

# ОБЪЕДИНЕННЫЙ ИНстИтУт ЯДЕРНЫХ ИССЛЕДОВАНИЙ 

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ALGEBRAIC ITERATIVE METHOD TO SOLVE BOUNDARY PROBLEMS OF ARBITRARY ELECTROSTATIC SYSTEMS SATISFYING THE LAPLACE EQUATION

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If we assume that all charges are located within or on the surface of the electrodes, the potential obeys the Laplace equation:

$$
\begin{equation*}
\Delta \phi=0 . \tag{1}
\end{equation*}
$$

The resulting problem is to find the solution of this equation which fulfils certain boundary condition. The Laplace equation is difficult to solve. Since an exact analytical solution cannot be found for most of the cases, numerical methods should be applied. The numerical methods for solving the Laplace equation can be classified into two groups:

1) Methods approximating the solution of the Laplace equation in the region of interest by discretisation (finite-element method, finite-difference method).
2) Methods approximating the boundary values by superimposing exact analytical solution of the Laplace equation (charge-simulation method or integral-equation method) [1].

The integral-equation method (IEM) is the most appropriate for determining the optical properties of the electron optics. The IEM approximates the potential distribution by a sum of exact analytical solutions of the Laplace equation. Since the electric field is also given by a sum of analytical functions, numerical differentiation is then avoided. Generally the calculation of electromagnetic fields in electron optical systems requires a numerical solution of the three-dimensional boundary-value problem. It is important to study all possibilities reducing dimension in actual field calculations which are then considerably simplified. Two-dimensional field calculations are quite familiar for the systems rotationally symmetric about the optical axis (z). The boundary values of the potential $V$ may depend on the azimuth $\varphi$. Determination of the field source distribution on a given two-dimensional boundary S implies a numerical solution of a Fredholm equation [2] for unknown $Y(r)$ while $U(r)$ is given:

$$
\begin{equation*}
\int_{S} K\left(r, r^{\prime}\right) Y\left(r^{\prime}\right) d^{2} r^{\prime}=U(r) \quad(r \in S) . \tag{2}
\end{equation*}
$$

The methods of the first group provide an alternative possibility for computing the electromagnetic fields in electron optical systems. In the rotationally symmetric system the potential distribution $\Phi(\mathrm{r}, \varphi, \mathrm{z})$ can be expressed as a Fourier series of harmonic
components $\Phi_{m}(r, z)[3,4]$. They can be calculated by minimizing the variational functional

$$
\begin{equation*}
J_{m}=\iint_{S} \frac{1}{2} \varepsilon_{0}\left[\left(\frac{d \Phi_{m}}{\partial r}\right)^{2}+\left(\frac{d \Phi_{m}}{\partial z}\right)^{2}+\left(\frac{m \Phi_{m}}{r}\right)^{2}\right] \pi r d r d z . \tag{3}
\end{equation*}
$$

For the solution of equations (2) and (3) the knowledge of special methods of mathematical physics is necessary.

The purpose of this paper is to present a new technique of solution that avoids the difficulties of FDM, FEM, and IEM described above thus making it more acceptable for general applications.

## 2. ALGEBRAIC ITERATIVE METHOD

The proposed algebraic iterative method is applicable to solve the boundary and main problems of electrostatics for the conductors of an arbitrary form assuming that conductor potentials satisfy the Laplace equation. The motivation of the method and some examples of the solutions of the boundary problems of electrostatics are given in [5]. The method is based on the uniquiness theorem saying that if there is any solution found for the potential satisfying the boundary conditions, it means that this solution is the only one.

The algebraic method is based on the fact, that there exist "image" auxiliary charges inside the electrodes which, in the region outside the electrodes, produce the same potential distribution as the real surface charges. Since the potential and electric field of these charges inside the electrodes are not of our interest, the unknown potential distribution outside the electrodes can often be calculated using a simpler distribution of "image" point charges inside the electrodes. To minimize the number of the charges, they must be adapted to the geometry of the problem. The total fields and potentials are obtained by a linear superposition of the fields and potentials due to these point charges. Therefore the method is based on the well-known formula for the potential at a point P produced by the point charge $Q: \Phi=Q / 4 \pi \varepsilon_{0} d$, where $\varepsilon_{o}$ is permittivity of free space and $d$ is the distance between the point charge and the point $P$.

The substitution of the real charges by the point ones placed inside the conductor volume substantially simplifies mathematical calculations when solving the boundary problem. It also avoids uncertainties which appear at $\mathrm{r} \rightarrow 0$. Similar method using the
linear charges inside the conductor was applied earlier to calculate electric fields, potentials and some other characteristics of multiwire particle detectors [6,7]. This approach lies in the basis of the computer code used to design the multiwire detectors for experiments in high energy physics [8]. It was also applied to solve boundary problems of electron optics [9]. However in [9] the rings, the wires and the point charges, all together forming the field, were used.

### 2.1. DESCRIPTION OF ALGORITHM

In the new proposed method all intermediate calculations are carried out only in relative units. Assume that the total number of charges is equal to $m$. The potentials are defined in control points on the electrode surface at the nearest distance from the appropriate charges.

Assuming that $u(i)$ is the relative potential at the control point of the electrode after $i$ th iteration, the charge in the next iteration is

$$
\begin{equation*}
q(i+1)=q(i) / u(i) . \tag{4}
\end{equation*}
$$

This expression (4) is in the basis of the algorithm for the solution of the boundary problem. Clearly, the necessary condition for the convergence of this iterative process is the existence of the limit $u(i) \rightarrow l$ at $i \rightarrow \infty$. Only under this condition it is possible to apply the expression

$$
\begin{equation*}
\dot{q}(k, i+1) q(k, i) / u(k, i) \tag{5}
\end{equation*}
$$

to calculate a new value of charge $q(k, i+1)$ using the charge $q\left(k_{i}\right)$ and also of potential $u(k, i)$ produced by all the charges in previous iteration. In (5) $k \in(1, m)$ is the number of point charges and control points, $i$ is the number of iteration. It is clear from equation (5) that the charge in the next iteration decreases if $u(k, i)>u(k, i-1)$, while it increases if $u(k, i)<u(k, i-I)$.

The algorithm for one charged conductor, of a potential $U_{o}$, consists of 8 steps and can be discribed as follows:

1. The calculation of the coordinates of the auxiliary charges and the control points on the conductor surface which are placed at the shortest distances from the corresponding auxiliary charges.
2. Value assignment $q=l$ to all the auxiliary charges.
3. The calculation of the relative potentials $u(k)$ at control points on the conductor surface.
4. Normalization of the all new potential values $u(k, i)$, obtained after each $i$-th iteration: $u(k, i)=u(k, i) / u(l, i), u(l, i)$ is the reference potential.
5. Calculation of the all new charge values for the next iteration using the expression $q(k, i+1)=q(k, i) / u(k, i)$.
6. Normalization of all the calculated charge values to the value of the reference one.
7. Repeating the points 3 to 6 until the normalized potential $u(k, i) \in(I-\delta u, I+\delta u)$ for all the points of the surface, $\delta u$ is a given accuracy.
8. The calculation of all new values of the charges $q(k)$ which will produce potential $u=1$ over all the surface with the given accuracy $\delta u$. Final result will be obtained according to expression $q(k)=q(k) \times U_{0}$.

The first index 1 or 2 denotes the first or second electrode. The second index 1 or 2 corresponds to the first or second stage. As a result of calculations we obtain a system of charges $Q(1,1)$ and $Q(2,1)$ for the case The problem of several charged conductors is solved in a similar way provided the absolute values of their potentials are equal.

### 2.2. ARBITRARY SYSTEM OF CHARGED CONDUCTORS

It is cler that equation (5) relating the charges and the potential:
$q(k, i+1)=q(k, i) / u(k, i)$ is absolutely not applicable for the systems containing at least one conductor with the zero potential. Let us consider two electrodes, the potential of one of them $u(l)=l$ and the second one having a potential equal to zero. To solve the problem, we can apply the superposition principle.

The solution is searched for in two stages. In the first stage we assume the equality of the potentials, the charges of both electrodes having the same sign. In the second stage we assume the electrodes with the same position of the charges but opposite sign potentials:

$$
\begin{equation*}
u(1,1)=u(2,1)=1 \quad u(1,2)=-u(2,2)=1 \tag{6}
\end{equation*}
$$

with equal potentials, and a system of charges $Q(1,2)$ and $-Q(2, \dot{2})$ for the case with the potentials of the electrodes equal in magnitude but opposite in sign.

The corresponding charges of the electrodes are then summed up in pairs with the weight $k=0.5$. As a result we obtain a system of charges $\mathrm{Q}(1)=\mathrm{k}(\mathrm{Q}(1,1)+\mathrm{Q}(2,1))$ for the
first electrode and $\mathrm{Q}(2)=\mathrm{k}(\mathrm{Q}(2,1)-\mathrm{Q}(2,2))$ for the second electrode, producing the required potentials $u(1)=I$ and $u(2)=0$.

To solve the problem for arbitrary potentials, let us consider a combination $\mathrm{Q}(1)$ of the charges for the first electrode and $Q(2)$ for the second one:

$$
\begin{equation*}
Q(1)=\alpha Q(1,1)+\beta Q(2,1), Q(2)=\alpha Q(1,1)-\beta Q(2,1) . \tag{7}
\end{equation*}
$$

These combinations of the charges $Q(1)$ and $Q 2$ ) produce potentials of the first and second electrodes respectively:

$$
\begin{equation*}
u(1)=(\alpha+\beta) u, u(2)=(\alpha-\beta) u . \tag{8}
\end{equation*}
$$

Equations (6) and (8) are generalized for a system of four conductors:

$$
\begin{align*}
& u(1,1)=u(2,1)=u(3,1)=u(4,1) \\
& u(1,2)=u(2,2)=u(3,2)=-u(4,2) \\
& u(1,3)=u(2,3)=-u(3,3)=-u(4,3)  \tag{9}\\
& u(1,4)=-u(2,4)=-u(3,4)=-u(4,4),
\end{align*}
$$

$$
\begin{align*}
& u(1)=(\alpha+\beta+\gamma+\delta) u, \quad u(2)=(\alpha+\beta+\gamma-\delta) u, \\
& u(3)=(\alpha+\beta-\gamma-\delta) u, u(4)=(\alpha-\beta-\gamma-\delta) u . \tag{10}
\end{align*}
$$

Equation (10) allow one to define the weights values $\alpha, \beta, \gamma, \delta$ and, using them, to find the charges producing the given potentials of the four charged conductors. Similarly to equation (7) the charges are determined from the following relations:

$$
\begin{align*}
& Q(1)=\alpha Q(1,1)+\beta Q(2,1)+\delta Q(3,1)+\gamma Q(4,1), \\
& Q(2)=\alpha Q(1,1)+\beta Q(2,1)+\delta Q(3,1)-\gamma Q(4,1),  \tag{11}\\
& Q(3)=\alpha Q(1,1)+\beta Q(2,1)-\delta Q(3,1)-\gamma Q(4,1), \\
& Q(4)=\alpha Q(1,1)-\beta Q(2,1)-\delta Q(3,1)-\gamma(Q(4,1) .
\end{align*}
$$

Based on the above examples, one can see the principle to form the system of equations solving the problem for $m$ conductors. Let us compose a matrix of signs + $+\boldsymbol{+} \ldots+\boldsymbol{+}$ and - for the system of $m$ conductors. Signs in the $i$-th matrix row $+++\ldots+-$
$+++\ldots-$ determine the signs of the terms in the $i$-th equations of the systems $+++\ldots$. . similar to $(9,10,11)$. The signs before the unit potentials of the system $++\ldots \ldots=-$ elements correspond to the matrix signs. The signs of the first matrix row $+\cdots \ldots-\cdots$ are taken for the first linear equation, signs of the second matrix row for the second one and etc. So, the stage of the matrix composition and the completion of the calculation of the charge values of the system from $m$ elements is the 9 -th
concluding step of the proposed algorithm solving the problem of electrostatics of the arbitrary 3D systems satisfying the Laplace equation.

## 3. APPLICATION OF METHOD TO SOLVE THE BOUNDARY PROBLEM FOR THE TWO-TUBE ELECTROSTATIC LENS.

As an example of the application of the proposed method, let us consider a solution of the boundary problem for a two-tube electrostatic lens. We put the inner diameter of each tube $D=10 \mathrm{~mm}$, the length of the cylindrical electrode $L=30 \mathrm{~mm}$, the value of the gap $\mathrm{s}=1 \mathrm{~mm}$.

Auxiliary charges were placed on the cylindrical surface with the radius of 5.4 mm . The potential was calculated in 80 control points located along the inner surface of the electrode. The total number of auxiliary charges was equal to $2 \times 60 \times 80$.

Fig. 1 shows the potential distribution at the control points in relative units. The non-regularities at the beginning and the end of the distribution (edge effects) can be suppressed by insignificant changes of the positions of the charges corresponding to these non-regularities [7]. The discrete character of the auxiliary charge distribution results in a wave-like potential surface. Its maxima are located at the positions closest to the point charges, the minima correspond to the center of the interval between neighbouring charges. Mathematical simulation has shown that $d$-distance from a point charge up to the surface should satisfy the inequality $d \geq a$, where $a$ is a distance between the neighbouring charges [7]. The influence of the discrete position of the point charges can be seen in fig. 2, where the potential distribution is shown along the part of the inner surface of the lens electrode. The distribution of the calculated potential along the axis of the lens electrode is shown in fig. 3. The calculated value of the electric field in the gap of the electrode along the radius is given in fig. 4.

In [4] a linear variation of the potential in the gap between adjacent electrodes was assumed thus making the calculations substantially easier. The real dependence is shown in fig. 5. It appears to be linear except for the regions near the electrodes. Fig. 6 shows the cross section of the surface of the electrode near the gap. The points denote the position of the auxiliary charges. The normal component of the electric field is connected with the surface charge density $\sigma$ by the following relation: $E_{n}=\sigma / \varepsilon_{0}$, where $\varepsilon_{0}$ is the permittivity of free space. Fig 7 shows the surface charge density as a function of the distance $\rho$ along the initial part of the electrode. The local minimum at

U rel


Fig.1. The calculated relative values of the potential at control points of one of the lens electrodes.


Fig.2. The calculated relative values of the potential along the inner part of the lens electrode. The distribution maxima are located at the positions closest to the corresponding point charges, the minima correspond to the center of the interval between the neighbouring charges.


Fig.3. Distribution of the calculated potential value in relative units along the axis of the tube electrode.

Ez


Fig.4. The radius dependence of $z$ component of the electric field calculated in the region between the electrodes.


Fig.5. Distribution of the calculated relative potential value in the gap between the lens electrodes.


Fig.6. Cross section of the potential surface of the lens electrode near the gap. Points show the position of the auxiliary charges.
$\sigma$

$\begin{array}{lllllll}0 & 0.2 & 0.4 & 0.6 & 0.8 & 1 & 1.2\end{array}$

Fig.7. Distribution of the calculated value of the surface charge density along the part of the electrode. The local minimum at the beginning of the curve corresponds to the flatted forward part of the electrode shown in fig. 6.

Et


Fig.8. Distribution of the electric field along the axis of the lens electrode calculated in relative units.


Fig.9. Distribution of the calculated the surface charge density along the part of the electrode where the electric field direction changes.

R mm


Fig.10. The equipotentials (a) and electric field lines (1-6) in the region where the electric field changes direction. Values of the potentials in the units relative to the potential of the electrode are: .9995; .9994; .9993; .9992;.99915; .9991. Potentials correspond respectively to the curves $1,2,3,4,5$, and 6 .


Fig.11. Equipotentials in a part of two-tube electrostatuc lens of 60 mm length; shown is the distribution to the left from the symmetric plane. The corresponding relative values of the potentials increase from left to right with a step of 0.1 starting from 0.1 .
the beginning of the curve corresponds to the flatted part of the electrode near the gap (fig. 6). The distribution of the electric field along the electrode axis of the lens is given in fig. 8. In the region where the direction of the electric field changes, the distribution of the surface charge density in arbitrary units along the surface electrode is shown in fig. 9. The value of the surface charges density in this region is approximately by 5000 times less than the value of the surface charge density in the gap of the tube electrodes.

Fig. 10 presents equipotential and field lines in the region where the direction of the electric field changes. The values of the potentials are shown in relative units. Fig. 11 shows the axial section through one electrode of the lens near the gap. The curves represent the equipotential lines of the physical model of the electrostatic lens. The corresponding relative values of the potentials increase from left to right with a step of 0.1 starting from 0.1 .

## 4. CONCLUSIONS

A simple method of the solution of the boundary problem in electrostatics is - proposed. It does not require the application of the usual rather complicated methods of mathematical physics. The corresponding computer code is quite easy to write, it doesn't require special programming skills. For the example calculations discussed here the computer code was written in C language. Total computing time for 100 iterations on PC-486 $(66 \mathrm{MHz})$ was $\approx 30$ minutes.

In comparison with the other methods for solving the problems of the electron optics: finite-difference method (FDM), finite-element method (FEM) and integralequation method (IEM), - the proposed method is universal and can be applied to arbitrary three-dimensional electrostatic systems.

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## References

[1] P.W. Hawkes and E. Kasper, Principes of Electron Optics, Vol. 1, Basic . Geometrical Optics, Academic Press, London, 1989.
[2] E. Kasper, Optic, 54, (1979) 135-169.
[3] E. Munro and H.C.Chu, Optik, 61, 1, p. 1-16, 1982.
[4] B. Lencova, Nucl. Inctr. and Meth., A 363 (1995) 190.
[5] M.D. Shafranov, JINR Communication, P11-98-103, Dubna, 1998.
[6] G.A. Erskine, Nucl. Inctr. and Meth., 105 (1972) 565.
[7] M.D. Shafranov, Nucl. Inctr. and Meth., A 367 (1995) 125.
M.D. Shafranov, JINR Communication, P13-96-355, Dubna, 1996.
M.D. Shafranov, JINR Rapid Communication, 6[74]-95, Dubna, 1995.
[8] R. Veenhof, GARFIELD, a drift-chamber simulation programm, CERN (1994).
[9] H. Hoch, E. Kasper and D. Kern, Optic, 50, (1978) 413.

## Шафранов М.Д.

Алгебраический итеративный метод решения краевых задач произвольных электростатических систем,
удовлетворяющих уравнению Лапласа
Предложен новый алгоритм и алгебраический итеративный метод решения краевых задач произвольных электростатических систем, удовлетворяюших уравнению Лапласа. Алгебраический метод основан на размещении «изображений» вспомогательных точечных зарядов внутри электродов, которые создают такое же потенциальное распределение, как и реальные поверхностные заряды. Электрические поля и потенциалы получаются линейной суперпозицией полей и потенциалов, создаваемых точечными зарядами. Метод базируется на известной формуле для потенциала точечного заряда $q$ : $u=q / 4 \pi \varepsilon_{0} d$, где $d$ - расстояние между точечным зарядом и некоторой точкой пространства.

В предположении того, что $u(i)$ - относительный потенциал в контрольной точке после i -й итерации, заряд для следующей итерации определяется из выражения $q(i+1)=q(i) / u(i)$. Это выражение является основой алгоритма решения краевых задач

В качестве примера рассмотрено применение предложенного метода к решению краевой и основной задач электростатики для двухэлектродной линзы.

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## Shafranov M.D

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Algebraic Iterative Method to Solve Boundary Problems
of Arbitrary Electrostatic Systems Satisfying the Laplace Equation
The new algorithm and algebraic iterative method to solve. boundary problem of arbitrary electrostatic systems satisfying the Laplace equation are proposed.

The algebraic method is based on the fact, that there exist «image» auxiliary point charges inside the electrodes which, in the region outside the electrodes, produce the same potential distribution as the real surface charges. The total fields and potentials are obtained by a linear superposition of the fields and potentials due to these point charges. Therefore the method is based on the well-known formula for the potential at a point $P$ produced by the point charge $q: u=q / 4 \pi \varepsilon_{0} d$, where $d$ is the distance between the point charge and the point $P$. The potentials are defined in control points on the electrode surface at the nearest distance from the appropriate charges.

Assuming that $u(i)$ is the relative potential at the control point of the electrode after i -th iteration, the charge in the next iteration is $q(i+1)=q(i) / u(i)$. This expression is in the basis of the algorithm for the solution of the boundary problem.

As an example of the application of this method, a solution of the boundary problem for a two-tube electrostatic lens is considered.

The investigation has been performed at the Laboratory of Particle Physics, JINR

