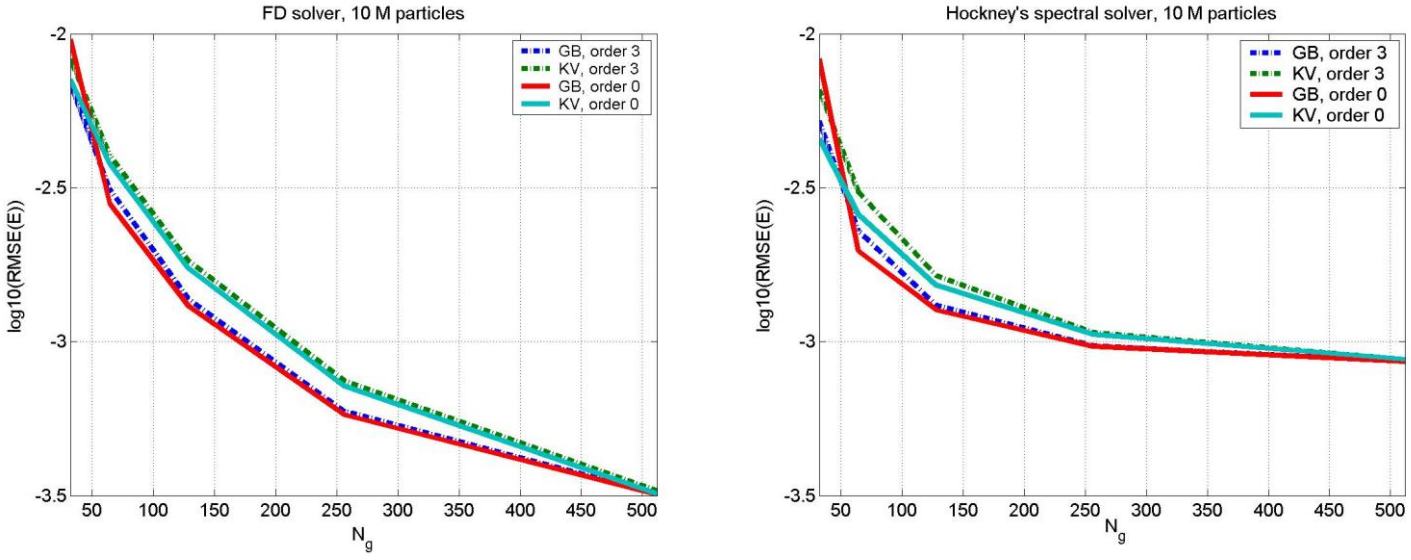
As one can see from the plots, the charge density predicted with higher-order weighting functions in PIC (Figure 1b) has less stochastic variation. Figure 2 presents the stochastic root mean squared error (RMSE) in electric field due to the charge deposition using flat-top and higher-order macroparticles as a function of the number of macroparticles on a 256x256 numerical grid.



a) b)

Figure 2. RMS error in electric field as a function of the number of macroparticles for the 256x256 numerical grid, FD vs. Hockney's spectral solver, a) FD solver, b) Hockney's spectral solver.

It can be seen from Figure 2 that for both GB and KV beams, the RMS error in electric field is consistently lower when the higher-order spline weighting function is used in the PIC charge assignment. In Figure 3, stochastic numerical error produced by FD and Hockney's spectral solvers is plotted against the grid resolution for 10 million macroparticles used in simulations.



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a) b)

Figure 3. Convergence of the RMS of stochastic error in the calculated electric field with respect to the grid refinement, a) FD vs. b) Hockney's spectral solver, for 10 million macroparticles.

As expected, the total computation time is found to scale approximately as $N_g^2 * \log_2(N_g^2)$, where N_g is the number of grid points along one of the axes of the numerical grid. For the same spatial resolution and the same boundary conditions, the Hockney's spectral algorithm was found to work marginally faster than the finite-difference method. On a parallel machine, this distribution of computation times may be different.

Discussion and Conclusions

Recent comparative studies of the numerical accuracy of Poisson solvers for space charge in particle beams conducted at CERN [8] have shown that finite-difference methods can provide better accuracy at the same spatial discretization and better convergence of the result with the increasing number of nodes than fast multipole methods. This suggests that the use of FD methods in space charge solvers can be beneficial to achieve more accurate long-term beam dynamics tracking. In this paper, in a similar fashion, the accuracy of the FD methods and spectral methods are compared, and our conclusion is that the FD Poisson solvers have greater potential for reducing simulation errors in space charge potentials and fields. FD methods can also handle various types on boundary conditions, describing conductor-dielectric and dielectric-dielectric interfaces. The current implementation of the space charge calculator in the Fermilab Synergia 2.0 particle-tracking code has some room for improvement. In particular, changing the Poisson solver algorithm from the current Hockney's spectral solver to a fast FD Poisson solver can help further reduce the E-field fluctuations due to numerical effects. Besides this, the use of higher order weighting functions in the charge assignment should allow significant reduction in the stochastic noise in the PIC charge assignment scheme.

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