# MPI BASED SIMULATION OF BEAM DYNAMICS IN INJECTION SYSTEMS WITH PARTICLE INTERACTIONS

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# Abstract

In this paper the problem of 3D beam dynamics simulation in injection systems is considered. Accelerating electrostatic field is simulated as a result of the solution of boundary value problem for Laplace equation by finite difference method. The computation of the beam field is based on the analytical solution of boundary value problem set for Poisson equation with use of MPI based parallel computations. High efficiency of the proposed computational method is shown in the examples.

#### Key words

Injection systems, 3D beam dynamics simulation, beam field simulation, electrostatic field simulation, MPI based parallel computations.

#### 1 Introduction

Currently, linear and circular accelerators, based on different principles of acceleration of charged particles, are widely used in various fields. In this regard, the increasing attention has been paid to the problems of designing, creating and optimization the accelerator complexes that provide a formation of precision beams.

Therefore, when developing an accelerator complex for certain applications, such as linear accelerator with spatially uniform quadrupole focusing or cyclotron, the injection system design is of importance, because it largely determines the output characteristics of the beam. For the design of such systems it is necessary to carry out numerical simulation and optimization of beam dynamics in the electromagnetic fields which necessitated the development and improvement of mathematical models of charged particle beams.

The questions of modeling and optimization of charged particle beam dynamics in linear accelerators has been widely discussed in various papers. In the papers of D.A. Ovsyannikov and his followers the theory of optimization of charged particle beam dynamics in linear accelerators, based on the analytical methods, has been developed [Ovsyannikov, 1990], [Ovsyannikov and Drivotin, 2003], [Ovsyannikov, Ovsyannikov, Antropov and Kozynchenko, 2005], [Ovsyannikov, Ovsyannikov, Svistunov, Durkin and Vorogushin, 2006], [Ovsyannikov, Ovsyannikov, 2011], [Ovsyannikov, 2012], [Ovsyannikov and Altsybeyev, 2013], [Ovsyannikov and Altsybeyev, 2014].

In the papers of O.I. Drivotin and D.A. Ovsyannikov the self-consistent distributions of charged particle beams have been studied [Drivotin and Ovsyannikov, 1994], [Drivotin and Ovsyannikov, 1998], [Drivotin and Ovsyannikov, 1999], [Drivotin and Ovsyannikov, 2004 1], [Drivotin and Ovsyannikov, 2004 2], [Drivotin and Ovsyannikov, 2006], [Drivotin and Ovsyannikov, 2009].

S.A. Kozynchenko and Yu.A. Svistunov investigated the problem of modeling, simulation and optimization of charged particle beam dynamics in the injection systems, using numerical methods [Kozynchenko and Svistunov, 2002], [Kozynchenko and Svistunov, 2006], [Kozynchenko and Svistunov, 2009]. A simulation software package for modeling and optimization of beam dynamics in injection systems allows to compute the external and internal beam field and beam dynamics, using numerical methods and taking into account the real geometry of the accelerating-focusing structure [Kozynchenko, 2012], [Kozynchenko, 2014], [Kozynchenko and Kozynchenko, 2014].

In the paper [Kozynchenko and Ovsyannikov, 2009] the formulation of the optimization problem of charged particle beam dynamics in the injection systems allowing the use of numerical optimization techniques is presented.

In the papers [Ovsyannikov, 2013 1], [Ovsyannikov, 2013 2], [Ovsyannikov, 2014] A.D. Ovsyannikov pro-

posed the formulation of the optimization problem of charged particle beam dynamics in the injection systems that allows the use of analytical methods for optimization.

In the papers of V.A.Kozynchenko the approximate analytical methods for calculating the Coulomb field of charged particle beams in linear accelerators are proposed. These methods are useful in applying together with analytical techniques of beam dynamics optimization and allow parallelization [Kozynchenko, 2007], [Kozynchenko, 2012], [Kozynchenko, 2014], [Kozynchenko and Boyko, 2014].

The issues of the computer simulation of charged particle beam dynamics were considered by many authors, including [Bondarev, Durkin, Ivanov, Shumakov, Vinogradov, Ovsyannikov and Ovsyannikov, 2001], [Ovsyannikov, Ovsyannikov, Antropov and Kozynchenko, 2005], [Kozynchenko and Svistunov, 2006], [Kozynchenko, 2012], [Kozynchenko, 2014], [Kozynchenko and Kozynchenko, 2014].

Under beam dynamics simulation an ensemble of model particles is usually used for the representation of the beam ('large' particle method). For the intense beam to take into account the Coulomb interaction between the particles is of great importance. The most effective numerical methods for charged particle beam field simulation are based on the solution of boundary value problem for the Poisson equation by the grid method. However, these methods are not applicable for beam dynamics optimization with analytical representation for the internal and external fields in the accelerating structures. Therefore, it seems urgent to develop mathematical models that admit an analytical representation for the Coulomb field of charged particles.

In this paper under simulation of charged particle beam dynamics in the injection system an external accelerating electrostatic field is obtained as a result of the solution by grid method of boundary value problem for the Laplace equation, taking into account the real geometry of the accelerating structure. We use both numerical and analytical methods for beam field computation. Numerical method is based on the solution by finite difference method of the Poisson equation for the beam field potential with the boundary conditions which take into account the actual geometry of the accelerating structure. Analytical method for beam field modeling is presented in the paper [Kozynchenko, 2012], where the beam of charged particles is represented by a set of annular cylinders. At each cylinder, the transverse beam charge density is assumed to be constant, and the longitudinal density is modeled by a trigonometric polynomial. For each cylinder, the Poisson equation is solved analytically with boundary conditions for the potential in the metal tube of a constant radius. Both longitudinal and transverse components of the beam field intensity are obtained in the form of trigonometric polynomials. This model suggests the possibility of MPI based parallel computations for the Coulomb field intensity.

The results for beam dynamics simulation in the injection system using both analytical and numerical methods for beam field computation are presented in this paper. We use analytical method together with MPI based parallel computations for beam field simulation. Analysis of beam dynamics simulation in the injection system shows high efficiency of both analytical method of beam field calculation and MPI based parallel computations.

# 2 Description of the Beam Dynamics Simulation Problem for Non-Relativistic Charged Particle Beam Injection Systems

In this paper we consider the accelerating-focusing structures consisting of  $n_e$  round electrodes in the form of thick disks with given potentials  $U_1^e,...,U_{n_e}^e$ .

Following D.A. Ovsyannikov [Ovsyannikov, 1990], the dynamics of the beam in the external field, taking into account the beam space charge, is described by integro–differential equations:

$$\begin{cases} \frac{dX}{dt} = V, \\ \frac{dV}{dt} = \frac{1}{m_p} f_1(t, X, u) + \\ \frac{1}{m_p} \int\limits_{M_t} f_2(t, X, V, \xi) \rho(t, \xi) d\xi = f_3(t, X, u), \\ X(t_0) = X_0, \quad V(t_0) = V_0, \quad (X_0, V_0) \in M_0, \end{cases}$$
(1)

$$\frac{\partial\rho(t,\eta)}{\partial t} + \frac{\partial\rho(t,\eta)}{\partial\eta}\tilde{g}(t,\eta,u) + \rho\,div_{\eta}\tilde{g} = 0, \quad (2)$$

$$\rho(t_0, \eta) = \rho_0(\eta). \tag{3}$$

Here  $t \in [t_0, T]$  — the independent variable (time); parameters  $t_0$ , T are fixed;  $m_p$ , — the mass,  $X(t) = (x, y, z) \in \mathbb{R}^3$  — the position,  $V(t) = (v_x, v_y, v_z) \in R^3$  — the velocity of a charged particle, respectively;  $\eta = (X, V) \in \mathbb{R}^6$ - the position of the charged particle in the phase space;  $u = u(x, y, z) \in C^{2}(G)$  — potential of the external field, where  $G \subset R^{3}$  — limited and open set; function  $f_{1}(t, X, u(X))$  describes the force, defined by external field; the choice of the function  $f_2(t, X, V, \xi)$  defines the way of modeling of the Coulomb interaction of charged particles; vector-function  $\tilde{g}(t, \eta, u) = (V(t), f_3(t, \eta, u));$  $\rho(t,\eta)$  — density distribution of particles due to the system (1);  $\rho_0(\eta)$  — given charge density in the space  $M_0$  at the moment  $t_0$ , where  $M_0 \subset R^6$ — bounded closed set of non-zero measure;  $M_t =$  $\{X = X(t, X_0), V = V(t, V_0) : (X_0, V_0) \in M_0\}$ image of the set  $M_0$ , due to system (1) a the moment t.

The potential of the external electrostatic field u(x, y, z), defined and continuous in  $\overline{G}$ , is a solution of the Dirichlet problem for the Laplace equation:

$$\begin{cases} \Delta u \left( x, y, z \right) = 0, \quad (x, y, z) \in \mathbf{G}, \\ u \left( x, y, z \right) |_{\Gamma_G} = u_0 \left( x, y, z \right), \end{cases}$$
(4)

where  $\Gamma_G = \bigcup_k \Gamma_k$  — the boundary of G, composed of piecewise-smooth curves  $\Gamma_k$ ;  $u_0(x, y, z)$  – known function.



Figure 1. Cross-sections of the electrode system in the planes xz and yz. Area G within the electrode system is edged by the dotted line. Cross- sections of the electrodes are shown in dark gray.  $U_1^e, ..., U_{n_e}^e$  – potentials of the electrodes.

The potential  $\varphi(x, y, z)$  of the beam field, defined and continuous in  $\overline{G}$ , is a solution of the boundary value problem for the Poisson equation:

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} = \frac{\rho\left(x, y, z\right)}{\epsilon_0}, \quad (x, y, z) \in G.$$
(5)

$$\varphi(x, y, z)|_{\Gamma_G} = \varphi_0(x, y, z), \qquad (6)$$

where  $\varphi_0$  — known function.

We consider an area G restricted by the dotted line shown in (Fig. 1). The boundary  $\Gamma_G(\hat{u}) = \bigcup_{i=1}^{n_{\Gamma}} \Gamma_i$ is defined by endpoints of the curves  $\Gamma_i$ , such as segments of straight lines, arcs, etc. The part of curvilinear boundary of the *i* - th electrode between the points A and B,  $i = \overline{1, n_e}$ , consists of curves  $\Gamma_p$ ,  $p = \overline{n_{\Gamma}^5, n_{\Gamma}^6},$  $2 < n_{\Gamma}^5, n_{\Gamma}^6 < n_{\Gamma} - 1$  (Fig. 1), in which the boundary condition (6) will be:

$$\varphi\left(x,y,z\right)|_{\Gamma_{p}} = U_{j}^{e}, \quad j = \overline{1, n_{e}}.$$

In the gaps between the electrodes on the straight sections of the boundary  $\Gamma_q$ , located between points C and D (Fig. 1)  $q = \overline{n_{\Gamma}^7, n_{\Gamma}^8}, 3 < n_{\Gamma}^7, n_{\Gamma}^8 < n_{\Gamma} - 2$ , the condition (6) can be written as follows:

$$\varphi\left(\hat{x}, \hat{y}, z\right)|_{\Gamma_{q}} = U_{i-1}^{e} + \left(U_{i}^{e} - U_{i-1}^{e}\right) \frac{z - z_{i-1}^{e}}{z_{i}^{e} - z_{i-1}^{e}}.$$

On the sections of the boundary  $\Gamma_G(\hat{u})$ , other than sections  $\Gamma_p$  and  $\Gamma_q$ , the boundary conditions (6) are expressed as follows:

$$\begin{cases} \varphi\left(x,y,\hat{z}\right)|_{\Gamma_{1}} = v_{0}, \\ \varphi\left(\hat{x},\hat{y},z\right)|_{\Gamma_{2}} = v_{0} + \left(U_{1}^{e} - v_{0}\right)\frac{z-z_{1}^{e}}{z_{2}^{e}-z_{1}^{e}}, \\ \varphi\left(\hat{x},\hat{y},z\right)|_{\Gamma_{n_{\Gamma}-k}} = U_{n_{e}}^{e} - U_{n_{e}}^{e}\frac{z-z_{n_{\Gamma}-k-1}}{z_{n_{\Gamma}-k}^{e}-z_{n_{\Gamma}-k-1}^{e}}, \\ \varphi\left(\hat{x},\hat{y},z\right)|_{\Gamma_{n_{\Gamma}-k+1}} = U_{n_{e}}^{e}, \end{cases}$$

where  $v_0$  — given value;  $\hat{x}$ ,  $\hat{y}$ ,  $\hat{z}$  are fixed.

Next we consider the solution of the boundary value problem (5), (6) by the finite difference method. Let us associate the computational domain G with a set of discrete points (grid)  $\Omega^h$ , formed by intersection of the planes parallel to the coordinate axes:  $x = x_i$ ,  $y = y_j$ ,  $z = z_k$ ,  $i = \overline{0, n_k^h}$ ,  $j = \overline{0, n_y^h}$ ,  $k = \overline{0, n_z^h}$ . The node (i, j, k) with coordinates  $(x_i, y_j, z_k)$  is referred to as an internal node relative to the domain G if  $(x_i, y_j, z_k) \in G$ , and as an external one otherwise. Let us introduce the notations:  $h_{ijk}^1 = h_{i-1}^x = x_i - x_{i-1}$ ;  $h_{ijk}^2 = h_{j-1}^y = y_j - y_{j-1}$ ;  $h_{ijk}^3 = h_i^x = x_{i+1} - x_i$ ;  $h_{ijk}^4 = h_j^y = y_{j+1} - y_j$ ;  $h_{ijk}^5 = h_{k-1}^z = z_k - z_{k-1}$ ;  $h_{ijk}^6 = h_k^z = z_{k+1} - z_k$ ;  $h = \max_{i,j,k} \{\sup h_{ijk}^r\}$ ;  $\Omega_0^h$  — set of internal nodes;  $\Omega_1^h$  — set of external nodes;  $\Omega_{\Gamma}^h$  — set of boundary points of the grid (points of intersection of coordinate grid lines with the boundary  $\Gamma$ ).

On the set of nodes  $\Omega^h$  we specify a grid function  $\psi = \{\psi(x_i, y_j, z_k)\} = \{\psi_{ijk}\}$  as a set of values, which can be presented in the form of  $n^h$  - dimensional vector;  $n^h$ — the total number of nodes considered. The boundary value problem (5), (6) can be written in an operator form:

$$L\varphi = g,\tag{7}$$

where L – differential operator defined on  $\{\varphi(x, y, z)\}$ .

The differential problem (7) is associated with a difference boundary value problem, which is equivalent to a system of linear equations:

A system of linear equations being equivalent to the difference boundary value problem can be written as follows:

$$A\psi = f$$

where  $\psi = \{\psi_k\}, f = \{f_k\}$  — vectors;  $k = \overline{1, n^h}$ ;  $A = \{a_{kl}\}$  — non-singular square matrix of order  $n^h$ . General view of a linear iterative method represented in the form:

$$\psi^{n+1} = B_n \psi^n + G^n, \tag{11}$$

where  $B_n = E - H_n A$  — transition matrix from the n - th to (n + 1) - th iteration(iteration step operator),  $H_0, H_1, H_2, \dots$  some sequence of the matrices.

For solving the system of difference equations the successive over relaxation (SOR) method can be used. Assume that A— symmetric matrix with diagonal block tridiagonal representation (A = D + M + N, where D— diagonal matrix, M— lower triangular matrix, and N— upper triangular matrix). Then the SOR method is defined as follows:

$$(D+M) \cdot \psi^{n+1} = \omega \cdot f - (N - (1 - \omega) \cdot A) \cdot \psi^n,$$

where  $\psi^n - n$  - th approximation of the solution (*n*-th iteration);  $\omega$  — relaxation parameter. The solution is carried out by SOR method when the order of the  $\psi$  components is consistent with the view of the tridiagonal matrix A.

## **3** Mathematical Model of a Cylindrical Beam of Charged Particles in a Metal Tube

We assume that the beam is unlimited and periodical in the longitudinal coordinate. Assume also that the beam is in a coaxial circular metal tube of radius *a* and has azimuthal symmetry. To determine the Coulomb field we consider the beam as a set of annular cylindrical coaxial layers. Each layer is non-uniform in the longitudinal coordinate and in each cross-section the layer density is constant. The intensity vector of the beam Coulomb field is calculated as the sum of the intensity vectors of each layer:

$$E = \sum_{i=0}^{N} E^{i},$$

where  $E^i$  — Coulomb field intensity vector of the *i*-th annular layer; N — the number of annular layers,

$$L_h\psi=f,$$

where  $\psi$ ,  $f - n^h$  - dimensional vectors whose components are defined as values of the grid function at the grid nodes  $\Omega^h$ ;  $L_h$  — finite difference operator defined on the grid functions  $\psi$ .

At the given grid, the following seven-point finite difference approximation to the Poisson equation is considered:

$$(\Lambda_7 \psi)_{ijk} = ((\Lambda_x + \Lambda_y + \Lambda_z) \psi)_{ijk} = 0, \quad (8)$$

$$(\Lambda_x \psi)_{ijk} = \alpha_1 = \alpha_2 + \alpha_3, \tag{9}$$

where

$$\alpha_1 = \frac{2\psi_{i-1,j,k}}{h_{i-1}^x \left(h_{i-1}^x + h_i^x\right)} - \frac{2\psi_{i,j,k}}{h_{i-1}^x h_i^x} + \frac{2\psi_{i+1,j,k}}{h_i^x \left(h_{i-1}^x + h_i^x\right)}$$

$$\alpha_2 = \left(\frac{\partial^2\psi}{\partial x^2}\right)_i + \frac{h_i^x - h_{i-1}^x}{3} \left(\frac{\partial^3\psi}{\partial x^3}\right)_i,$$

$$\alpha_{3} = \frac{(h_{i}^{x})^{2} - h_{i}^{x}h_{i-1}^{x} + (h_{i-1}^{x})^{2}}{12} \left(\frac{\partial^{4}\psi}{\partial x^{4}}\right)_{i} + O(h^{3})$$

Difference operators  $\Lambda_y$  and  $\Lambda_z$  are defined similarly to  $\Lambda_x$ . The difference equation (8) approximates the Poisson equation (5) with an error of the first order for a non-uniform grid, and the second order - on a uniform grid. At the nodes near boundary, to construct the difference analogue of the differential operator on a uniform or non-uniform grid the nearest points from  $\Omega_{\Gamma}^h$  are used. In this case, a system of difference equations contains the values of the grid function at all internal nodes, as well as at the boundary nodes of the grid, and in the latter case the boundary condition (6) is approximated exactly:

$$\psi(x_i, y_j, z_k) = \varphi_0(x_i, y_j, z_k), \ (x_i, y_j, z_k) \in \Omega_{\Gamma}^h.$$
(10)

The error of approximation of the difference equation at a node near boundary, as well as the error of the difference problem (8) – (10), is defined by O(h).

zero layer — axial cylindrical layer. This model allows to take into account both longitudinal and transverse beam heterogeneity under calculation of its Coulomb field.

We introduce a cylindrical coordinate system  $(z, \theta, r)$ , where Oz axis coincides with the axis of symmetry of the tube. We assume that an annular layer has an azimuthal symmetry, i.e. coordinates and velocities of the particles do not depend on the polar angle  $\theta$ . We assume also that the space charge density within an annular cylinder is a periodic function of the longitudinal coordinate z and is a constant in the cross-section. In this case, the potential  $\varphi(z, r)$  satisfies the Poisson equation:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\varphi\left(z,r\right)}{\partial r}\right) + \frac{\partial^{2}\varphi\left(z,r\right)}{\partial z^{2}} = f\left(z,r\right), \quad (12)$$

where

$$f\left(z,r\right) = -\frac{\rho\left(z,r\right)}{\varepsilon_{0}}$$

$$\rho(z,r) = \begin{cases} 0, r \leq R_1, \\ \frac{\tau(z)}{\pi \left(R_1^2 - R_2^2\right)}, R_1 < r \leq R_2, \\ 0, r > R_2, \end{cases}$$

 $\tau\left(z\right)$  — charge of the beam per unit length, and the boundary conditions

$$\begin{cases} \varphi\left(z,a\right) = 0 \quad \forall z \in R, \\ \frac{\partial \varphi(z,r)}{\partial r}|_{r=0} = 0 \quad \forall z \in R, \\ \varphi\left(z,r\right) = \varphi\left(z+L,r\right) \quad \forall z \in R, \quad \forall r \in [0,a], \\ \frac{\partial \varphi(z,r)}{\partial z}|_{z=p} = \frac{\partial \varphi(z,r)}{\partial z}|_{z=p+L} \forall z \in R, \quad \forall r \in [0,a]. \end{cases}$$

We assume that functions  $\varphi(z,r)$ ,  $\partial \varphi(z,r)/\partial r$ ,  $\partial \varphi(z,r)/\partial z$  are continuous at  $r = R_1$  and  $r = R_2$ . We introduce the notation:

$$\varphi(r) = \begin{cases} \eta(r), & 0 < r \le R_1, \\ \nu(r), & R_1 < r \le R_2, \\ w(r), & R_2 < r \le a. \end{cases}$$

Because of the beam periodicity along the longitudinal coordinate, we consider the function f(z,r) as periodic in zwith period L. For modeling of the function f(z,r) we introduce on the axis Oz the grid  $S = \{z_i = hi, h = L/N, i = \overline{0, N}\}$  with number of nodes N. At the nodes of the grid S we define the function of the beam charge per unit length  $\tau(z)$  based on the location of model particles. By formulas (12) we calculate the value of a function f(z, 0) at the nodes of the grid S. We model the function f(z, r) by trigonometric polynomial whose values at the nodes of the grid S coincide with the known ones  $f_i = f(z_i, 0)$ :

$$f(z,r) = \frac{1}{2} f_0^c + \sum_{k=1}^M (f_k^c(r) \cos(\omega_k z) + f_k^s(r) \sin(\omega_k z)),$$

where

$$\omega_k = \frac{2\pi k}{L}, \, M = \frac{N_z - 1}{2},$$

$$f_{k}^{c}(r) = \begin{cases} 0, \ 0 < r \le R_{1}, \\ f_{k}^{c}, \ R_{1} < r \le R_{2}, \\ 0, \ R_{2} < r \le a, \end{cases}$$

$$f_k^s(r) = \begin{cases} 0, \ 0 < r \le R_1, \\ f_k^s, \ R_1 < r \le R_2, \\ 0, \ R_2 < r \le a, \end{cases}$$

$$f_0^c = \frac{2}{N_z} \sum_{i=0}^{N_z - 1} f_i,$$
(13)

$$f_k^c = \frac{2}{N_z} \sum_{i=0}^{N_z - 1} f_i \cos \frac{2\pi ki}{N_z},$$
 (14)

$$f_k^s = \frac{2}{N_z} \sum_{i=0}^{N_z - 1} f_i \sin \frac{2\pi ki}{N_z}.$$
 (15)

Then the expressions for the longitudinal and transverse components of the intensity vector of the Coulomb field of the cylindrical axially symmetric beam taking into account heterogeneity and periodicity of the charge density in the longitudinal coordinate will look like:

$$E_{z}(z,r) = \sum_{k=1}^{M} \omega_{k} \left( u_{k}^{c}(r) \sin \omega_{k} z - u_{k}^{s}(r) \cos \omega_{k} z \right),$$

 $E_r\left(z,r\right) = \beta_1 - \beta_2,$ 

$$\beta_1 = -\frac{1}{2} \frac{du_0^c\left(r\right)}{dr},$$

$$\beta_2 = \sum_{k=1}^{M} \left( \frac{du_k^c(r)}{dr} \cos \omega_k z + \frac{du_k^s(r)}{dr} \sin \omega_k z \right),$$

where the functions  $u_{k}^{c}(r)$ ,  $u_{k}^{s}(r)$ ,  $\frac{du_{0}^{c}(r)}{dr}$ ,  $\frac{du_{k}^{c}(r)}{dr}$ ,  $\frac{du_{k}^{c}(r)}{dr}$ ,

$$u_{0}^{c}\left(r\right) = \begin{cases} \beta_{3} + \beta_{4}, 0 \leq r \leq R_{1}, \\ \beta_{5} + \beta_{6} + \beta_{7}, R_{1} \leq r \leq R_{2}, \\ \frac{f_{0}^{c}}{2} \left(R_{1}^{2} - R_{2}^{3}\right) \ln \frac{r}{a}, R_{2} \leq r \leq a, \\ \beta_{3} = \frac{f_{0}^{c}}{4} \left(2 \left(R_{1}^{2} - R_{2}^{3}\right) \ln \frac{R_{2}}{a}\right), \\ \beta_{4} = \frac{f_{0}^{c}}{4} \left(2R_{1}^{2} \ln \frac{R_{1}}{R_{2}} + R_{2}^{2} - R_{1}^{2}\right), \\ \beta_{5} = -\frac{f_{0}^{c}r^{2}}{4} + \frac{R_{1}^{2}f_{0}^{c}}{2} \ln r, \\ \beta_{6} = \frac{f_{0}^{c}}{4} \left(2 \left(R_{1}^{2} - R_{2}^{3}\right) \ln \frac{R_{2}}{a}\right), \\ \beta_{7} = -\frac{f_{0}^{c}}{4} \left(2R_{1}^{2} \ln R_{2} + R_{2}^{2}\right), \end{cases}$$

$$u_{k}^{c}(r) = \begin{cases} f_{k}^{c}C_{3}I_{0}(\omega_{k}r), \ 0 \leq r \leq R_{1}, \\ \beta_{8} + \beta_{9} + \beta_{10}, \ R_{1} \leq r \leq R_{2}, \\ \beta_{11} + \beta_{12}, \ R_{2} \leq r \leq a, \\ \beta_{8} = f_{k}^{c}\frac{1}{\omega_{k}^{2}}, \\ \beta_{9} = f_{k}^{c}C_{1}I_{0}(\omega_{k}r), \\ \beta_{10} = f_{k}^{c}C_{2}K_{0}(\omega_{k}r), \\ \beta_{11} = f_{k}^{c}C_{5}I_{0}(\omega_{k}r), \\ \beta_{12} = f_{k}^{c}C_{6}K_{0}(\omega_{k}r), \end{cases}$$

$$u_{k}^{s}(r) = \begin{cases} f_{k}^{s}C_{3}I_{0}(\omega_{k}r), \ 0 \leq r \leq R_{1}, \\ \beta_{13} + \beta_{14} + \beta_{15}, \ R_{1} \leq r \leq R_{2}, \\ \beta_{16} + \beta_{17}, \ R_{2} \leq r \leq a, \\ \beta_{13} = f_{k}^{s}\frac{1}{\omega_{k}^{2}}, \\ \beta_{14} = f_{k}^{s}C_{1}I_{0}(\omega_{k}r), \\ \beta_{15} = f_{k}^{s}C_{2}K_{0}(\omega_{k}r), \\ \beta_{16} = f_{k}^{s}C_{5}I_{0}(\omega_{k}r), \\ \beta_{17} = f_{k}^{s}C_{6}K_{0}(\omega_{k}r), \end{cases}$$

$$\frac{du_0^c(r)}{dr} = \begin{cases} 0, 0, 0 \le r \le R_1, \\ -\frac{f_0^c r}{2} + \frac{R_1^2 f_0^c}{2r}, R_1 \le r \le R_2, \\ \frac{f_0^c}{2r} \left(R_1^2 - R_2^3\right), R_2 \le r \le a, \end{cases}$$

$$\frac{du_{k}^{c}\left(r\right)}{dr} = \begin{cases} f_{k}^{c}\omega_{k}C_{3}I_{1}\left(\omega_{k}r\right), \ 0 \leq r \leq R_{1}, \\ \beta_{18} + \beta_{19}, \ R_{1} \leq r \leq R_{2}, \\ \beta_{20} + \beta_{21}, \ R_{2} \leq r \leq a, \\ \beta_{18} = f_{k}^{c}\omega_{k}C_{1}I_{1}\left(\omega_{k}r\right), \\ \beta_{19} = f_{k}^{c}\omega_{k}C_{2}K_{1}\left(\omega_{k}r\right), \\ \beta_{20} = f_{k}^{c}\omega_{k}C_{5}I_{1}\left(\omega_{k}r\right), \\ \beta_{21} = f_{k}^{c}\omega_{k}C_{6}K_{1}\left(\omega_{k}r\right), \end{cases}$$

$$\frac{du_{k}^{s}\left(r\right)}{dr} = \begin{cases} f_{k}^{s}\omega_{k}C_{3}I_{1}\left(\omega_{k}r\right), \ 0 \leq r \leq R_{1}, \\ \beta_{22} + \beta_{23}, \ R_{1} \leq r \leq R_{2}, \\ \beta_{24} + \beta_{25}, \ R_{2} \leq r \leq a, \\ \beta_{22} = f_{k}^{s}\omega_{k}C_{1}I_{1}\left(\omega_{k}r\right), \\ \beta_{23} = f_{k}^{s}\omega_{k}C_{2}K_{1}\left(\omega_{k}r\right), \\ \beta_{24} = f_{k}^{s}\omega_{k}C_{5}I_{1}\left(\omega_{k}r\right), \\ \beta_{25} = f_{k}^{s}\omega_{k}C_{6}K_{1}\left(\omega_{k}r\right), \end{cases}$$

$$C_{2} = \begin{cases} \frac{I_{1}(\omega_{k}R_{1})}{\omega_{k}^{2}(\beta_{26}+\beta_{27})}, \\ \beta_{26} = K_{0}(\omega_{k}R_{1}) I_{1}(\omega_{k}R_{1}), \\ \beta_{27} = K_{1}(\omega_{k}R_{1}) I_{0}(\omega_{k}R_{1}), \end{cases}$$

$$C_{1} = \begin{cases} C_{2} \frac{\beta_{28} - \beta_{29}}{(\beta_{30} - \beta_{31})} - \frac{1}{\omega_{k}^{2}(\beta_{30} - \beta_{31})\gamma}, \\ \beta_{28} = \frac{K_{1}(\omega_{k}R_{2})}{(I_{1}(\omega_{k}R_{2})K_{0}(\omega_{k}a) + I_{0}(\omega_{k}a)K_{1}(\omega_{k}R_{2}))}, \\ \beta_{29} = \frac{K_{0}(\omega_{k}R_{2})}{(I_{0}(\omega_{k}R_{2})K_{0}(\omega_{k}a) - I_{0}(\omega_{k}a)K_{0}(\omega_{k}R_{2}))}, \\ \beta_{30} = \frac{I_{0}(\omega_{k}R_{2})K_{0}(\omega_{k}a) - I_{0}(\omega_{k}a)K_{0}(\omega_{k}R_{2}))}{(I_{1}(\omega_{k}R_{2})K_{0}(\omega_{k}a) + I_{0}(\omega_{k}a)K_{1}(\omega_{k}R_{2}))}, \\ \beta_{31} = \frac{I_{1}(\omega_{k}R_{2})}{(I_{1}(\omega_{k}R_{2})K_{0}(\omega_{k}a) - I_{0}(\omega_{k}a)K_{1}(\omega_{k}R_{2}))}, \\ \gamma = I_{0}(\omega_{k}R_{2})K_{0}(\omega_{k}a) - I_{0}(\omega_{k}a)K_{0}(\omega_{k}R_{2}), \end{cases}$$

$$C_{3} = \frac{C_{1}I_{1}(\omega_{k}R_{1}) - C_{2}K_{1}(\omega_{k}R_{1})}{I_{1}(\omega_{k}R_{1})}$$

$$C_{5} = \frac{K_{0}(\omega_{k}a)(C_{1}I_{1}(\omega_{k}R_{2}) - C_{2}K_{1}(\omega_{k}R_{2}))}{I_{1}(\omega_{k}R_{2})K_{0}(\omega_{k}a) + I_{0}(\omega_{k}a)K_{1}(\omega_{k}R_{2})}$$

$$C_6 = C_5 \frac{I_0\left(\omega_k a\right)}{K_0\left(\omega_k a\right)},$$

 $f_0^c, f_k^c, f_k^s$  defined by (13) – (15).

# 4 On the Use of an Annular Cylinder Model Under Simulation of Beam Dynamics in the Injection Systems

This section discusses the applicability of the annular cylinder model, considered in Section 3 of this paper, for the calculation of a beam field in injection system performed both with and without the use of parallel computing. We consider an injection system of ions  $H^-$  for cyclotron consisting of  $n_e = 5$  electrodes with given potentials  $U_1^e = 15kV$ ,  $U_2^e = 10kV$ ,  $U_3^e =$ 20kV,  $U_4^e = 25kV$  and  $U_5^e = 103kV$ . At the input of the electrode system, the axially-symmetric beam with initial energy of 25keV and current of 15mA is considered. The characteristics of this beam are presented in

Fig. 2. The beam energy at the injection system output is 100keV. The  $H^-$  ion beam in the injection system is shown in Fig. 3, having 90 percent of particles involved in subsequent acceleration process in cyclotron (Fig. 4).



Figure 2. Characteristics of an axially-symmetric beam of ions  $H^-$  at the outlet of the plasma-surface ion source. (a) the phase portrait of the beam in the plane xx', (b) the phase portrait of the beam in the plane yy', (c) particles density distribution in the plane xy.



Figure 3. The cyclotron injection system for axially-symmetric beams of ions  ${\cal H}^-$ 



Figure 4. Characteristics of an axially-symmetric beam of ions  $H^-$  at the output of the injection system, shown in Fig. 3. On the figures (a) and (b) the cyclotron acceptance is shown kneeling solid ellipse. (a) the phase portrait of the beam in the plane xx', (b) the phase portrait of the beam in the plane yy', (c) particles density distribution in the plane xy.

We also consider in the injection system, an ensemble of ions  $H^-$  is simulated consisting of five "bunches" (for taking into account a beam periodicity along the longitudinal coordinate) and having both a longitudinal and transverse heterogeneity, as well as an azimuthal symmetry relative to the symmetry axis Oz (see Fig. 5). In the "bunch" cross-section, the charge density has a normal distribution.

To test the applicability of the annular cylinder model the field of considered ensemble of charged particles has been computed. Some results of comparison of the longitudinal components of the field of the particle ensemble acting on the axis of symmetry within the central bunch are shown in Fig. 6. The calculations were performed both using an annular cylinder beam model and by solving the boundary value problem for the Poisson equation by the finite difference method.

Also the calculations were performed for the longitudinal component of the field of the particle ensemble, which acts on the axis of symmetry of the infinite cylindrical tube of radius a, with a different number of annular cylinders. The results of calculations are shown in Fig. 7. In this case, we consider an ensemble of charged particles consisting of one central bunch (see Fig. 5) having a normal transverse charge density distribution. It is seen from Fig. 7 that, in case of an inhomogeneous radial beam and 6 cylinders, the longitudinal field component on the axis of symmetry of the injection system can increase three-fold as compared to the same value when using one cylinder, which substantiates the usage of the annual cylinder model to calculate the beam field in injection systems.



Figure 5. Ensemble of ions  $H^-$  in the injection system of a linear accelerator. The cross-section in xz - plane is shown.



Figure 6. Graphs of the longitudinal component of the field force of an ensemble of ions  $H^-$  acting on Oz - axis of system symmetry. The force obtained through the annular model is shown by red, black color marks the force obtained by solving the boundary value problem for the Poisson equation.



Figure 7. Graphs of the longitudinal component of the field of the ensemble of ions  $H^-$  acting on the Oz - axis for various numbers of annular cylinders.

Table 1.	The run time of compu	ting the longitudinal component of
the field o	of ensemble of ions $H^-$	at $Oz$ – axis for various numbers
of annula	r cylinders.	

number of	time	time
cylinders	without	with
	MPI, sec.	MPI, sec.
2	3.272	4.197
4	4.025	1.973
8	5.576	1.037
16	8.687	0.798
32	15.368	0.751
64	28.205	0.690

We investigated a possibility of using parallel computing based on the MPI-1 communication protocol to simulate a field of the ensemble of ions  $H^-$  using the annual cylinder model. Run times of computing the longitudinal component of the field of the particle ensemble along Oz - axis both with and without the use of parallel computing for different numbers of annual cylinders are shown in Table 1. In the case of parallel computations for the cylinders being involved to a beam, both fields and forces are calculated in parallel in separate processes.

Table 1 shows that with increasing the number of cylinders the run time of calculating the field with parallel computing is reduced compared to the run time without parallelization. This demonstrates the applicability and efficiency of the parallel computation based on the MPI-1 to calculate the fields of the ensemble of charged particles in the injection systems using annular model.

The studies carried out show the suitability of the annular model for calculation of the field of charged particle ensembles in the injection systems of accelerators.

#### 5 Conclusion

The paper presents the calculations of the internal Coulomb field of the ensemble of ions  $H^-$  in the injection system using both analytical and numerical methods for modeling the internal field. Comparison of the results of calculations using numerical and analytical modeling techniques shows the effectiveness of the analytical method of calculation in injection systems, including the effectiveness of parallelization.

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