Advanced Software Package for Estimation Boundary Trajectories of Electron Beams and Other Practical Applications

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- Abstract: The article describes advanced computer software for numerical simulation, interpolation, extrapolation, and approximation of electron beam boundary trajectories. From a mathematical point of view, the distinguishing feature of the proposed software is the use of different-order root-polynomial functions for estimating the boundary trajectories of electron beams. The accuracy of estimation is very high. The level of interpolation and extrapolation errors is a range of a few percent, and in some cases, it is a fraction of a percent. For obtaining a minimal level of error estimation and guaranteeing the convergence of the choosing function, the method of including the positive deviation into root-polynomial functions is proposed and verified. Corresponding examples are also given. Particularities of realizing computer software in the Python programming language are also considered. Using manual input of digital data for interpolation and approximation is also possible. Elaborated computer software is supplied by a well-developed graphic user interface, and for simplicity of working with it, different simulation tasks are located in the separate bookmarks. Transferring numerical data between different tasks using the corresponding interface components is also possible. The program interface is created using advanced means of Python programming and software standards, and for this reason, it is easy for understanding by users and working with it. Therefore, elaborated computer software can also be used for solving other significant practical tasks connected with interpolation, approximation, and extrapolation of stiff ravine dependences.

1 INTRODUCTION

Solving the problems of interpolation, extrapolation and approximation of stiff ravine dependences is very important task today. Analyses of such dependences is often necessary for solving different optimization task in problems of physics, economy, psychology, social science and other. Therefore, analyzing of ravine dependences is the special problem in the data science and computer algorithms, including egression analyze [1-3].

A special task in this aspect is analyzing the boundary trajectories of Electron Beams (EB). Generally, this task is corresponded to basic laws of electro-physics and electron optics [4 - 10], and have been considered in papers [11 - 17]. Generally, this approach firstly has been applied to research and further development of high voltage glow discharge electron guns, which are widely applied in industry today in electronics [18 - 20] and mushing-building

industry [21 - 33]. Generally, principle of operation such type of electron guns is given in papers [23 - 33].

The approach of estimation short-focus EB trajectories, proposed in papers [11 - 17], is based on for interpolation, using approximation and extrapolation of the boundary trajectory of electron beam, former by of high voltage glow discharge electron guns, by root-polynomial functions (RPF). General conception of interpolation by such functions is described in paper [11, 12], and it has been pointed out in this works, that using this approach by the suitable position of reference point in the symmetric ravine date sets obtaining high accuracy of interpolation, range of fraction of percent relatively to obtained numerical data, is really possible. Examples of data approximation using this approach are given in papers [13, 14]. Generally, it based on two different approaches: approximation by the reference points [14] and by the tangents [17]. In the papers [15, 16]

the method of extrapolation of EB trajectories and advanced method of interpolation using slightly different location of reference points, generally taking from the extrapolation task [16], have been described.

Theoretical background of using proposed interpolation and approximation methods, based on the mathematical particularities of RPF and they derivatives, is given in paper [16]. In the work [18] on the base of proposed theoretical approach another possible application of RPF was described. The main applications of this approach, have been considered in [18], are probability theory tasks [34, 35] and fuzzy-logic tasks [36 – 42].

But as noted in [11, 12], the magnitude of the interpolation error strongly depends on the position of the base points in the numerical data sets, and if the value of the interpolated set near the minimum is close to zero, then the RPFs usually diverge. Basic structure of elaborated software package has been described in work [15, 16]. Some practical recommendations in terms of avoiding the problem of RPF divergence, which was pointed out in works [15, 16], have been given in [17], however this problem has not been completely solved till today.

Therefore, the purpose of this paper is to describe the included changes in the developed software package that allow obtaining guaranteed convergence of the algorithms for calculating RPF coefficients when solving practical problems related to the interpolation and extrapolation of stiff ravine digital data sets. Some corresponding examples are also given.

2 STATEMENT OF PROBLEM

As it has been pointed out in the papers [11, 12], in the general form RPF for the known set of basic points on longitudinal coordinate *z* and transversal coordinate $r \{P_1(z_1, r_1), P_2(z_2, r_2), ..., P_{n+1}(z_{n+1}, r_{n+1})\}$ is written as follows:

$$r_b(z) = \sqrt[n]{C_n z^n + C_{n-1} z^{n-1} + \ldots + C_1 z + C_0},$$
 (1)

where where *n* is the degree of the polynomial and the order of the root-polynomial function, and $C_0 - C_n$ are the polynomial coefficients.

Generally, the problem of defining polynomial coefficients is very simple and, with known coordinate of basic points \mathbf{P} it led to solving the set of linear equation [11, 12]:

$$\begin{cases} C_n z_1^n + C_{n-1} z_1^{n-1} + \dots + C_1 z_1 + C_0 = r_1^n; \\ C_n z_2^n + C_{n-1} z_2^{n-1} + \dots + C_1 z_2 + C_0 = r_2^n; \\ \dots & \dots; \\ C_n z_n^n + C_{n-1} z_n^{n-1} + \dots + C_1 z_n + C_0 = r_n^n; \\ C_n z_{n+1}^n + C_{n-1} z_{n+1}^{n-1} + \dots + C_1 z_{n+1} + C_0 = r_{n+1}^n. \end{cases}$$
(2)

Clear, that the set of equation (2) is linear and can be simply solved analytically using well-known Gauss – Seidel methods of exclusion the variables [43, 44]. The analytical relations, which have been obtained for calculation the coefficients $C_0 - C_n$ for the RPF from second to sixth order are given in the works [14 – 17]. Generally, now namely these relations are used for calculation the polynomial coefficients in elaborated computer software Electron Beam Trajectories Interpolation, Approximation and Extrapolation (EBTIAE). Basic structure of these computer software is given in works [15 – 17].

But as have been pointed out in the works [15,16], for small values of r in the region of minimum proposed algorithms of calculation are usually divergence with the small values of r near the region of minimum. Corresponded result, has been obtained manually for the set of basic points (r; z): (0; 0.01), (0.01; 0.007), (0.02; 0.003), (0.03; 0.001), (0.04; 0.003), (0.05; 0.007), (0.06; 0.01), is shown in Fig. 1. In this dataset all values on z coordinate are given in meters, and on r coordinate – in millimeters. Clear that value $r_4 = 0.001$ mm = 10^{-6} m in the region on minimum is very small. The result, presented in Figure 1, has been obtained for sixth-order RPF.



Figure 1: Illustration of divergence the algorithm of calculation the sixth-order RPF coefficients for ravine dataset with extra-small value near the minimum region.

In general, this problem is explained simply by the fact that in relation (1) the polynomial is under the root of degree n, and accordingly, for negative values of the coordinate r, the given problem generally has no solution. Therefore, it is obvious that the condition r > 0 is necessary for the convergence of the algorithms for calculating the RPF coefficients, but, unfortunately, it is not sufficient. As the conducted studies have shown, for values of r close to zero, the usually proposed computational algorithms still diverge. This problem has been generally formulated in the works [16, 17], but correct solution for its

solving wasn't find rill today. It also should be pointed out, that generally for the stiff functions finding the minimum, which value is close to zero, is always the sophisticated problem for different numerical method and such task usually has to be solved very carefully with analyzing the precision of provided iterative calculations [45-49].

Therefore, advanced method for obtaining guaranteed convergence of calculation RPF coefficients by analytical relations, which have been obtained early, will be proposed and analyzed in the next section of this work.

3 USE DEVIATION AND ADVANCED FORM OF ROOT-POLYNOMIAL FUNCTION

3.1 Basic Conception and Corresponding Example

Really, the solution is very simple, when the relation (1) is rewritten in advanced form with positive deviation δ as follows:

$$r_b(z) = \sqrt[n]{C_n z^n + C_{n-1} z^{n-1} + \ldots + C_1 z + C_0} - \delta.$$
(3)

In this case the set of basic points for calculation polynomial coefficients is rewritten with deviation as follows:

$$\{P_1(z_1, r_1 + \delta), P_2(z_2, r_2 + \delta), ..., P_{n+1}(z_{n+1}, r_{n+1} + \delta)\}.$$

In Figure 2 presented the result of interpolation for the same set of points, as in pervious section, but using deviation $\delta = 0.01$. It is clear, that in this case divergence of RPF is not observed and solution, which has been obtained, is generally correct.



Figure 2: Illustration of convergence the algorithm of calculation the sixth-order RPF coefficients for ravine dataset with extra-small value near the minimum region in the case of using deviation $\delta = 0.01$.

Corresponding sixth-order RPF is written as follows:

$$r(z) = \int_{0}^{-7.2608025 \cdot 10^{-20}z^{6} + 1.30694445 \cdot 10^{-20}z^{5} - - -8.59362525 \cdot 10^{-22}z^{4} + 2.4706836 \cdot 10^{-23}z^{3} - -2.10426 \cdot 10^{-25}z^{2} - 3.616736445 \cdot 10^{-27}z + -6.410 \cdot 10^{-29}$$

3.2 Use Deviation for Interpolation and Extrapolation the Boundary Trajectory of Electron Beams

Generally, the stiff ravine function with the values, which in the region of minimum are close to zero, are corresponding to the trajectory of EB in the case of high acceleration voltage and small beam current [4 - 10]. Certainly, using deviation in such case for guaranteed convergence of calculation RPF coefficients is necessary.

In the papers [15, 16], it has also been pointed out that a small error of interpolation using RPF is possible only in the case of a treatment-symmetric ravine dataset. In the case of asymmetry, the value of the error is, generally, greatly raised.

On the physical point of view, the boundary trajectory of short-focus EB, propagated in ionized gas, is described by following set if algebradifferential equations [4 - 10, 14]:

$$\begin{split} f &= \frac{n_e}{n_{i0} - n_e}; C = \frac{I_b \left(1 - f - \beta^2\right)}{4\pi\varepsilon_0 \sqrt{\frac{2e}{m_e}} U_{ac}^{1.5}}; \frac{d^2 r_b}{dz^2} = \frac{C}{r_b}; \theta = \frac{dr_b}{dz} + \theta_s; \\ n_e &= \frac{I_b}{\pi r_b^2}; \ v_e = \sqrt{\frac{2eU_{ac}}{m_e}}; \\ n_{i0} &= r_b^2 B_i p n_e \sqrt{\frac{\pi M \varepsilon_0 n_e}{m_e U_{ac}}} \exp\left(-\frac{U_{ac}}{\varepsilon_0 n_e r_b^2}\right); \quad (4) \\ \gamma &= \sqrt{1 - \beta^2}; \ \tan\left(\frac{\theta_{\min}}{2}\right) = \frac{10^{-4} Z_a^{4/3}}{2\gamma \beta^2}; \ \tan\left(\frac{\theta_{\max}}{2}\right) = \frac{Z_a^{3/2}}{2\gamma \beta^2}; \\ \overline{\theta^2} &= \frac{8\pi (r_b Z_a)^2 dz}{n_e} \ln\left(\frac{\theta_{\min}}{\theta_{\max}}\right), \ \beta &= \frac{v_e}{c}, \end{split}$$

where U_{ac} is the accelerating voltage, I_b is the EB current, p is the residual gas pressure in the region of EB propagation, z is the longitudinal coordinate, dz is the electron path in the longitudinal direction at the current iteration, r_b is the radius of the boundary trajectory of the electron beam, n_e is the beam electrons' concentration, n_{i0} is the concentration of residual gas ions on the beam symmetry axis, ε_0 is permittivity, v_e is the average velocity of the beam electrons, m_e is the electron mass, c is the light velocity, γ is the relativistic factor, f is the residual gas ionization level, B_i is the gas ionization level, θ_{\min} and θ_{max} are the minimum and maximum scattering angles of the beam electrons, corresponding to Rutherford model, θ is the average scattering angle of the beam electrons, Z_a is the nuclear charge of the residual gas atoms.

Corresponded analytical relation for error estimation is follows [11, 12]:

$$\varepsilon(z) = \frac{\left|r_{num}(z) - r_{E}(z)\right|}{r_{num}(z)} \cdot 100\%,\tag{4}$$

where r_E is the result of estimation using relation (1) and set of equations (2), r_{num} is the result of solving the set of algebra-differential equation (4) using four order Runge – Kutt method [43 – 47].

Let's considering now the tasks of interpolation and extrapolation boundary trajectory of EB with such simulation parameters: $U_{ac} = 25$ kV, $I_b = 0.6$ A, p = 7 Pa, start EB radius $r_{b0} = 3$ mm, start longitudinal coordinate $z_0 = 0.1$ m, start angle of EB convergence $\alpha = 12^0$, last longitudinal coordinate $z_0 = 0.15$ m, number of calculated points N = 120000. Corresponding simulation result is given at Figure 3.



Figure 3: Illustration of solving simulation task for $U_{ac} = 25$ kV, $I_b = 0.6$ A, and $r_{b0} = 3$ mm.

Clear, that EB trajectory in this case is very stiff and, generally, similar to the function of absolute value $r(z) = 0.2179 \cdot |z - 0.1148|$. But, in contrary on absolute value function, the derivative in the point of minimum $z_{\min} = 0.1148$ m is $\frac{dr}{dz} = 0$.

The result of solving interpolation task for such parameters of EB is given in Figure 4a, the deviation is $\delta = 2.5$ mm. Since ravine function is left-hand asymmetric, the significant error is existed in the region of minimum, range of 100 %. In contrary, for combined interpolation-extrapolation task [15, 16], minimal error is significantly smaller, range of 3-4 %, but it also corresponding to the region of EB focus position. The value of deviation for this task is $\delta = 1.4 \text{ mm.}$ Graphic dependences, have been obtained for this combined interpolationextrapolation task, are given in Figure 4b.

In the case of solving combined interpolationextrapolation task obtained sixth order RPF is written as follows:

$$r(z) = \int_{0}^{2.332142 \cdot 10^{-4} z^{6} - 1.607568 \cdot 10^{-4} z^{5} + 4.6247388 \cdot 10^{-5} z^{4} - 7.107475 \cdot 10^{-6} z^{3} + 6.1542275 \cdot 10^{-7} z^{2} - 2.84664851 \cdot 10^{-8} z + 5.495177647 \cdot 10^{-10}} - 1.4.$$

Clear, that, in any case maximal relative interpolation error correspond to the region of minimum because the numerical values of function r_{num} in this region are very small. Therefore, such result is in agreement with relation (4).



Figure 4: Illustration of solving interpolation task (a) and combined interpolation-extrapolation task (b) for EB boundary trajectory with simulation task parameters: $U_{ac} = 25$ kV, $I_b = 0.6$ A, and $r_{b0} = 3$ mm.

Another approach to refining the parameters of relativistic EB in powerful accelerators in the strong microwave electromagnetic fields has been proposed in papers [50, 51]. This approach is based on using microcomputers and careful statistical analyze of experimental results.

4 PARTICULARITIES OF ELABORATED COMPUTER SOFTWARE

Generally, the particularities of elaborated software package EBTIAE, created using the advanced means of Python programing language [52 - 55], just have been considered early in works [13 - 17]. The package EBTIAE is created by the means of

functional programing in one module, and for providing sophisticated numerical calculations and creating scientific graphics advanced Python libraries, such as numpy and matplotlib has been used [52-55]. From the library numpy has been effectively used the advanced means of large digital arrays treatment, including methods of matrix programming. And for realizing data transferring between different tasks the means of describing global variables have been used.

But the main particularity of the elaborated EBTIAE package is the location of all independent

tasks on the separate tabs of the canvas, formed in the graphic interface window. And in these tabs the specific textboxes are located for input numerical data and the buttons for providing calculations and data transferring [14 - 16]. Generally, such approach is fully corresponded to conception of functional programming [52 - 55]. And since new function of using deviation has been realized in the EBTIAE package, corresponding tabs "Interpolation" and "Extrapolation" have been slightly modified. The appearances of these two tabs on the computer screen with all the elements of the interface window are shown in Figure 5.



b)

Figure 5: The tabs "Interpolation" (a) and "Extrapolation" (b) of elaborated computer software EBTIAE. Screen copies.

The main differences of these tabs from the figures, given in works [14 - 16], are the appearance of the textbox "Deviation" and the button "+", which are located in both tabs in the upper right corner. In the textbox "Deviation" the corresponding value of deviation has to be typing, and in case of pressing on the button "+" the typing value of deviation is added to the basic points on *r* coordinate, which are located on the top of both tabs in the second row. But the button "+" button included only for providing manual calculations. Calculation the boundary trajectory of EB is provided by the same way, as early, namely, after events of pressing to the buttons "Import from SDE Task", which are also located in both tabs in the upper right corner (see Figure 5a and 5b).

The deviation value is read from the text window and passed to the function for calculating the EB trajectory. If the value of this parameter is incorrect, a corresponding error message is issued. Thus, only minor changes have been introduced into the interface of the developed computer software, which simplifies the work of ordinary users with it.

5 CONCLUSIONS

The conducted studies have shown that, in general, with the correct choice of the deviation value, the minimum value of the interpolation error and extrapolation of the EB boundary trajectory can be achieved using the RPF of different orders, from the second to the sixth. In reality, the reduction in the interpolation error with using deviation can be by several orders of magnitude. But, most importantly, by correctly selecting the deviation, it was possible to completely solve the problem of the RPF divergence at radial coordinate values close to zero.

The corresponding interpolation and extrapolation RPF were obtained for all EB parameters, including for problems with a high degree of rigidity, which correspond to high values of the accelerating voltage and low beam current.

The use of functional programming tools in the Python language allowed us to make appropriate changes to the program interface with minor changes in the algorithms and computational procedures.

Interesting, that it is also possible to interpolate and extrapolate numerical data in manual mode, which significantly expands the range of tasks to be solved by elaborated computer software. In particular, using the developed software, it is possible to solve problems of probability theory and fuzzy logic, where functional dependencies with a high degree of rigidity are often used for accurate data processing.

The obtained theoretical and practical results are of great practical interest to a wide range of specialists in the fields of interpolation and extrapolation theory, computational algorithms, and processing of large data arrays.

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