On finding the analytic dependencies of the external field potential on the control function when optimizing the beam dynamics

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Abstract. When developing a particle accelerator for generating the high-precision beams, the injection system design is of importance, because it largely determines the output characteristics of the beam. At the present paper we consider the injection systems consisting of electrodes with given potentials. The design of such systems requires carrying out simulation of beam dynamics in the electrostatic fields. For external field simulation we use the new approach, proposed by A.D. Ovsyannikov, which is based on analytical approximations, or finite difference method, taking into account the real geometry of the injection system. The software designed for solving the problems of beam dynamics simulation and optimization in the injection system for non-relativistic beams has been developed. Both beam dynamics and electric field simulations in the injection system which use analytical approach and finite difference method have been made and the results presented in this paper.

1. Introduction
The paper mostly focuses on exploring the ways of algorithmic and software realization of the optimal design methodology in the beam dynamics area, which is proposed in [1-3] and intended to be applied in the injection systems producing the high-precision beams. The development of the optimal design methodology for beam dynamics is considered to be rather complex and laborious problem. It has given rise to a large and growing body of research [4-14].

The main issue in the optimal design techniques that we try to address in the paper consists in finding an analytical expression of the control potential function $\phi(\eta)$ defined over the domain contour, together with developing an algorithm that could compute the electrostatic field $U_\xi$ inside the working domain using this control function. The control function is to be used in further optimization procedures. The paper starts with some algorithmic study relating to the numerical solution of the integral of Cauchy type that is applied in the given problem to calculate the electrostatic field. Then we consider a case study model of the axial symmetrical field in an injection system. Some numerical data obtained in the C++ computer simulation are presented.

2. A possible basic algorithm of finding the integral of Cauchy type
Let us consider a three-dimensional simply connected bounded domain having the axial symmetry and let $G$ be its diametric cross section. This two-dimensional domain $G$ is bounded by a contour $L$ that is supposed to be a smooth closed curve. Hereinafter the real plane $\mathbb{R}^2$ containing the domain $G$ will be
identified with the complex plane \( C \). Let a continuous complex function \( \phi(\eta) \) be defined over the contour \( L \). The complex potential of the external electrostatic field inside the domain \( G \) can be evaluated with the use of an integral of Cauchy type

\[
F(\xi, \phi) = \frac{1}{2\pi i} \int_{L} \frac{\phi(\eta)}{\eta - \xi} d\eta, \quad \xi \not\in L,
\]  

where \( \xi = z_G + i \cdot r_G \in G, \eta = x_L + i \cdot y_L \in L \). Then the complex potential of the three-dimensional external field can be represented as follows (see [3], p. 97):

\[
H(z, r, \phi) = \frac{1}{2\pi} \int_{0}^{2\pi} F(z + i \cdot r \cos \alpha, \phi) d\alpha.
\]

The real part of \( H \), i.e. the function \( U = \text{Re} H \), will be considered as a function determining the electrostatic field in the three-dimensional domain. The complex contour integral (1) can be written as

\[
F(\xi, \phi) \equiv \frac{1}{2\pi i} \int_{L} f(z) dz = \frac{1}{2\pi i} \left[ \int_{L} u(x, y) dx - v(x, y) dy + i \int_{L} v(x, y) dx + u(x, y) dy \right],
\]

where \( f(z) = u(x, y) + i \cdot v(x, y) \) is a function of a complex variable \( z = x + i \cdot y \). Therefore, the potential function \( U \) can be defined as a real line integral

\[
U(x, y) = \frac{1}{2\pi} \int_{L} v(x, y) dx + u(x, y) dy
\]

taken over the same contour \( L \) as the complex integral. Let us consider the simplest case when the function \( \phi \equiv \phi_0 \) is a constant. Then the following expressions can be written

\[
f(z) = \frac{\phi_0}{z}, \quad u(x, y) = \frac{x}{x^2 + y^2}, \quad v(x, y) = -\frac{y}{x^2 + y^2},
\]

and the real part of the integral (1) is evaluated as follows

\[
U \equiv \text{Re} F(\xi, \phi_0) = \frac{\phi_0}{2\pi} \left[ \int_{L} -\frac{yd\alpha}{x^2 + y^2} + \int_{L} \frac{x d\alpha}{x^2 + y^2} \right],
\]

where \( x = x_L - z_G \), \( y = y_L - r_G \).

Let us take the domain \( G \) as a rectangle \( ABCD \) shown in Fig.1.
The integral (3) can be represented as a sum of four integrals to be evaluated counter-clockwise over the horizontal and vertical segments $AB, BC, CD, DA$ of the closed contour $L$. Actually, these segments can be treated as vectors. Thus, on the vector $\overrightarrow{AB}$ it turns out that $dy = 0$ and the integral (3) takes the form

$$ U_{AB} = -\frac{\phi_0}{2\pi} \int_{-a}^{a} \frac{y \, dx}{x^2 + y^2}. $$

Given an arbitrary position of the point $\xi$ in the domain $G$, the variables $x$ and $y$ are defined as $x = x_L - x_G, \ y = y_L - y_G$.

So, we have

$$ U_{AB} = -\frac{\phi_0}{2\pi} \int_{-a}^{a} \frac{y \, dx}{x^2 + y^2} = -\frac{\phi_0}{2\pi} \int_{-a}^{a} \frac{d(x/y)}{x^2 + y^2 + 1} = -\frac{\phi_0}{2\pi} \left[ \arctan \left( \frac{x}{y} \right) \right]_{-a}^{a} = -\frac{\phi_0}{2\pi} \left[ \arctan \left( \frac{a - x_G}{-b - y_G} \right) - \arctan \left( \frac{-a - x_G}{-b - y_G} \right) \right]. $$(4)

In a similar manner, we obtain other constituents of potential $U_{BC}, U_{CD}, U_{DA}$:

$$ U_{BC} = \frac{\phi_0}{2\pi} \int_{a}^{b} \frac{(x_L - x_G) \, d(y_L - y_G)}{(x_L - x_G)^2 + (y_L - y_G)^2} = \frac{\phi_0}{2\pi} \left[ \arctan \left( \frac{b - y_G}{a - x_G} \right) - \arctan \left( \frac{-b - y_G}{-a - x_G} \right) \right], $$(5)

$$ U_{CD} = -\frac{\phi_0}{2\pi} \int_{a}^{b} \frac{(y_L - y_G) \, d(x_L - x_G)}{(x_L - x_G)^2 + (y_L - y_G)^2} = -\frac{\phi_0}{2\pi} \left[ \arctan \left( \frac{-a - x_G}{-b - y_G} \right) - \arctan \left( \frac{a - x_G}{b - y_G} \right) \right], $$(6)

$$ U_{DA} = \frac{\phi_0}{2\pi} \int_{a}^{b} \frac{(x_L - x_G) \, d(y_L - y_G)}{(x_L - x_G)^2 + (y_L - y_G)^2} = \frac{\phi_0}{2\pi} \left[ \arctan \left( \frac{-b - y_G}{-a - x_G} \right) - \arctan \left( \frac{b - y_G}{a - x_G} \right) \right]. $$(7)

So, at the point $\xi$ the potential $U_\xi$ equals to

Fig. 1. Finding the potential $U_\xi$ inside the conducting rectangle with the use of integral of Cauchy type
\[ U_\xi = U_{AB} + U_{BC} + U_{CD} + U_{DA} \]  

This expression evidently contains the pairs of terms in which the arguments of the function \( \arctan \) are inverse ones. Taking into account the following trigonometric identity

\[
\arctan x + \arctan \frac{1}{x} = \begin{cases} 
\frac{\pi}{2}, & \text{if } x > 0 \\
-\frac{\pi}{2}, & \text{if } x < 0 
\end{cases}
\]

we can represent (8) as a sum of binomials forming such a pair of terms. For instance, taking the first term from (5) and the second from (6), we get

\[
\frac{\phi_0}{2\pi} \arctan \left( \frac{b - y_G}{a - x_G} \right) + \frac{\phi_0}{2\pi} \arctan \left( \frac{a - x_G}{b - y_G} \right) = \frac{\phi_0}{2\pi} \frac{\pi}{2} = \frac{\phi_0}{4}, \quad \text{as } b - y_G > 0 \text{ and } a - x_G > 0.
\]

Similarly, summing the first term from (4) and the second from (5) gives

\[
-\frac{\phi_0}{2\pi} \arctan \left( \frac{a - x_G}{b - y_G} \right) + \left( -\frac{\phi_0}{2\pi} \arctan \left( \frac{b - y_G}{a - x_G} \right) \right) = -\frac{\phi_0}{2\pi} \left( -\frac{\pi}{2} \right) = \frac{\phi_0}{4}, \quad \text{as } a - x_G < 0 \text{ and } b - y_G < 0.
\]

Finally, the summation of all four pairs in (8) gives us the potential value in an arbitrary point \( \xi \) of the domain \( G \):

\[ U_\xi = 4 \cdot \frac{\phi_0}{4} = \phi_0. \]

This result undoubtedly matches the electrostatics fundamentals: if a plane closed contour (e. g., made from a conducting wire) has been charged to the potential \( \phi_0 \), then any point inside the contour has the same potential.

It seems to be worth attempting to apply the above scheme in the case of non-constant potential function \( \phi(\eta) \) over the closed contour \( L \). The possible solution could consist in representing the smooth contour by a sequence of horizontal and vertical directed segments - vectors, together with making the approximation of the function \( \phi(\eta) \) by a step function \( \phi_s(\eta) \) that is a constant at each segment. A contribution of each segment into the whole potential at a point \( \xi \) in \( G \) can be computed using one of the formulas (4), (5), (6), or (7) depending on the orientation of the segment.

Needless to say, considering more exact, linear, approximation of the boundary potential seems to be appropriate as well. Let us assume that the boundary potential on some horizontal line segment \( ab, \quad x_{ab} \in [x_{Li}, x_{Li+1}] \) is defined by a linear function \( \phi = k_0 + k_i x_L \), \( y_L = y_{L_{i+1}} = y_L \). The integrand \( f(z) \) takes the following form

\[ f(z) = \frac{\phi}{z} = \frac{k_0 + k_i x_L}{x + i \cdot y} = u(x, y) + i \cdot v(x, y), \]

where \( u(x, y) = \frac{(k_0 + k_i x_L) x}{x^2 + y^2}, \quad v(x, y) = -\frac{(k_0 + k_i x_L) y}{x^2 + y^2}. \)

By analogy with the derivation of the formula (4), and taking into account that \( x = x_L - x_G, \quad y = y_L - y_G \), we can get the following expression chain
\[ U_{ab}(x_G, y_G) = \text{Re} \left[ \frac{1}{2\pi i} \int_{\gamma_G} f(z)dz \right] = \frac{1}{2\pi} \int_{x_G}^{x_G+iy} v(x, y)dx = -\frac{k_0}{2\pi} \int_{x_G}^{x_G+iy} \frac{ydx}{x^2 + y^2} - \frac{k_1}{2\pi} \int_{x_G}^{x_G+iy} \frac{x_Lydx}{x^2 + y^2} = \]
\[ \frac{(k_0 + k_1x_G)}{2\pi} \left[ \arctan \left( \frac{x_L(x+1)}{y_L-y_G} \right) - \arctan \left( \frac{x_L-x_G}{y_L-y_G} \right) \right] - \frac{k_1}{4\pi} \ln \left[ \frac{(x_L(x+1))^2 + (y_L-y_G)^2}{(x_L-x_G)^2 + (y_L-y_G)^2} \right] \]

Note that the formula (4) can be thought as a special case of (9) if the boundary potential \( \phi \) is constant, i.e. when \( k_1 = 0 \).

3. Algorithm description and a case study simulation

An algorithm considered in the paper includes the following stages:

- Computing the electrostatic field in the working domain of an injection system under the given initial configuration and potentials of electrodes. The computation is carried out using, e.g., the iterative Liebmann’s procedure on a square grid, [15], as is done in the paper.
- On moving along the piece-wise contour bounding the working domain, the reference potential profile \( \varphi(\eta) \) over the boundary of the working domain is formed. This set of exact values is used for finding the approximate boundary control function \( \phi(\eta) \).
- A suitable type of an approximating function is chosen and its parameters are computed by one of the methods of solving the systems of linear equations.
- In order to find a potential at any point of the domain, the integrals of Cauchy type are computed at each grid cell side (horizontal or vertical) around the domain contour using the formulas (4-7), where \( \phi_h = 0.5 \cdot [\varphi(\eta) + \varphi(\eta),] \).

Let us consider these stages in greater detail. As an example in the case study we take an axially-symmetric working domain for an injection system with three electrodes, which cross-section is shown in Fig. 2. The rectangle \( \text{AFF}, \text{A} \), of length \( \text{AF} = 400 \text{ mm} \) and height \( \text{AA} = 80 \text{ mm} \) is covered with a square grid with a cell side \( h = 0.5 \text{ mm} \). Potentials of electrodes are \( U_1 = 100 \text{ kV}, U_2 = 45 \text{ kV}, U_3 = 87 \text{ kV} \).
The simulation model has been developed in C++, where a class *Field* defines the model parameters and contains all necessary member functions. One of them computed the electrostatic field in a cylindrical coordinate system by the iterative Liebmann’s method with the maximal error $\varepsilon = 0.001\%$. It takes ca. 88360 iterations. Another function scans the grid nodes that bound the top half of the contour, namely $A_0A_1L_2K_2H_2G_2L_1G_1LHGF,F_0$, and collects the potentials into an array of size $1173 = L_n$. The reference profile $\phi(\eta)$ is shown in Fig. 3, curve 1.

To approximate the profile of the contour potential, we have chosen a rational-fraction approximation:

$$
\phi(\eta) = \left( a_0 + \sum_{i=1}^{4} a_i \eta^i \right) \left( 1 + \sum_{j=1}^{5} b_j \eta^j \right).
$$

For finding the unknown parameters $a_i, b_j$, the least squares method that minimizes a weighted mean-square approximation error has been used. It handles the over-determined matrix with $M = 15$ rows (i.e., equations) and $N = 10$ columns (unknowns). The approximating function $\phi(\eta)$ is shown in Fig. 3, curve 2.

Finally, the potential function $U_{ax}(x)$ over the domain axis has been calculated using the reference profile $\phi(\eta)$ (see Fig. 4, curve 1), the approximate profile $\phi(\eta)$ (curve 2) and based on the Liebmann’s method (curve 3).
Calculations were performed using both stepwise and piecewise linear approximations of the boundary potential. The corresponding values of the potential function on the axis, calculated on the basis of these approximations, differ very slightly (less than 0.1%), that is, apparently, due to using the fine mesh.

**4. Conclusions**
The numerical technique using the integral of Cauchy type and intended for calculating the electrostatic field inside the axially symmetric domain has been considered. The simulation results have shown that the given approach seems to be practicable but requires some theoretical and algorithmic studies to achieve better accuracy. The algorithm proposed in the paper can be used in computing and optimization of beam dynamics in the injection systems (see, e.g., [16]).

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