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THE APPLICATION OF THE ALTERNATING PROCEDURE OF H.A. SCHWARZ FOR COMPUTING THREE-DIMENSIONAL ELECTROSTATIC FIELDS IN ELECTRON-OPTICAL SYSTEMS

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Abstract

The numerical solution of three-dimensional electrostatic field problems in electron-optical devices with complicated boundaries requires the use of very large and fast computers. A numerical counterpart of the Alternating Procedure by H.A.Schwarz (SAP) makes efficient use of both storage space and time available on the computer and therefore represents a useful new method in this context. In this method, the domain of solution is decomposed into independent subdomains where the appropriate individual methods of solution may be chosen. Correspondingly, the original boundary value problem is decomposed into a sequence of boundary value problems in these subdomains. SAP requires no explicit influence matrix and uses little storage space. Time requirements depend essentially on the methods applied in the respective subregions. SAP is particularly useful in obtaining analytical formulas for field distributions in "large" regions of empty space (such as in fringe field regions). Numerical results obtained with a computer program treating an electrostatic quadrupole lens problem show that a high degree of accuracy can be obtained with this method.

Key words: Alternating Procedure, three-dimensional, electrostatic field, potential theory, numerical, quadrupole lens, fringe field, subregion.

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Introduction

In the computer design of electron-optical devices, the Laplace equation $\Delta U=0$ arises when electrostatic and magnetostatic fields are to be calculated. The complexity of boundaries encountered in realistic devices requires the use of numerical methods for solving the corresponding boundary value problems. Three numerical methods in common use are the Finite-Difference Method (FDM) [2,4], the Finite-Element Method (FEM) [12], and the Integral Equation Method (IEM) [1;6].

We shall be concerned in particular with electrostatic field computation in complicated devices *not* possessing rotational symmetry. Moreover, since we want to consider fringe field problems, we must allow for domains of definition D for the potential U which are unbounded. An example for this type of problem is furnished by the electrostatic quadrupole lens pictured in fig. 1, consisting of four cylindrical electrodes arranged symmetrically as shown but held at the respective potentials $+V_0$ and $-V_0$. Though D is bounded by a grounded shielding in the x- and y-directions, it is assumed to be unbounded in the z-direction, and a fringe field must be taken into account.

Applied to this class of problems, each of the three methods mentioned gives rise to certain difficulties. In the following, we investigate briefly the pros and cons of each method. The applicability of each method is closely related to the geometry of the domain it is to be used in.

An FDM is adequate for "small" bounded domains enclosed by irregular boundary surfaces (perhaps containing edges and corners). For "large" domains, the dimension of the associated linear system grows too large, requiring too much storage space and computer time during iterative solution. Code is simple and short. The desired field is obtained from stored potential data using interpolation techniques. This requires much storage space but produces the field at little time expenditure. Smoothness of the field depends on meshwidth and interpolation formulae in use. For rectangular domains of reasonable size, fast solvers may be quite useful. (An account of fast direct methods in rectangular 2-d regions is found in [5]. Many of these methods "have a natural extension to three dimensions".)

Most of these considerations equally apply to the FEM. However, the FEM is more flexible both regarding domain size and irregularity of boundaries, at the cost of more complex code. (For a comparison of the FDM and the FEM with respect to electron-optical applications, see [7].)

An IEM is adequate for treating an exterior or mixed interior and exterior boundary value problem (e.g. any electrostatic field problem in unbounded space arising from potential values being posed on arbitrarily positioned electrodes). The associated code is flexible. An IEM is inadequate if the boundary surfaces are "large" in total surface area, as the dimension of the associated linear system grows too large and the matrix of coefficients

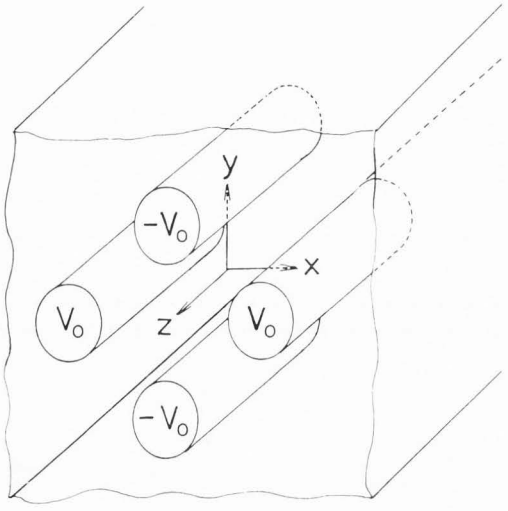

Fig. 1: Electrostatic quadrupole lens with cylindrical electrodes and shielding

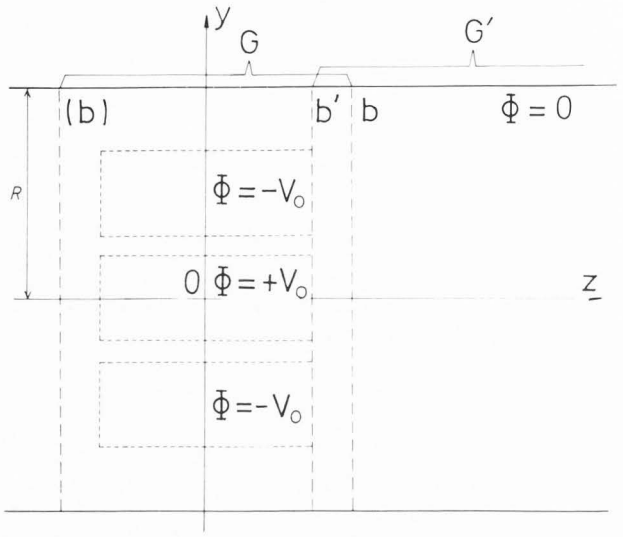

Fig. 2: Cross-section $x=0$ through the electrostatic quadrupole lens. Definition of surfaces b,b' and subregions G,G'.

is dense. The resulting potential is defined continuously and is "smooth", and the field and derivatives of higher order may be computed analytically. However, potential and field computation are expensive on computer time, and accuracy deteriorates near boundaries.

In practical 3-d field problems, different methods may seem appropriate to use in different parts of the domain D. Moreover, a certain advantage of one method may seem desirable in a certain region of D (such as obtaining an analytical solution). The method we are presenting allows one to decompose D into a finite number of subdomains. In each subdomain, the appropriate method of solving the Dirichlet problem associated with the Laplace equation is chosen. Instead of solving the original Dirichlet problem, a sequence of Dirichlet problems with different boundary conditions is solved in each subdomain. Besides combining the advantages of several methods, the proposed method has two notable properties: it requires storing values of functions only on surfaces, not in volumes (which is also true for the IEM) but requires no storage space for a matrix of coefficients. In fact, this matrix is never explicitly set up.

This method originally was conceived as a theoretical tool in potential theory by H.A.Schwarz in 1870 [11] and is referred to as "Alternating Procedure" (SAP). Its numerical counterpart has been employed by F.Lenz (private communication) since the early 1950's, and more recently by Kern [8] and the author [9,10].

In the first section of this paper, SAP is illustrated and discussed in the physical context of a typical fringe field problem in three dimensions. Only the case of two subdomains is treated there. The following section defines the precise algorithm to proceed by in the case of $n \geq 2$ subdomains. (The associated proofs may be found in [9,10].) The results of an application of SAP to the electrostatic-field problem associated with a quadrupole lens are reported in a final section.

Fringe field determination through SAP

As an example, suppose we were to determine the electrostatic field induced in the quadrupole lens pictured in fig. 1. A longitudinal cross-section $x=0$ through that system is shown in fig. 2. The dotted lines (-----) represent the projection of the contours of the electrodes. While the electrodes have a finite length of $2L$, the shielding is assumed to extend infinitely in the $\pm z$-directions. The shielding is of square cross-section, and its sides are perpendicular to the x- and y-axes, respectively, each having a distance R to the z-axis. Let D denote the domain of solution of the associated Dirichlet problem (DP; the boundary value problem of Dirichlet boundary conditions being imposed on a solution of the Laplace equation is referred to as DP. Dirichlet boundary conditions prescribe the values of the potential on the boundary ∂D of D.).

We artificially introduce two plane surfaces b' and b which are perpendicular to the z-axis (indicated by dotted lines (-.-.-.-) in fig. 2). This enables us to define two overlapping subregions of D: G, a bounded region enclosing the electrodes, and G', an unbounded fringe field region. From the figure it should be clear that G extends from boundary b (left) to boundary b (right), and that G' extends from b' to infinity. We are assuming for simplicity that that problem is symmetric with respect to the x,y-plane ($z=0$).

In G', the desired potential Φ may be represented analytically using the following series:

$$\Phi(x,y,z) = \sum_{m,n=1}^{\infty} A_{mn} \cos\left[(2m-1)\frac{\pi}{2}\frac{x}{R}\right] \cos\left[(2n-1)\frac{\pi}{2}\frac{y}{R}\right] \cdot$$

$$\cdot \exp\left(-\sqrt{(2m-1)^2+(2n-1)^2}\,\frac{\pi}{2}\frac{z-L}{R}\right) \qquad (1)$$

If the potential values $\Phi(x,y,L)$ ($|x|, |y| < R$) were known, the coefficients A_{mn} could readily be determined by evaluating the iterated integrals

$$A_{mn} = \frac{4}{R^2}\int_0^R\int_0^R \Phi(x,y,L) \cos\left[(2m-1)\frac{\pi}{2}\frac{x}{R}\right] \cdot$$

$$\cdot \cos\left[(2n-1)\frac{\pi}{2}\frac{y}{R}\right] dx\,dy \quad (m,n \geq 1) \qquad (2)$$

More generally, we may prescribe on b' arbitrary smooth boundary values $V(x,y)$ (which exhibit the required symmetry) and obtain a series solution (1) to the associated Dirichlet problem by substituting these values $V(x,y)$ for $\Phi(x,y,L)$ in (2).

Correspondingly, let us assume that we are capable of solving the Dirichlet problem in G associated with arbitrary boundary values posed on b.

Consider the following alternating sequence of Dirichlet problems posed in G and G':

1) Solve the DP associated with zero boundary values on b and the originally imposed boundary values on all other boundaries of G. Denote the solution by $U^{(0)}$.

2) Restrict $U^{(0)}$ to b', denote these values defined on b' by $U^{(0)}_{b'}$. Let $V^{(0)}$ be the solution of the DP in G' which is defined by the values $U^{(0)}_{b'}$ on b' and the original (vanishing) values on the remainder of $\partial G'$, the boundary of G'.

3) Restrict $V^{(0)}$ to the surface b, denote these values by $V^{(0)}_b$. Let $U^{(1)}$ be the solution of the DP in G which is defined by the values $V^{(0)}_b$ on b and zero boundary values on the remainder of ∂G, the boundary of G.

4) Restrict $U^{(1)}$ to b', denote these values by $U^{(1)}_{b'}$. Let $V^{(1)}$ be the solution of the DP in G' defined by the values $U^{(1)}_{b'}$ on b' and zero boundary values on the remainder of $\partial G'$. ...

Continuing in this fashion yields two sequences $(U^{(i)})_{i=1,2,...}$, $(V^{(i)})_{i=1,2,...}$ of harmonic functions defined in G and G', respectively. The series

$$\sum_{i=0}^{\infty} U^{(i)}(x,y,z) \quad and \quad \sum_{i=0}^{\infty} V^{(i)}(x,y,z)$$

converge uniformly in G and G', respectively, and their sums are equal to the desired potential values $\Phi(x,y,z)$ in the respective regions. The rate of convergence is one of a geometric series $\Sigma_i q^i$ with $0<q<1$; q becomes smaller as the overlap becomes larger and vice versa. For exact solutions $U^{(i)}$ and $V^{(i)}$, this is the assertion of the Alternating Procedure. (For a proof, see [3].) A precise description of how the procedure is performed discretely (on the computer) will be given in the next section. This includes a sufficient condition of convergence in the discrete case.

SAP prescribes a repeated performance of the following four steps: Solve a DP in G; evaluate the solution on $b' \subset G$; solve a DP in G'; evaluate the solution on $b \subset G'$. Following this procedure on the computer, only one of the two subroutines for solving a DP in G and G' is kept in the high-speed store at a time. For SAP to proceed after the i-th iteration in G, there is no need to evaluate and store all values of the solution $U^{(i)}$ in G; only the values $U^{(i)}_{b'}$ are of immediate interest. The same is true for $V^{(i)}$ and G'; i is any current value of the iteration parameter. Keeping stored, say, the sum

$$\sum_{k=0}^{i} U^{(k)}_{b'},$$

after a sufficient number M of iterations,

$$\Phi \cong \sum_{k=0}^{M} U^{(k)}_{b'} \ ;$$

from these approximated values of Φ on b', Φ can later be determined anywhere in G' (and hence in G). Analytical solutions like the functions $V^{(i)}$ in G' are particularly convenient; they allow the determination of the values $V^{(i)}_b$ without computing any other values of $V^{(i)}$ in G'. This means that very little storage space is required to obtain the values $V^{(i)}_b$ on b corresponding to the solution $V^{(i)}$ of the i-th DP in G'. Comparing SAP to conventional methods, the reduction in storage space stems from the fact that potential values need not be computed and stored in volumes but only on surfaces (b and b'). In this respect, SAP resembles the IEM. However, no matrix of coefficients for the unknown values of Φ on these surfaces is explicitly set up; the Alternating Procedure is merely followed, employing the two subroutines for solving the respective Dirichlet problems in G and G'.

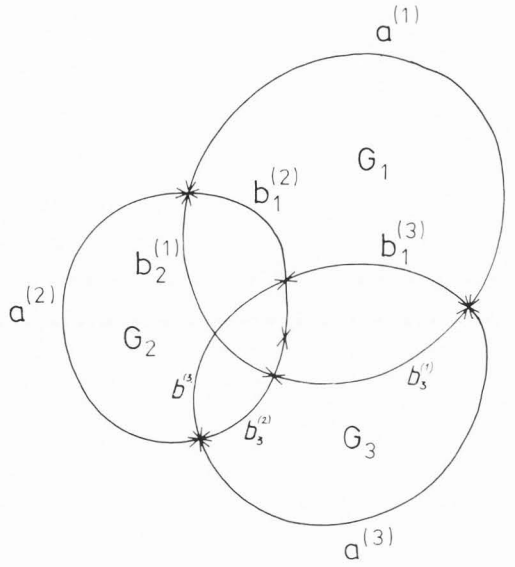

Fig. 3: Decomposition of a 2-d domain into three subregions G_1, G_2, G_3. Definition of boundary segments $a^{(i)}$ and $b^{(i)}_j$.

The other major advantage of SAP is that the domain of definition D is divided into subregions where individually, the appropriate methods of solution can be applied. In the fringe field region, for example, an analytical solution seems appropriate since the region is unbounded and its geometry is simple. On the other hand, in a bounded region such as G containing a complicated device, a flexible discrete method like the FDM seems most suitable. SAP tells us how to join the separate solutions "harmonically".

All these arguments apply equally well to the case of $n \geq 2$ subregions, treated in the next section.

The general Alternating Procedure

In this section, it is shown how a given domain D is properly decomposed into n overlapping subdomains and how SAP is performed step by step, making use of existing methods of solution in the individual subdomains. A condition is stated which each method must satisfy for SAP to converge. No proofs are issued in this paper; they may be found in [9] or [10]. No analytical estimate of the approximation error of SAP is offered by this author. It will depend on the accuracy of the individual methods in use.

Consider decomposing an open and connected region (domain) D in 3-space into $n \geq 2$ overlapping subdomains G_i $(i=1,...,n)$:

$$D = \bigcup_{i=1}^{n} G_i$$

(fig. 3 illustrates a two-dimensional case where n=3). Let ∂D denote the boundary of D. Each boundary $\Gamma_i = \partial G_i$ of G_i consists of two complementary parts

$$a^{(i)} := \Gamma_i \cap \partial D \quad and \quad b^{(i)} := \Gamma_i \cap D; \quad \Gamma_i = a^{(i)} \cup b^{(i)} \ .$$

(Perhaps $a^{(i)} = o$ but $b^{(i)} \neq o$.) By $\bar{b}^{(i)}$ we refer to the closure $\bar{b}^{(i)} = b^{(i)} \cup \partial b^{(i)}$ of an open surface segment $b^{(i)}$. Each surface $b^{(i)}$ is divided into $n-1$ open surface segments

$$b^{(i)}_1, b^{(i)}_2, ..., b^{(i)}_{i-1}, b^{(i)}_{i+1}, ..., b^{(i)}_n$$

such that for each $j=1,\ldots,i-1,i+1,\ldots,n$, $b_j^{(i)}$ is contained in the interior of the region G_j:

$$b_j^{(i)} \subset G_j .$$

More precisely,

$$\overline{b}^{(i)} = \bigcup_{j=1;j\neq i}^{n} \overline{b}_j^{(i)} \quad but \quad b_j^{(i)} \cap b_k^{(i)} = o \quad if \quad j\neq k$$

$$(j,k=1,\ldots,i-1,i+1,\ldots,n)$$

Of course, this division of each $b^{(i)}$ generally is not unique and is only possible if the following vital condition is satisfied:

Overlap condition. For every subdomain G_i $(i=1,\ldots,n)$, that part $b^{(i)}$ of its boundary surface Γ_i which is located in the interior of the original domain D must satisfy the following condition: every point of $b^{(i)}$ must lie within at least one of the other subdomains G_j $(j\neq i)$.

Next, consider distributing a finite number of mesh points P_k in some uniform manner over the complete set of (open!) boundary surface segments $b_j^{(i)}$ $(i=1,\ldots,n;\ j=1,\ldots,i-1,i+1,\ldots,n)$. With these points we associate an array of variables x_k used in SAP. The array x_k constitutes most of the storage space required by SAP. Certain subsets of this array will sometimes be referred to as "the values associated with" one or the other surface segment.

Assume that for each subdomain G_i, a numerical method (implemented as a computer subroutine) is available which will solve a given DP in G_i. Any such method will linearly associate with a complete set of boundary values x_l (corresponding to a complete set of mesh points P_l located on Γ_i), any required set of interior values x_m (corresponding to points P_m located in the interior of G_i). If the discrete set of boundary values x_l approximates some set of boundary values continuously defined on Γ_i, the values x_m should approximate the potential values $U(P_m)$ of the associated exact solution U.

For convergence of SAP, only one condition is required of each of the numerical methods employed in the respective subdomains: it must be subject to the discrete counterpart of the fundamental maximum-minimum principle for harmonic functions. It is stated below.

Discrete maximum-minimum principle: if $M_1 \leq x_l \leq M_2$ at every boundary point $P_l \in \Gamma_i$, solving the DP in G_i numerically leads to values $M_1 < x_m < M_2$ at any $P_m \in G_i$. It has been assumed that: 1) $M_1 < M_2$, and that $M_1 \leq 0 \leq M_2$ if G_i is unbounded; 2) the boundary values x_l are not constant.

As in the case of n=2 subregions, the general Alternating Procedure prescribes moving from subdomain to subdomain in a defined sequence. In each subdomain, a current set of (discrete) boundary values defines a DP, this DP is solved, and the solution is evaluated at certain mesh points on surface segments lying within the current subdomain. The following initial and general steps define this procedure.

By $\psi_j^{(i)}$ denote the array of variables x_k associated with a surface segment $b_j^{(i)}$ $(i=1,\ldots,n;\ j=1,\ldots,i-1,i+1,\ldots,n)$. Let G_{i_0} be any subregion where after the completion of SAP, the solution is required $(1 \leq i_0 \leq n)$. For each $j=1,\ldots,i_0-1,i_0+1,\ldots,n$, let $\phi_j^{(i_0)}$ denote an independent array of variables associated with the set of mesh points located on $b_j^{(i_0)}$.

Initial procedure

Set the values associated with all surfaces $b^{(i)}$ $(i=1,\ldots,n)$ equal to zero. Let the parameter i run from 1 to n in steps of 1. For each i, carry out the following step completely (before increasing i):

Solve the DP in G_i. The boundary values on $a^{(i)}$ are the values inherited from those prescribed on ∂D, the boundary values on $b_j^{(i)}$ $(j=1,\ldots,i-1,i+1,\ldots,n)$ are those currently stored in connection with $b_j^{(i)}$. Restrict the obtained solution ψ to all surfaces $b_i^{(j)} \subset G_i$ $(j=1,\ldots,i-1,i+1,\ldots,n)$ and store these values $\psi_i^{(j)}$ in connection with $b_i^{(j)}$. If $i\neq i_0$, let $\phi_i^{(i_0)} := 0$.

General procedure

For $i=1,2,\ldots,n,1,2,\ldots,n,1,2,\ldots$ perform the following step:

Solve the DP in G_i. The boundary values on $a^{(i)}$ are zero, the boundary values on $b_j^{(i)}$ $(j=1,\ldots,i-1,i+1,\ldots,n)$ are those currently stored in connection with $b_j^{(i)}$. Restrict the obtained solution ψ to all surfaces $b_i^{(j)} \subset G_i$ $(j=1,\ldots,i-1,i+1,\ldots,n)$ and replace the old values associated with $b_i^{(j)}$ by the new values $\psi_i^{(j)}$. If $i\neq i_0$, update $\phi_i^{(i_0)} := \phi_i^{(i_0)} + \psi_i^{(i_0)}$. When the values $\psi_i^{(i_0)}$ have become uniformly "small", stop the procedure.

The solution in G_{i_0} may now be obtained by solving a final DP in G_{i_0} with the original boundary values posed on $a^{(i_0)}$ and the values $\phi_j^{(i_0)}(j=1,\ldots,i_0-1,i_0+1,\ldots,n)$ posed on $b_j^{(i_0)}$. Consider any quantity representing a linear functional operating on the potential in G_{i_0} (such as the value of this potential at any specific interior point or any coefficient in some series representation of this potential). Such quantities may replace the arrays $\phi_j^{(i_0)}$ and make solving the final DP in G_{i_0} unnecessary if these quantities were the only information required with respect to this subdomain.

Numerical results obtained with SAP

Using SAP, a program has been developed which computes the electrostatic potential in a quadrupole lens as shown in fig. 1. The domain of solution D has been decomposed into $n=6$ overlapping subdomains, four of which are rectangular and have been treated using analytical (series) solutions. The FDM serves to solve the respective Dirichlet problems in each of the remaining two. More details of this program, including some plots of equipotential lines in various sections across D, may be found in [10].

Some figures which may serve to estimate the accuracy of the computed potential are presented in table 1.

Table 1: Maximum error of computed potential

Run no.	1	2	3
$\Delta_r(\Delta_a)$ in T_1	.00071(.00005)	.00019(.00002)	.00014(.00001)
T_2	.00072(.00017)	.00019(.00006)	.00014(.00005)
T_3	.00096(.00033)	.00039(.00010)	.00025(.00007)
T_4	.00164(.00070)	.00064(.00026)	.00045(.00017)
No. of iterations	23	25	24
Time (h:min)	0:19	2:47	10:08

The columns of this table correspond to various runs of the program with differing degrees of precision. In lines two through five we find the maximum relative error Δ_r (in parentheses: the maximum absolute error Δ_a) within four plane square regions of test T_1-T_4 in the fringe field area of the lens:

$$T_i = \{(x,y,z) \mid z = z_0; \mid x \mid, \mid y \mid \leq r_i\}.$$

(See fig. 1 for the orientation of the coordinate system. The origin is located at the center of the lens.) Let a denote the distance of the electrodes from the optical axis. z_0 has been chosen such that:

$$\frac{(z_0 - L)}{a} \cong 1.2$$

The numbers r_i are defined as follows:

$$r_1 = \frac{a}{4}\ ; r_2 = \frac{a}{2}\ ; r_3 = \frac{3a}{4}\ ; r_4 = \frac{11a}{12}\ .$$

The absolute error Δ_a is given with respect to unit potential values ± 1 on the electrodes. The relative error at a point $P \in D$ is defined as

$$\Delta_r(P) = \frac{\Delta_a(P)}{\mid \Phi(P) \mid}.$$

In the last two lines are reported the number of iterations performed, i.e. the number of times a DP is solved in *each* subdomain (with the boundary values uniformly growing smaller each iteration), and the computer time required on a Sperry-Univac 1100/80 computer. With respect to these time requirements, we would like to emphasize that a high speed store of 480 KBytes was used and no peripheral storage space was required. We note that even with respect to complicated electrostatic field problems, SAP could be used on smaller computers where storage space is sparse while computer time is cheap.

Acknowledgements

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