COMPARATIVE ANALYSIS OF THE FINITE DIFFERENCE METHOD AND THE MATRIZANT METHOD OF A BEAM DYNAMICS SIMULATION IN ELECTROSTATIC STRUCTURES WITH AXIAL SYMMETRY

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A study and further simulation of the dynamics of an ion beam in an accelerating structure, which is part of an immersion probe-forming system, has been carried out. The matrizant method is used for such simulation, which employs an approximate solution of the equations of motion of ions in electrostatic structures with axial symmetry. Take to account that deviations from the axis of ion trajectories can be significant, it is necessary to carry out a comparative analysis of the finite difference method, which uses exact equations of motion, as a reference method, and the matrizant method under beam dynamics simulation.

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INTRODUCTION

At the Institute of Applied Physics of the National Academy of Sciences of Ukraine, a compact nuclear microprobe based on an immersion probe-forming system is being developed [1–4]. This development offers several advantages, including compact dimensions, low power consumption, reduced cost, and higher spatial resolution compared to conventional microprobe systems.

The present simulation aims to investigate ion beam dynamics within the accelerating structure that is part of the immersion probe-forming system. The matrizant method [5–8], which provides an approximate solution to the equations of motion for ions in axially symmetric electrostatic structures is employed. Since ion trajectories can deviate significantly from the axis, a comparative analysis with the finite difference method is required. The finite difference method, which uses the exact equations of motion, serves as the reference for evaluating the accuracy of the matrizant method.

A key advantage of the matrizant method is relatively low computational cost for calculating the trajectory of a single ion, which is two orders of magnitude lower than that of the finite difference method. This enables to carry out the analysis of a beam dynamic consisting of 10^6...10^7 ions in trajectory phase space with minimal computational effort.

For the comparative analysis, an accelerating structure in the form of a triplet of standard NEC accelerating tubes [9] was selected. Proton beam dynamics were simulated within this structure, and the beam envelope was chosen as a quantitative measure for given parameters of the beam phase volume at the entrance to the structure. Comparison of the envelopes obtained by both methods showed that the root-mean-square deviation between them does not exceed 1%, confirming the reliability of the matrizant method for efficient beam dynamics simulations.

1. FINITE DIFFERENCE METHOD

The equation of motion of a positively charged particle in an axially symmetric electrostatic structure was taken in the form

$$r'' = \frac{\left(E_r(r,z) - r'E_z(r,z)\right)\left(1+r'^2\right)}{2\left(p_0^2/2mq + \varphi(r,0) - \varphi(r,z)\right)}, \qquad (1)$$

where p_0, m, q – initial momentum, mass and charge of the beam particle, respectively; $p_0^2/2mq$ – is the initial kinetic energy of the particle at the entrance to the electrostatic structure; E_r *u* E_z – are the radial and axial components of the electric field in the electrostatic structure. The potential φ has the form [10]

$$\varphi(r,z) = U(z) - U''(z)r^2/4 + U^{IV}(z)r^4/64 \qquad (2)$$

the field is expressed through potential $\vec{E}(r,z) = -grad(\varphi)$.

For the numerical solution of equation (1), the Everhart integration scheme [11], implemented in the RADA subroutine, is employed. This scheme possesses high accuracy and was originally developed for the calculation of spacecraft trajectories. In the numerical simulation, a piecewise-constant approximation is adopted for the potential and its derivatives, with values equal to the mean at the endpoints of each interval along the z-axis.

2. MATRIZANT METHOD

An axially symmetric electrostatic structure is considered, in which the electric potential in the Cartesian coordinate system is given by [10]

$$\varphi(x, y, z) = U(z) - U''(z)\frac{x^2+y^2}{4} + U^{IV}(z)\frac{(x^2+y^2)^2}{64} - \ldots \qquad (3)$$

The transition to the Cartesian coordinate system is motivated by the fact that the electrostatic structures will subsequently be used in conjunction with optical elements having quadrupole symmetry.

For $\hat{U}(z) = p_0^2/2mq - U(z)$ the expressions for the projections of the electrostatic field intensity vector will be as follows [12]

$$E_x = -\frac{\partial\varphi(x,\,y,\,z)}{\partial x} = -\hat{U}''(z)\frac{x}{2} + \hat{U}^{IV}(z)\frac{x(x^2+y^2)}{16},$$
$$E_y = -\frac{\partial\varphi(x,\,y,\,z)}{\partial y} = -\hat{U}''(z)\frac{y}{2} + \hat{U}^{IV}(z)\frac{y(x^2+y^2)}{16}, \quad (4)$$
$$E_z = -\frac{\partial\varphi(x,\,y,\,z)}{\partial z} = \hat{U}'(z) - \hat{U}'''(z)\frac{(x^2+y^2)}{4}.$$

The square of the particle momentum during its motion in the electrostatic structure can be approximated to second order in the phase coordinates as

$$p^2 \approx 2mq\left(2\tilde{u}\delta + \hat{U}(z) - \hat{U}''(z)\frac{(x^2+y^2)}{4}\right) = \\ = 2mq\hat{U}(z)\left(1 + \frac{2\tilde{u}}{\hat{U}(z)}\delta - \frac{\hat{U}''(z)}{4\hat{U}(z)}(x^2+y^2)\right), \quad (5)$$

where δ – relative momentum spread of particles, $\tilde{u} = p_0^2/2mq$.

As the phase volume of the beam is inversely proportional to its energy during acceleration, to conserve this invariant, the transition is performed from the transverse stationary phase coordinates (x, x', y, y') to the normalised coordinates (x_1, x_2, y_1, y_2) according to the following relations

$$x_1 = x, \quad x_2 = x'\sqrt{\frac{\hat{U}(z)}{\tilde{u}}}, \\ y_1 = y, \quad y_2 = y'\sqrt{\frac{\hat{U}(z)}{\tilde{u}}}. \quad (6)$$

Consequently, the following relations can be written

$$x_1' = x_2\sqrt{\frac{\tilde{u}}{\hat{U}(z)}}, \\ x_2' = \left(x'\sqrt{\frac{\hat{U}(z)}{\tilde{u}}}\right)' = x''\sqrt{\frac{\hat{U}(z)}{\tilde{u}}} + x_2\frac{\hat{U}'(z)}{2\hat{U}(z)}, \quad (7) \\ y_1' = y_2\sqrt{\frac{\tilde{u}}{\hat{U}(z)}}, \quad y_2' = y''\sqrt{\frac{\hat{U}(z)}{\tilde{u}}} + y_2\frac{\hat{U}'(z)}{2\hat{U}(z)}.$$

The system of equations of motion that describes the motion of a particle in a normalised space with coordinates (x_1, y_1, x_2, y_2) has the form.

$$x_1' = \tau\cdot x_2, \\ y_1' = \tau\cdot y_2, \\ x_2' = \frac{qm}{\tau\cdot p^2}(E_x - \tau\cdot E_z x_2)\left(1 + (\tau x_2)^2 + (\tau y_2)^2\right) + x_2\frac{U'(z)}{2\hat{U}(z)}, \quad (8) \\ y_2' = \frac{qm}{\tau\cdot p^2}(E_y - \tau\cdot E_z y_2)\left(1 + (\tau x_2)^2 + (\tau y_2)^2\right) + y_2\frac{\hat{U}'(z)}{2\hat{U}(z)},$$

where $\tau = \sqrt{\frac{\tilde{u}}{\hat{U}(z)}}$.

Substituting the dependence for p^2 from (5) and expanding the resulting expression into a series in phase moments (10), while leaving terms no higher than third-order moments, we obtain the equations of motion in the form

$$x_1' = \tau\cdot x_2, \\ y_1' = \tau\cdot y_2, \\ x_2' = \sum_{i=1}^{15} X_i\tilde{\Phi}_{xi}, \quad (9) \\ y_2' = \sum_{i=1}^{15} Y_i\tilde{\Phi}_{yi},$$

where the phase moments have the form

$$\tilde{\mathbf{\Phi}}_x = \|\tilde{\Phi}_{xi}\|_{i=1\ldots15} = (x_1,\, x_2, \delta,\, x_1\delta, x_2\delta, x_1^3,\, x_1^2x_2, \\ x_1x_2^2,\, x_2^3, x_1y_1^2,\, x_1y_1y_2,\, x_1y_2^2,\, x_2y_1^2,\, x_2y_1y_2,\, x_2y_2^2)^T \quad (10)$$

$\tilde{\mathbf{\Phi}}_y$ is obtained by replacing $x \leftrightarrow y$ in $\tilde{\mathbf{\Phi}}_x$.

Vectors $\vec{\mathbf{X}} = \vec{\mathbf{Y}}$

$$X_1 = -\hat{U}''/(4\tau\hat{U}); \quad X_4 = \tau\hat{U}''/2\hat{U}; \\ X_5 = \tau^2\hat{U}'/\hat{U}; \quad X_6 = \left(\hat{U}\hat{U}^{IV} - 2\hat{U}''^2\right)/\left(32\tau\hat{U}^2\right); \\ X_7 = \left(\hat{U}\hat{U}''' - \hat{U}'\hat{U}''\right)/8\hat{U}^2; \quad X_8 = -\tau\hat{U}''/4\hat{U}; \\ X_9 = -\tau^2\hat{U}'/2\hat{U}; \; X_{10}=X_6; \; X_{12}=X_8; \; X_{13}=X_7; \; X_{14}=X_9$$

the remaining elements of the vectors $\vec{\mathbf{X}}, \vec{\mathbf{Y}}$ are equal to zero.

The construction of the system of linear differential equations in the phase moment space (10), limited by the third order of smallness, is carried out by applying a formal procedure of immersing equations (9) into the phase moment subspace [7, 8, 12], which has the form

$$\frac{d\tilde{\mathbf{\Phi}}_x}{dz} = \mathbf{P}(z)\cdot\tilde{\mathbf{\Phi}}_x. \quad (11)$$

For an electrostatic structure, the longitudinal distribution of potential and it's higher derivatives on the axle can be calculated with sufficient accuracy based on the geometry of the electrodes and the potentials set on them. Therefore, in this case, the matrizant is calculated numerically using the shuttle-sum method, in which, to ensure the conservativeness of the method, the elements of the main diagonal of the matrix $\mathbf{P}$ in the system of equations (11) must be equal to zero. This is what causes the transition to the normalised phase space.

The equation for the matrizant has the same structure as (11)

$$\frac{d\tilde{\mathfrak{R}}_x}{dz} = \mathbf{P}(z)\cdot\tilde{\mathfrak{R}}_x. \quad (12)$$

However, the complete matrizant of the beam formation system, which contains various types of active ion-optical elements, is calculated in the usual stationary phase space. Therefore, before calculating the matrizant of the electrostatic structure, it is necessary to switch to the input of the normalised space $\tilde{\mathbf{\Phi}}_x$, and, at the output, perform the reverse transformation from the normalised phase space to the usual stationary $\mathbf{\Phi}_x$. Thus, the matrizant of the electrostatic structure, which performs the transformation of stationary coordinates of phase moments, has the form

$$\mathfrak{R}_x(z_{out} \leftarrow z_{in}) = \hat{T}\left(\tilde{\mathbf{\Phi}}_x(z_{out}) \rightarrow \mathbf{\Phi}_x(z_{out})\right); \\ \cdot\hat{\mathfrak{R}}_x(z_{out} \leftarrow z_{in})\cdot\hat{T}\left(\mathbf{\Phi}_x(z_{in}) \rightarrow \tilde{\mathbf{\Phi}}_x(z_{in})\right), \quad (13)$$

where z_{in}, z_{out} coordinates at the entrance and exit of the

electrostatic structure, and square matrices $\hat{T}\left(\mathbf{\Phi}_x(z_{in}) \to \tilde{\mathbf{\Phi}}_x(z_{in})\right)$ and $\hat{T}\left(\tilde{\mathbf{\Phi}}_x(z_{out}) \to \mathbf{\Phi}_x(z_{out})\right)$ perform coordinate transformation from the space of stationary phase moments to the normalised space and vice versa, respectively

$$\hat{T}_{i,k}\left(\mathbf{\Phi}_x(z_{in}) \to \tilde{\mathbf{\Phi}}_x(z_{in})\right) = \begin{cases} \tilde{\Phi}_{xi}\Big|_{x_1=y_1=1,\,x_2=y_2=\sqrt{\hat{U}(z_{in})/\tilde{u}}}, & i=k \\ 0, & i \neq k, \end{cases},$$

$$\hat{T}_{i,k}\left(\tilde{\mathbf{\Phi}}_x(z_{out}) \to \mathbf{\Phi}_x(z_{out})\right) = \begin{cases} \tilde{\Phi}_{xi}\Big|_{x_1=y_1=1,\,x_2=y_2=\sqrt{\tilde{u}/\hat{U}(z_{out})}}, & i=k \\ 0, & i \neq k, \end{cases}, \quad (14)$$

$i = 1\ldots15,\ k = 1\ldots15.$

It is worth noting that, because of the axial symmetry, the matrizants $\mathfrak{R}_x$ and $\mathfrak{R}_y$ possess the same structure.

3. ELECTROSTATIC ACCELERATING STRUCTURE

The accelerating structure under consideration was a triplet of the NEC accelerating tube [9]. The computational scheme of the structure is presented in Fig. 1, which shows the electrode geometry of the tube. The potential distribution across the electrodes varies uniformly in the range of 0...100 kV.

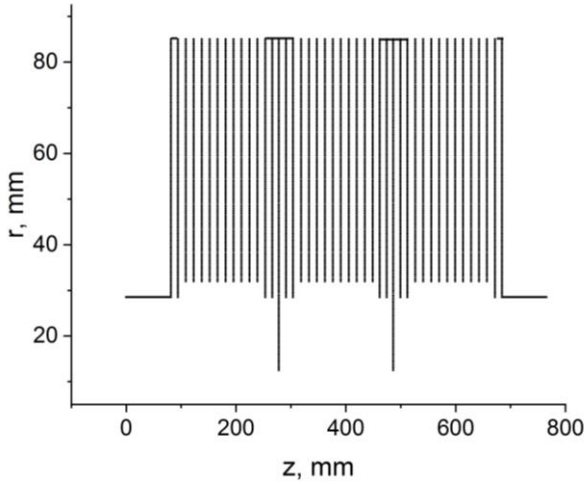

Fig. 1. Computational scheme of the accelerating structure

The distribution of the potential along the axis and its higher-order derivatives were computed using the integral equation method for potential theory by boundary elements method. The results of the calculation are shown in Fig. 2.

The beam dynamics simulation was carried out with the following beam parameters. The beam at the entrance to the structure was represented as a crossover with parameters r_0=0.000020 m, r'_0=0.00175 rad. The phase ellipse was represented as 400 points. The average initial energy was 3000 eV, with a momentum spread of 10^{-3}. The beam dynamics simulation was carried out using both the finite difference method and the matrizant method. The analysis of the beam envelope in both cases showed that the difference amounts to approximately 0.5%. Fig. 3 shows the beam envelopes in both cases, which do not differ due to their small difference.

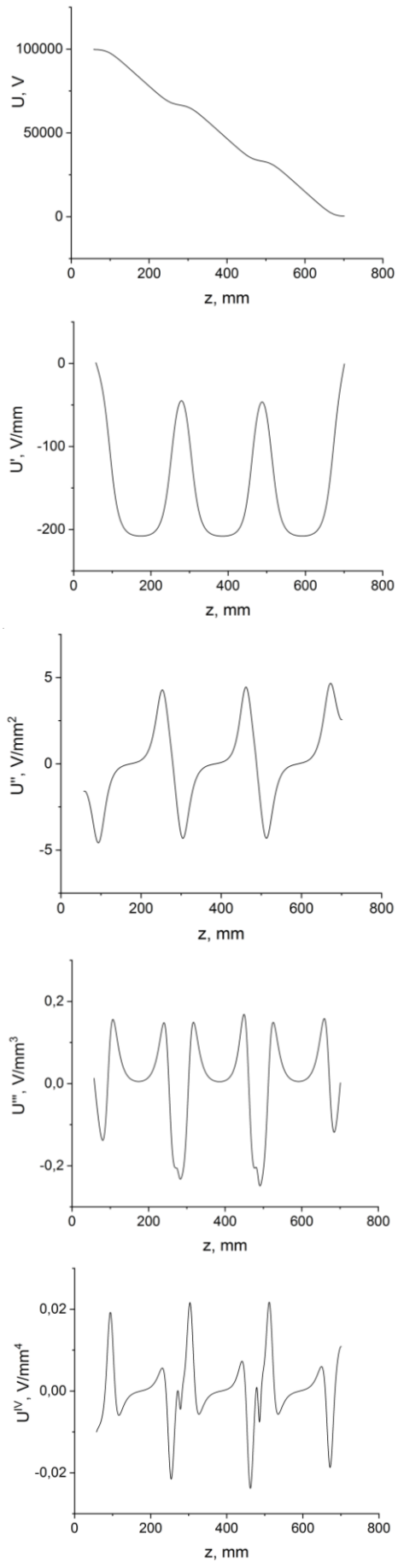

Fig. 2. Distribution of the potential along the axis and its higher-order derivatives in the accelerating structure

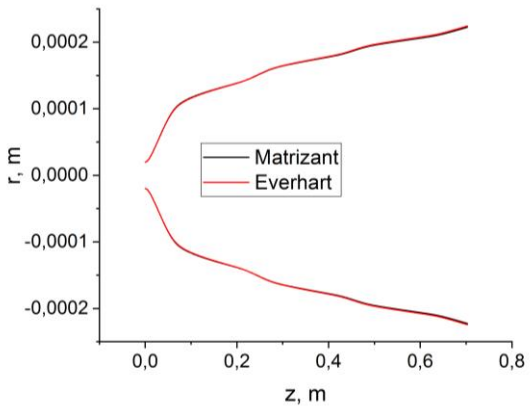

Fig. 3. Beam envelopes during motion in an electrostatic accelerating structure obtained using the finite difference method and the matrizant method

CONCLUSIONS

To simulate the dynamics of an ion beam in an axially symmetric electrostatic accelerating structure that forms part of an immersion probe-forming system, both the matrizant method and the finite difference method employing the Everhart scheme were used. Since the finite difference method employs the exact equations of motion of charged particles in an electric field, it was adopted as the reference method. The root-mean-square deviation of the beam envelope for the matrizant method ($r_{i,matr}$) with respect to the reference envelope from the finite difference method ($r_{i,fd}$) was computed as a result of the simulation in electrostatic accelerating tube NEC. Based on the results obtained, it can be concluded that the matrizant method is a reliable approach for simulating ion beam dynamics in an accelerating structure. The approximations employed in this method reduce the computational cost by two orders of magnitude while yielding results with minimal errors of less than 1%, making it a powerful and reliable tool for beam dynamics calculations.

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ПОРІВНЯЛЬНИЙ АНАЛІЗ МЕТОДУ СКІНЧЕНИХ РІЗНИЦЬ І МЕТОДУ МАТРИЦАНТІВ ПРИ МОДЕЛЮВАННІ ДИНАМІКИ ПУЧКА В ЕЛЕКТРОСТАТИЧНИХ СТРУКТУРАХ З АКСІАЛЬНОЮ СИМЕТРІЄЮ

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Проведено дослідження та подальше моделювання динаміки іонного пучка в прискорювальній структурі, яка входить до складу імерсійної зондоформуючої системи. Для такого моделювання застосовується метод матрицантів, в якому використовується наближене рішення рівнянь руху іонів в електростатичних структурах з аксіальною симетрією. Враховуючи те, що відхилення від осі траєкторій іонів можуть бути значними, потрібно виконати порівняльний аналіз методу скінчених різниць, який використовує точні рівняння руху, в якості реперного методу і методу матрицантів при моделюванні динаміки пучка в таких структурах.