ACCURACY AND EFFICIENCY OF 2D AND 3D FAST POISSON'S SOLVERS FOR SPACE CHARGE FIELD CALCULATION OF INTENSE BEAM

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Abstract

Design of particle accelerators with intense beams requires careful control of space charge problem. To obtain accurate treatment of the problem, solution of the Poisson's equation for electrostatic potential created by an arbitrary space charge distribution of the beam is required. Numerical routines developed for 2D and 3D space charge field calculation of high current beam are examined. Two numerical techniques are used: (i) finite-difference method, combining Fourier expansion and Gauss elimination and (ii) spectral method, utilizing Fourier expansion of electrostatic potential. Accuracy and time consuming for calculation of test problem are compared.

1 NUMERICAL ERRORS AND CONSERVATION LAW

Particle-in-cell code BEAMPATH has been developed for study of wide range of problems with intense beams [1]. Space charge field of the beam at every time step of particle trajectories integration is calculated from the Poisson's equation $\Delta U = - Q$, where U is a space charge potential and Q is a space charge density of the beam. Calculation includes distribution of space charge of macroparticles among the grid nodes, solution of Poisson's equation on a grid, and differentiation of grid potential function to find components of electrostatic field of the beam.

Important point in numerical simulations is a balance between accuracy and required resources of computer to get an efficient solution of the problem. Good accuracy in space charge problem is obtained, if number of macroparticles per cell is large enough and if a mesh size is much smaller, than the beam size. Meanwhile, even if these conditions are fulfilled, the following errors are unavoidable: (i) errors due to discrete charge representation in particle method, (ii) errors due to substitution of exact derivatives of Poisson's equation by approximation formulas, (iii) errors of differentiation of potential function to obtain values of electric field components, and (iiii) computer round-off errors.

To control errors of calculations, the following parameter can be used

$$g = \left| 1 - \int_S \vec{E}\, d\vec{S} \Big/ \int_V Q\, dV \right| , \qquad (1)$$

which has a meaning of error of the Gauss theorem. It is clear, that in exact calculations parameter g=0. In Eq. (1) the denominator is equal to the total charge of the beam, which is known exactly and does not depend on numerical method. The numerator in Eq. (1) depends on solution of the Poisson's equation and includes all errors, arising at the stage of space charge calculations. Control of the Gauss theorem, Eq. (1), gives an integral numerical error. Meanwhile, the Gauss theorem does not provide information about fluctuation of solution in detail. An extra criteria like averaged deviation from the exact solution is required. Below we consider numerical technique and typical errors of numerical solution of Poisson's equation in different coordinate systems.

2 SPACE CHARGE SOLVER IN 2D CARTESIAN COORDINATES

Space charge field of a z-uniform beam is calculated from the Poisson equation in two-dimensional Cartesian coordinates (see Fig. 1a)

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = - Q(x,y) , \; U(\Gamma) = 0 , \qquad (2)$$

with Dirichlet boundary condition for potential U at the surface of an infinite pipe, Γ. Unknown potential of the beam at grid points, $U(x_i, y_j)$, is represented as Fourier series:

$$U_{ij} = \sum_{n=1}^{N_x-1} \sum_{m=1}^{N_y-1} \bar{U}_{nm} \sin\left(\frac{\pi n i}{N_x}\right) \sin\left(\frac{\pi m j}{N_y}\right) , \qquad (3)$$

similar for space charge density, $Q(x_i, y_j)$. After substitution of expansions (3) into Poisson's equation (2), Fourier coefficients of space charge, $\bar{Q}_{nm}$, and potential, $\bar{U}_{nm}$, are connected by an algebraic relationship

$$\bar{U}_{nm} = \frac{\bar{Q}_{nm}}{\left(\frac{\pi n}{a}\right)^2 + \left(\frac{\pi m}{b}\right)^2} , \qquad (4)$$

which gives solution of the problem.

In Table 1 the error of the Gauss theorem as well as the round-off error for the test problem with random initial data are presented. As seen, parameter g has a value of $\sim 10^{-2} - 10^{-4}$.

3 SPACE CHARGE SOLVER IN 2D CYLINDRICAL COORDINATES

Space charge field of the train of axial-symmetric bunches is calculated from the Poisson equation in two-dimensional cylindrical coordinates:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial U}{\partial r}\right) + \frac{\partial^2 U}{\partial z^2} = - Q(r,z) , \qquad (5)$$

with Dirichlet boundary conditions at the surface of the tube, Neumann condition at the axis and periodic condition in z-direction (see Fig. 1b):

$$U(a,z) = 0\ ;\ \frac{\partial U}{\partial r}(0, z) = 0\ ,\ U(r,z) = U(r,z + L)\ . \qquad (6)$$

Poisson's equation (5) is substituted by finite-difference analog:

$$U_{k,j+1}\left(1+\frac{1}{2(j-1)}\right) - 2U_{k,j}\left(1+\frac{h_r^2}{h_z^2}\right) + U_{k,j-1}\left(1-\frac{1}{2(j-1)}\right)$$

$$+ U_{k+1,j}\left(\frac{h_r}{h_z}\right)^2 + U_{k-1,j}\left(\frac{h_r}{h_z}\right)^2 = -Q_{k,j}\,h_r^2\ . \qquad (7)$$

Calculations start with Fourier expansion of unknown potential, $U_{k,j}$, in z-direction

$$U_{k,j} = \sum_{m=1}^{N_z} \overline{U}_m(j)\exp\left(-i\,\frac{2\pi\,(k-1)\,(m-1)}{N_z}\right)\ , \qquad (8)$$

similar for space charge density, $Q_{k,j}$. Coefficients of Fourier expansion, $\overline{U}_m(j)$, are calculated via inverse Fourier transform:

$$\overline{U}_m(j) = \frac{1}{N_z}\sum_{k=1}^{N_z} U_{kj}\exp\left(i\,\frac{2\pi\,(k-1)\,(m-1)}{N_z}\right)\ , \qquad (9)$$

similar for $\overline{Q}_m(j)$. Substitution of expansion (8) into the finite-difference analog of the Poisson's equation (7), results in a three-diagonal matrix equation:

$$\alpha_j\,\overline{U}_m(j+1) + \beta_j\,\overline{U}_m(j) + \gamma_j\,\overline{U}_m(j-1) = w_j\ , \qquad (10)$$

which is solved utilizing the Gauss elimination method [2]. After that, the potential in grid points is calculated using Fourier series (8).

In Table 2 results of numerical solution of the test problem for axial-symmetric bunch with Gaussian distribution

$$Q = \frac{1}{(2\pi)^{3/2}\,\sigma^2\,\sigma_z}\exp\left(-\frac{x^2+y^2}{2\sigma^2} - \frac{z^2}{2\sigma_z^2}\right)\ , \qquad (11)$$

are presented. Potential of the Gaussian bunch is given by

$$U = \int_0^{\infty} \frac{dq}{4\pi^{3/2}(2\sigma^2+q)\sqrt{(2\sigma_z^2+q)}}\exp\left[-\frac{x^2+y^2}{(2\sigma^2+q)} - \frac{z^2}{(2\sigma_z^2+q)}\right]. \qquad (12)$$

In every point the numerical solution is different from the exact one. The accumulated error among all particles, normalized on the maximum value of space charge, gives an averaged error:

$$\varepsilon = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\left|\vec{E}^{(i)}_{numer}(r,z)\right| - \left|\vec{E}^{(i)}_{analyt}(r,z)\right|}{\left|\vec{E}_{max}\right|}\right)\ . \qquad (13)$$

which has a value of 10^{-2} - 10^{-3} for the considered case.

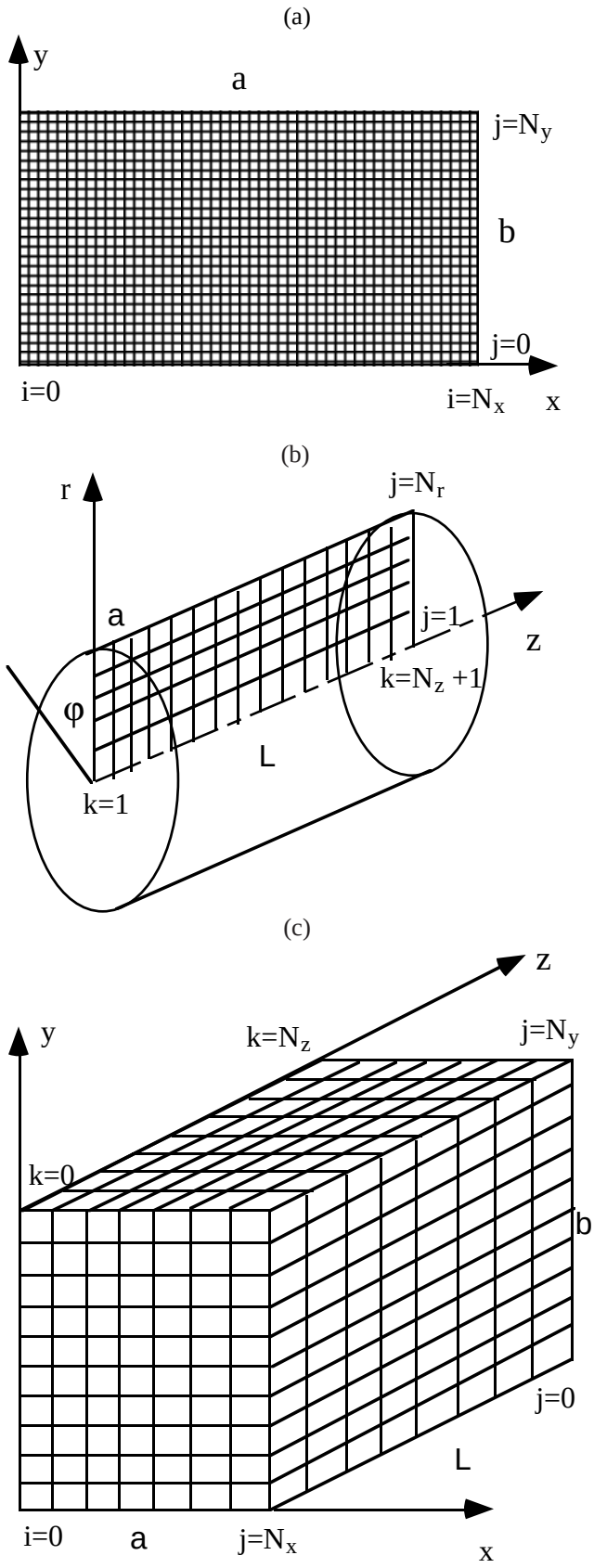

Fig. 1. On space charge calculations for :
(a) z-uniform beam, (b) axial-symmetric beam, (c) beam with 3D particle distribution.

4 SPACE CHARGE SOLVER IN 3D CARTESIAN COORDINATES

Space charge field of the bunched beam with 3D quadrupole symmetry is calculated from Poisson's equation in three-dimensional Cartesian coordinates (see Fig. 1c):

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} = - Q\,(x, y, z)\ , \qquad (14)$$

$$U(\Gamma) = 0\ ,\ U\,(x,y,z) = U\,(x,y,z + L)\ , \qquad (15)$$

with Dirichlet boundary condition for potential U at the surface of the rectangular pipe and periodic conditions in longitudinal direction [3]. The method of solution of Poisson's equation is similar to that of 2D case. Unknown potential function is represented as Fourier series:

$$U_{ijk} = \frac{1}{2} \sum_{n=1}^{N_x-1} \sum_{m=1}^{N_y-1} \bar{U}^{(c)}_{mno} \sin\left(\frac{\pi n i}{N_x}\right) \sin\left(\frac{\pi m j}{N_y}\right) +$$

$$\sum_{n=1}^{N_x-1} \sum_{m=1}^{N_y-1} \sum_{l=1}^{\frac{1}{2}N_z-1} \left[\bar{U}^{(c)}_{mnl} \sin\left(\frac{\pi n i}{N_x}\right) \sin\left(\frac{\pi m j}{N_y}\right) \cos\left(\frac{2\pi k l}{N_z}\right) +\right.$$

$$\left. + \bar{U}^{(s)}_{mnl} \sin\left(\frac{\pi n i}{N_x}\right) \sin\left(\frac{\pi m j}{N_y}\right) \sin\left(\frac{2\pi k l}{N_z}\right)\right] +$$

$$\frac{(-1)^k}{2} \sum_{n=1}^{N_x-1} \sum_{m=1}^{N_y-1} \bar{U}^{(c)}_{mn\frac{N_z}{2}} \sin\left(\frac{\pi n i}{N_x}\right) \sin\left(\frac{\pi m j}{N_y}\right)\ , \qquad (16)$$

similar for space charge expansion. After substitution of Fourier expansion (16) into Poisson's equation (14), coefficients of space charge and potential expansion are connected by algebraic relationship:

$$\bar{U}^{(c,s)}_{mnl} = \frac{\bar{Q}^{(c,s)}_{mnl}}{\left(\frac{\pi n}{a}\right)^2 + \left(\frac{\pi m}{b}\right)^2 + \left(\frac{2\pi l}{L}\right)^2}\ , \qquad (17)$$

which gives the solution of the space charge problem.

In Table 3 results of the same test problem for Gaussian beam, as for 2D axial-symmetric bunch, are presented. As seen, error, ε, is in the interval of $(1.5 - 5)\cdot 10^{-2}$. From results of the test problem the computing time, required for 3D space charge simulations on VAX Alpha computer is

$$t = (1.3\cdot M + 3\cdot N)\cdot 10^{-5}\ \text{sec}, \qquad (18)$$

where $M = \frac{1}{2} N_x \cdot N_y \cdot N_z$ is a number of grid points. Required computing time linearly changed with number of grid points, M, and number of macroparticles, N , which is typical for fast methods of space charge calculations [4].

Table 1. Results of 2D test problem in Cartesian coordinates with random numbers

Grid $N_x \cdot N_y$	Time, arbitr. unit	Max round-off error	Error of Gauss theorem
32 x 32	0.5	$2\cdot 10^{-4}$	$4\cdot 10^{-2}$
64 x 64	2.0	$3\cdot 10^{-3}$	$3\cdot 10^{-2}$
128 x 128	8. 0	$5\cdot 10^{-3}$	$1\cdot 10^{-2}$
256 x 256	32.0	$6\cdot 10^{-2}$	$4\cdot 10^{-4}$

Table 2. Error, ε, of 2D space charge field calculation of Gaussian bunch with $\sigma/\sigma_z = 1/4$.

Grid	Number of particles, N		
$N_r \cdot N_z$	$5\cdot 10^3$	$5\cdot 10^4$	$5\cdot 10^5$
32 x 32	$7.6\cdot 10^{-2}$	$7.4\cdot 10^{-2}$	$7.3\cdot 10^{-2}$
64 x 64	$2.9\cdot 10^{-2}$	$2.6\cdot 10^{-2}$	$2.5\cdot 10^{-2}$
128 x 128	$1.9\cdot 10^{-2}$	$1.3\cdot 10^{-2}$	$1\cdot 10^{-2}$
256 x 256	$2\cdot 10^{-3}$	$9.4\cdot 10^{-3}$	$6.7\cdot 10^{-3}$
512 x 512	$2.2\cdot 10^{-3}$	$8.9\cdot 10^{-3}$	$5\cdot 10^{-3}$

Table 3. Error, ε, and CPU time, t, sec, of VAX Alpha for space charge calculation of the Gaussian beam with $\sigma/\sigma_z = 1/4$.

Grid	Number of particles, N					
	$5\cdot 10^3$		$5\cdot 10^4$		$5\cdot 10^5$	
$\frac{N_x}{2}\cdot N_y \cdot N_z$	ε	t	ε	t	ε	t
16·32·64	$4.8\cdot 10^{-2}$	0.5	$3.5\cdot 10^{-2}$	1.6	$3.5\cdot 10^{-2}$	12.0
16·32·128	$4.7\cdot 10^{-2}$	0.9	$3.2\cdot 10^{-2}$	2.3	$3.2\cdot 10^{-2}$	16.0
32·64·64	$3.7\cdot 10^{-2}$	1.6	$2.1\cdot 10^{-2}$	3.1	$2.0\cdot 10^{-2}$	16.0
32·64·128	$3.7\cdot 10^{-2}$	3.2	$1.9\cdot 10^{-2}$	4.7	$1.8\cdot 10^{-2}$	20.8
32·64·256	$3.8\cdot 10^{-2}$	6.5	$2.0\cdot 10^{-2}$	8.7	$1.8\cdot 10^{-2}$	30.5
64·128·128	$3.9\cdot 10^{-2}$	13.5	$1.9\cdot 10^{-2}$	15.9	$1.6\cdot 10^{-2}$	37.0
64·128 ·256	$4.2\cdot 10^{-2}$	28	$2.0\cdot 10^{-2}$	30.6	$1.6\cdot 10^{-2}$	58.0

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