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A THREE-DIMENSIONAL SPACE-CHARGE CALCULATION METHOD

by

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ABSTRACT

We present a method for calculating space-charge forces on individual particles in a particle tracing simulation code. We solve Poisson's equation in three dimensions with boundary conditions specified on an arbitrary surface. When the boundary condition is defined by an impressed radio-frequency field, the external electric fields as well as the space-charge fields are determined. We use a least squares fitting procedure to calculate the coefficients of expansion functions, which need not be orthogonal nor individually satisfy the boundary condition.

I. PROBLEM

To determine the space-charge forces in an accelerator particle tracing simulation we would like to solve the Poisson equation,

$$\nabla^2 \phi = -\rho \quad , \tag{1}$$

with the potential specified on a surface S.

$$\phi(\vec{x}) = \phi_0(\vec{x}) \text{ on } S \quad . \tag{2}$$

We present a method that solves this problem in three dimensions for arbitrary surfaces and a charge density that is represented by a collection of macroparticles. (Other types of boundary conditions can be included also, if desired. Other equations can be done. In particular, we could include the rest of Maxwell's equations to the above to do the complete electromagnetic problem).

II. METHOD

Expand the potential in a finite set of functions ϕ_i.

$$\phi = \sum_{i=1}^{n} a_i \phi_i \ . \tag{3}$$

The coefficients a_i are to be determined. We do not require that the ϕ_i's be orthogonal nor individually satisfy the boundary condition.

We solve the problem by minimizing a χ^2 function, I, defined below.

$$I = \int_V dV \left(\sum_{i=1}^{n} a_i \ \nabla^2 \phi_i + \rho \right)^2 + w \int_S ds \left(\sum_{i=1}^{n} a_i \phi_i - \phi_o \right)^2 \ . \tag{4}$$

The volume integral will be a minimum where the potential represented by the series expansion most nearly satisfies Poisson's equation for the given particle distribution. The surface integral over the boundary is minimized when the boundary condition is nearly satisfied by the series expansion. The weight w can be adjusted according to the desired relative importance of the two conditions. (The quantity w is not a Lagrange multiplier because the surface integral is not a constraint but rather a function to be minimized.) We minimize I by requiring

$$\frac{\partial I}{\partial a_k} = 0 \quad , \ k = 1,2, \ \ldots, \ n \ . \tag{5}$$

This gives

$$\int_V dV \sum_{i=1}^{n} a_i \nabla^2 \phi_i \nabla^2 \phi_k + w \int_S dS \sum_{i=1}^{n} a_i \phi_i \phi_k$$

$$+ \int_V dV \rho \nabla^2 \phi_k - w \int_S dS \phi_o \phi_k = 0 \ . \tag{6}$$

Let

$$M_{ik} = M_{ki} = \int_V dV\, \nabla^2 \phi_i \nabla^2 \phi_k + w \int_S dS\, \phi_i \phi_k \tag{7}$$

$$N_k = w \int_S dS\, \phi_o \phi_k \tag{8}$$

$$S_k = - \int_V dV \rho \nabla^2 \phi_k \tag{9}$$

so that the condition for minimum in I, Eq. (6), becomes

$$\sum_{i=1}^{n} M_{ki}\, a_i = N_k + S_k \quad . \tag{10}$$

The matrix M_{ik} and the external source vector N_k depend only on the boundary condition and can be computed numerically (if necessary) for arbitrary three-dimensional shapes. The source term S_k depends on the charge distribution and must be computed at every time step in the particle tracing simulation. Fortunately, the source term is easy to compute for the discrete particle distribution; the result is

$$S_k = - \sum_{\text{particles}} \nabla^2 \phi_k \left(\vec{x}_p\right) \tag{11}$$

where $\vec{x}_p$ is the particle coordinate. The desired coefficients are given by

$$a_i = \sum_{k=1}^{n} \left(M^{-1}\right)_{ik} \left(S_k + N_k\right) \quad . \tag{12}$$

The space-charge potential is given by Eq. (3) and this solves the problem. Because the ϕ_i are known functions, we can easily obtain the gradient of the potential that gives the space-charge force on the particles. Perhaps higher order integration methods for calculating particle trajectories will become useful because of the ease in determining derivatives of the forces.

III. COORDINATE SYSTEM

We feel that cylindrical coordinates should be chosen for the type of structures we are interested in (drift-tube linac, radio-frequency quadrupole (RFQ), disk and washer). If the longitudinal (z) coordinate is expressed in units of $\beta\lambda$, then M_{ik} and N_k are often constant along the entire structure (especially for drift-tube linacs). Even if the boundary is slowly changing, only a few evaluations of M_{ik} and N_k are required because intermediate points can be determined by interpolation.

IV. EXPANSION FUNCTIONS AND BOUNDARY CONDITIONS

All structures of concern are nearly periodic in z and contain nearly periodic particle distributions. We therefore plan to use Fourier terms to describe the z-behavior of the potential function. This choice automatically takes into account the space-charge forces of adjacent bunches. Because of the exact periodicity in θ for all distributions, a Fourier expansion in θ is also appropriate. Because these periodic boundary conditions are satisfied by the individual expansion functions there is no need for these conditions to appear in Eq. (4). The best expansion in r might depend on the specific structure of interest (power series, Bessel functions). Therefore

$$\phi_i(\vec{x}) = f_i(r) \begin{bmatrix}\cos\\ \sin\end{bmatrix}(m_i\,\theta) \begin{bmatrix}\cos\\ \sin\end{bmatrix}(2\pi k_i z) \tag{13}$$

where the m_i and k_i are integers and f_i is some function of r. (Remember that z is in units of $\beta\lambda$.) With such expansion functions, the surface on which the boundary condition is specified could be expressed as $r = r(\theta,z)$. If this radius function is single-valued, then the surface integrals are easy to compute. For circular cylindrical geometry, the matrix M_{ik} becomes block

diagonal because the Fourier functions and their Laplacians are orthogonal in this geometry. Of course, some set of functions other than Eq. (13) may turn out to be more useful for some problems. Note that this method does not require that the functions factor into separate functions of each coordinate.

To determine which terms to include in the expansion, we must consider the effect of an additional term on the reduced χ^2

$$I_{reduced} = I/N_{deg} \tag{14}$$

where N_{deg} is the number of degrees of freedom for the system. Each additional term reduces N_{deg} by unity. Terms that have little effect or increase $I_{reduced}$ should not be included in the expansion.

For the RFQ, the rf electric field is known in the form of a potential function ϕ_{RFQ}. We can therefore calculate the external source term by setting $\phi_0 = \phi_{RFQ}$ in Eq. (8). Only the boundary value is required. The resulting solution for the potential function includes both the space-charge potential and the potential from the rf fields. Thus, this procedure can give the total force seen by a particle in the distribution.

V. POSSIBLE PROBLEMS

A poor choice of expansion functions could result in one of three problems. First, there could be no solution to Eq. (10) because the matrix M_{ik} is singular. This means the functions chosen were not independent for the given geometry. Second, there could be a solution to Eq. (10), but no minimum; that is, a maximum or saddle point was found. Third, a minimum was found, but it is large. If such problems arise, choose a different set of functions.

Another problem can arise because the finite number of particles that describes the distribution introduces an unreal structure into the fitted potential. Structure that is not statistically justified can be removed by the following smoothing procedure. If the statistical error in a given coefficient is larger than the magnitude of the coefficient, we set the coefficient equal to zero. These statistical errors are handled in a natural way using the chi-square procedure.

Boundary conditions are not satisfied exactly by the fitted potential function. Because the error in the boundary condition depends on the charge distribution, there is a beam-wall interaction that is not real. This "rubber wall" effect can be investigated by varying w.

VI. TESTS

To check this method, we can simply write down a function for ϕ and take its Laplacian to generate its source. Then, using this source, we can check how well this method reproduces the potential ϕ. The only constraint on ϕ is that $\nabla^2\phi$ be of one sign throughout the region of interest, because all particles in the simulation codes have the same charge. So far, the only example we have tried is the trivial case corresponding to a uniform charge density in a circular cylinder, $\phi = 1 - r^2$. The procedure worked as expected.

VII. SUMMARY

We have presented a method that can be used to solve the Poisson equation in three dimensions for arbitrary boundary conditions. Wall image charges and adjacent bunches can therefore be included by specifying the proper boundary conditions. When the rf field is known on the boundary, the external electric fields, as well as the space-charge fields, are determined.

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